CDCF 50

29.06 - 03.07, 2025 - Pisa

5th ECPC

Book of Abstracts

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EuChemS
European Chemical Society
Division of Physical Chemistry

We are pleased and proud to welcome you to the Joint 50th Congress of the Physical Chemistry Division of the Società Chimica Italiana and the 5th European Conference on Physical Chemistry (**CDCF50&5thECPC**, Pisa, 29 June – 3 July 2025).

This conference, jointly promoted by the Physical Chemistry Divisions of the **Società Chimica Italiana** and **EUCHEMS**, is hosted by the **University of Pisa**. It provides an outstanding forum for physical chemists to exchange knowledge and ideas, and to foster strong scientific collaborations.

Leading researchers from across Europe and Italy, representing all areas of physical chemistry, are attending the conference and presenting their latest achievements. The topics addressed include, but are not limited to: energy, environment, materials, soft matter, life sciences, catalysis, cultural heritage, spectroscopy, thermal and calorimetric analyses, computational methods, and advanced characterization techniques.

Opportunities for oral and poster presentations have been offered to researchers at all career stages. In particular, poster presenters were also invited to showcase their work through flash presentations during dedicated poster round-table sessions.

Beyond the scientific program, a variety of engaging social events enable participants to strengthen personal and professional relationships, while enjoying Italian cuisine and the renowned monuments of Pisa.

The chairs of the Conference
Marco Geppi and Sefik Suzer

Società Chimica Italiana
Divisione di Chimica Fisica

EuChemS
European Chemical Society
Division of Physical Chemistry

Golden wedding this year for the Conference of the Physical Chemistry Division (PCD) of the Società Chimica Italiana. This anniversary will be celebrated holding a joint conference with the European Physical Chemistry Division of EUCHEMS. Founded in 1986, PCD received the legacy of the Italian Physical Chemistry Association (AICF), founded in 1966. The activity of PCD is mainly devoted to the organization of schools, dedicated to PhD students and young researchers, to monitor the teaching and research activity in Physical Chemistry, and the organization of an annual conference. In this 50th Physical Chemistry Division Conference in Pisa, PCD awards the Bonino Prize to researchers that gave important contributions to the discipline, the Semerano Prize (best PhD thesis), the Distinguished and Young Scientist Prizes (best Conference lectures), and the Senatore Prize (best Conference poster communication).

The board of the Physical Chemistry Division of the Società Chimica Italiana

The Physical Chemistry Division of the EuCheMS had emerged, during 2009-2011, and was officially founded in 2011. The 1st Conference of this series was organized in Catania, Italy, by Giovanni Marletta (15-18 September 2015), followed by the 2nd Meeting in Borgo-Corsica, France by Carole Duboc. The 3rd event was organized by Wolfgang Kautek of University of Wien, jointly with the Bunsen Meeting in Jena, Germany (May 30-June 01, 2019). The 4th Meeting took place in Dornbirn, Austria (09-11 October 2023), organized again by Wolfgang Kautek. For the 5th Meeting, we have joined our forces with the Physical Chemistry Division of the Società Chimica Italiana for this exciting event in Pisa.

The board of the Physical Chemistry Division of the EuCheMS

Conference Program

CDCF50

29.06 - 03.07, 2025 - Pisa

5th ECPC

SUNDAY 29/06

18.30-19.30	REGISTRATION		
19.30	WELCOME COCKTAIL		

MONDAY 30/06

	Room A	Room B	Room C
8.30-9.30	**REGISTRATION + REFRESHMENT**		
9.30-10.20	**Opening**		
	Chair: G. Marletta		
10.20-11.00	PL1 - Antonietti		
11.00-11.10	SL1 - COLAVER		
	Environment	**Soft Matter**	**Advanced Characterisation**
	Chair: F. Ridi	*Chair: M. Scorciapino*	*Chair: A. Beneduci*
11.10-11.30	OC1 - Mulas	OC2 - Cappelletti	OC3 - Lang
11.30-11.50	OC4 - Rizzuto	OC5 - Fazzi	OC6 - Tofoni
11.50-12.10	OC7 - Muniz Miranda	OC8 - Campione	OC9 - Guiotto
12.10-12.30	OC10 - Marangon	OC11 - Greco	OC12 - Lo Presti
12.30-14.00	**LUNCH & POSTERS**		
	Chair: L. Marchese	*Chair: M. Venanzi*	*Chair: P. Ugliengo*
14.00-15.20	**Poster round table: Energy & Environment**	**Poster round table: Bio & Pharma**	**Poster round table: Theory & Characterization**
	FC1 - Cavallo FC2 - Cignolo FC3 - Della Latta FC4 - Di Giorgio FC5 - Edebali FC6 - Giovanelli FC7 - Scorciapino FC8 - Suzer	FC9 - De Matteis FC10 - Fasulo FC11 - Gelli FC12 - Ghelardi FC13 - Ledesma-Motolinía FC14 - Perilli FC15 - Poggetti	FC16 - Bedogni FC17 - Bedogni FC18 - Cirillo FC19 - D'Amore FC20 - Kautek FC21 - Sahin FC22 - Tani FC23 - Tomassoli
	Energy	**Spectroscopy**	**Computational Methods**
	Chair: M. Antonietti	*Chair: A. Maris*	*Chair: L. Pedraza González*
15.20-15.40	OC13 - Dini	OC14 - Nardelli	OC15 - Gentili
15.40-16.00	OC16 - Paradisi	OC17 - Slimani	OC18 - Dogan
16.00-16.20	OC19 - Coppola	OC20 - Bardi	OC21 - Vigna
16.20-16.40	OC22 - Ersoz	OC23 - Tancredi	OC24 - Grimblat
16.40-17.20	**COFFEE BREAK & POSTERS**		
	Materials	**Life Science**	**Catalysis**
	Chair: S. Pizzanelli	*Chair: C.A. Bortolotti*	*Chair: G. Lang*
17.20-17.40	OC25 - Saladino	OC26 - Baldelli Bombelli	OC27 - Hatay Patir
17.40-18.00	OC28 - Fernandes	OC29 - Pezzola	OC30 - Aslan
18.00-18.20	OC31 - Giannini	OC32 - Troisi	OC33 - Mazzucato
18.20-18.40	OC34 - Laudani	OC35 - Ferrero	OC36 - Viacava
19.30	**COCKTAIL for YOUNG PARTICIPANTS**		

TUESDAY 01/07

	Room A	Room B	Room C
	Chair: P. Ugliengo		
9.00-9.40	PL2 - Daidone		
	Environment	**Cultural Heritage**	**Computational Methods**
	Chair: M. Ferretti	*Chair: G. Poggi*	*Chair: I. Daidone*
9.40-10.00	OC37 - Gübbük	OC38 - Kautek	OC39 - Caricato
10.00-10.20	OC40 - Lettieri	OC41 - Lob	OC42 - Semmeq
10.20-10.40	OC43 - Ancora	OC44 - Armetta	OC45 - Nottoli
10.40-11.00	OC46 - Campagiorni	OC47 - Mastrangelo	OC48 - Perrero
11.00-11.40	**COFFEE BREAK & POSTERS**		
	Environment	**Soft Matter**	**Materials**
	Chair: E. Selli	*Chair: C. Della Volpe*	*Chair: M. Meneghetti*
11.40-12.00	OC49 - Beneduci	OC50 - Chiessi	OC51 - Giribaldi
12.00-12.20	OC52 - Campisi	OC53 - Rossi	OC54 - Finelli
12.20-12.40	OC55 - Baglioni	OC56 - Avanzini	OC57 - Americo
12.40-13.00	OC58 - Sciacca	OC59 - Di Muzio	OC60 - Secci
13.00-13.20	OC61 - Maurelli	OC62 - Balestri	OC63 - De Santis
13.20-15.00	**LUNCH & POSTERS**		
	Chair: S. Borsacchi		
15.00-15.40	PL3 - Grandinetti		
15.40-15.50	SL2 - BRUKER		
	Energy	**Spectroscopy**	**Life Science**
	Chair: P. Grandinetti	*Chair: S. Bordiga*	*Chair: F. Baldelli Bombelli*
15.50-16.10	OC64 - Murgia	OC65 - Yaman	OC66 - Tuccitto
16.10-16.30	OC67 - Scarperi	OC68 - Aarabi	OC69 - Boi
16.30-16.50	OC70 - Langella	OC71 - Sodomaco	OC72 - Mastrogiacomo
18.00	**SOCIAL EVENT PIAZZA dei MIRACOLI**		

WEDNESDAY 02/07

	Room A	Room B	Room C
	Chair: C. Giancola		
9.00-9.40	PL4 - Matulis		
	Environment	**Life Science**	**Thermal and Calorimetric Analyses**
	Chair: I.H. Gübbük	*Chair: E. Rühl*	*Chair: D. Matulis*
9.40-10.00	OC73 - Rizzi	OC74 - Rabe	OC75 - Corrente
10.00-10.20	OC76 - Vanuzzo	OC77 - D’Aria	OC78 - Lowe
10.20-10.40	OC79 - Maccarino	OC80 - Marzano	OC81 - Pelosi
10.40-11.00	OC82 - Locardi	OC83 - Bona	OC84 - Czerska
11.00-11.40	**COFFEE BREAK & POSTERS**		
	Energy	**Spectroscopy**	**Materials**
	Chair: M.L. Curri	*Chair: S. Melandri*	*Chair: A. Massaro*
11.40-12.00	OC85 - Tseberlidis	OC86 - Maris	OC87 - Zoccante
12.00-12.20	OC88 - Alberti	OC89 - Das	OC90 - Brancato
12.20-12.40	OC91 - Piscino	OC92 - Mendolicchio	OC93 - Azzarelli
12.40-13.00	OC94 - Lasala	OC95 - Ricci	OC96 - Briganti
13.00-13.20	OC97 - Fracchia	OC98 - Vinti	OC99 - Mercedi
13.20-15.00	**LUNCH & POSTERS**		
	Chair: L. Calucci		
15.00-15.40	PL5 - Bordiga		
15.40-15.50	SL3 - ALFATEST		
	Spectroscopy	**Soft Matter**	**Catalysis**
	Chair: L. Latterini	*Chair: E. Fratini*	*Chair: D. Peddis*
15.50-16.10	OC100 - Suzer	OC101 - Graziano	OC102 - Andreu
16.10-16.30	OC103 - Litti	OC104 - Gubitosa	OC105 - Manca
16.30-16.50	OC106 - Sambucari	OC107 - D’Annibale	OC108
16.50-17.30	**COFFEE BREAK & POSTERS**		
17.30-19.30	**ASSEMBLY OF THE DIVISION OF PHYSICAL CHEMISTRY OF SCI**		
20.30	**SOCIAL DINNER (restaurant La Clessidra)**		

THURSDAY 03/07

	Room A	Room B	Room C
	Chair: W. Kautek		
9.00-9.40	PL6 - Brett		
	Energy	**Life Science**	**Materials**
	Chair: E. Carignani	*Chair: M. Rabe*	*Chair: C.M.A. Brett*
9.40-10.00	OC109 - Ferrara	OC110 - Bortolotti	OC111 - Robson
10.00-10.20	OC112 - De Bonis	OC113 - Pantaleone	OC114 - Maltoni
10.40-11.00	OC115 - Bartoli	OC116 - Vitaliti	OC117 - Costa
11.00-11.40	**COFFEE BREAK**		
	Environment	**Soft Matter**	**Computational Methods**
	Chair: F. Martini	*Chair: B. Pignataro*	*Chair: F. Lipparini*
11.40-12.00	OC118 - Meroni	OC119 - Scorciapino	OC120 - Tabacchi
12.00-12.20	OC121 - Cambiotti	OC122 - Oliva	OC123 - Ribaldone
12.20-12.40	OC124 - Fichera	OC125 - Ruffino	OC126 - Dal Cin
	Chair: M. Venanzi		
12.40-13.10	Physical Chemistry and Society: Della Volpe		
13.10-13.30	**CLOSING and MEETING AWARDS**		
13.30-15.00	**LUNCH**		

List of Contributions

Plenary Lectures

1. Markus Antonietti: *About artificial photosynthesis, new electrochemistry, and artificial ion pumps. Organic heterojunctions for physical chemistry* — [PL1, p.1]
2. Silvia Bordiga: *Understanding surfaces using probe molecules and in situ spectroscopies* — [PL5, p.2]
3. Christopher Brett: *Advances in nanomaterial and nanostructured material modified electrodes* — [PL6, p.3]
4. Isabella Daidone: *Intermolecular photoinduced electron transfer in biosystems: impact of conformational transitions and multiple channels on kinetics* — [PL2, p.4]
5. Claudio Della Volpe: *Physical chemistry and society: from industry to phylosophy and viceversa* — [PL7, p.5]
6. Philip J. Grandinetti: *Inverse methods for nuclear magnetic resonance of non-crystalline materials* — [PL3, p.6]
7. Daumantas Matulis: *Biothermodynamics for the characterization of proteins and their interactions with biologically important molecules in solution* — [PL4, p.7]

Sponsor Lectures

1. Carmen Camelia Buju: *Colaver SRL: processing and production of glass and quartz articles for laboratories* — [SL1, p.8]
2. Graziella Gariano: *Advanced techniques for the physico-chemical characterizaiton of materials* — [SL3, p.9]
3. Manuela Liberi: *Benchtop magnetic resonances: EPR and NMR research on your table (with no cryogenics)* — [SL2, p.10]

Oral Communications

1. Mohammad Aarabi: *Exploring chiral sensitivity of truecars signal: monitoring ultrafast electronic coherences spawned by enantiomerically equivalent S_0/S_1 conical intersections in cis-trans photoisomerization of a retinal chromophore model* — [OC68, p.11]
2. Stefano Alberti: *Study of TiO_2-based photocatalysts coupled with magnetic zeolites and carbon nanomaterials for H_2 production* — [OC88, p.12]
3. Stefano Americo: *Lattice dynamics and polar domain structure of giant-refraction $K_{0,997}Li_{0,003}Ta_{0,64}Nb_{0,36}O_3$ solid solution* — [OC57, p.13]
4. Gioele Ancora: *Hierarchical zeolites from top-down approach: a systematic investigation of their structural and adsorption properties* — [OC43, p.14]

5. Teresa Andreu: *CO_2 electroreduction and glycerol oxidation electrocatalysts fabricated by electrodeposition* — [OC102, p.15]
6. Francesco Armetta: *Deep learning for spectral data modelling in cultural heritage* — [OC44, p.16]
7. Emre Aslan: *Catalysis of hydrogen evolution reaction using bio-inspired WC-based catalysts in biphasic reactions* — [OC30, p.17]
8. Francesco Avanzini: *Nonequilibrium thermodynamics of non-ideal reaction-diffusion systems: implications for active self-organization* — [OC56, p.18]
9. Simone Azzarelli: *Zn_2SiO_4:Eu^{3+} as smart multicolor visible emitter* — [OC93, p.19]
10. Michele Baglioni: *Biocompatible hydrogels loaded with brassicaceae extracts for the controlled disinfection of agricultural soils* — [OC55, p.20]
11. Francesca Baldelli Bombelli: *Fluorinated nanostructures as bioimaging tools and delivery agents* — [OC26, p.21]
12. Arianna Balestri: *Fusogenic PNIPAM-stabilized lipid nanoparticles for enhanced anticancer drug delivery* — [OC62, p.22]
13. Brunella Bardi: *Solid state solvation: a fresh view* — [OC20, p.23]
14. Mattia Bartoli: *Hydrogen production through thermal degradation of confined ammonia borane* — [OC115, p.24]
15. Amerigo Beneduci: *Water remediation from heavy metals and organic pollutants using cellulose-derived adsorbents* — [OC49, p.25]
16. Sara Boi: *The interplay of key parameters in the transport process of small synthetic chloride carriers* — [OC69, p.26]
17. Beatrice Lucia Bona: *Self-assembly and biological properties of highly fluorinated oligonucleotide amphiphiles* — [OC83, p.27]
18. Carlo Augusto Bortolotti: *Electrolyte gated organic tansistors for the detection of biomarkers for personalized medicine* — [OC110, p.28]
19. Antonio Brancato: *Laser-modified MoS_2 structures for improved semiconductor SERS sensing* — [OC90, p.29]
20. Debora Briganti: *Fine-tuning amorphous magnesium calcium phosphate particles: how polyacrylic acid prevents aggregation and crystallization* — [OC96, p.30]
21. Elena Cambiotti: *Oleic acid-induced dissolution of semiconductor nanocrystals* — [OC121, p.31]
22. Luca Campagiorni: *Physico-chemical properties of ternary slag cement with low clinker and high limestone filler content with superplasticizers* — [OC46, p.32]
23. Paola Campione: *Poly(3-hexylthiophene)-based smart biointerfaces for biomedical applications* — [OC8, p.33]
24. Sebastiano Campisi: *A physicochemical approach to hydroxyapatite extraction from ashes: linking processing parameters to functional properties* — [OC52, p.34]
25. Giuseppe Cappelletti: *Oxides-stabilized pickering emulsions: influence of surface properties, in-situ functionalization, and stimuli-induced responsiveness* — [OC2, p.35]
26. Marco Caricato: *Optical and chiroptical linear response properties of materials* — [OC39, p.36]
27. Ester Chiessi: *Polymer behavior in aqueous solution across the lower critical solution temperature: insights from molecular dynamics simulation* — [OC50, p.37]
28. Carmen Coppola: *Towards the prediction of novel and more efficient dye candidates for indoor dye-sensitized solar cells via a combined machine learning and density functional theory strategy* — [OC19, p.38]
29. Giuseppina Anna Corrente: *Natural gums-based materials for advanced technological applications: anti-counterfeiting and thermochemical energy storage* — [OC75, p.39]

30. Jessica Costa: *Physico-chemical characterization of biobased materials with active biofillers obtained via solvent-casting and extrusion methods* — [OC117, p.40]
31. Angelika Magdalena Czerska: *Tensimetric determination of activity and partial mixing properties of urea in type III deep eutectic solvents* — [OC84, p.41]
32. Valeria D'Annibale: *The stereochemical effect in driving the aggregation behaviour of porphyrin-cholic acid derivatives* — [OC107, p.42]
33. Federica D'Aria: *Physicochemical studies of modified aptamers targeting ephrin receptor tyrosine kinase A2 (EphA2) in glioblastoma stem cells* — [OC77, p.43]
34. Pietro Dal Cin: *Correlated QM/MM calculations for the determination of spectral properties of biomimetic photoswitches in solution* — [OC126, p.44]
35. Ankita Das: *Biomolecule adsorption on smart switchable germanium surfaces* — [OC89, p.45]
36. Martina De Bonis: *Design and development of novel nanocomposite anion exchange membranes for fuel cells and electrolysers* — [OC112, p.46]
37. Ilaria De Santis: *Unveiling the mesoscale assembly of gold nanoparticles on soft templates via nanoplasmonic isosbestic points* — [OC63, p.47]
38. Simone Di Muzio: *Investigation of tetrabutylammonium-based deep eutectic solvents: the influence of counterions and H-bond donor on the formation of liquid phase* — [OC59, p.48]
39. Danilo Dini: *Analysis of the dynamics of photogenerated carriers at the* $MAPbBr_3/SrTiO_3$ *interface with IR synchrotron radiation: a study for hybrid photovoltaics* — [OC13, p.49]
40. Berna Dogan: *Combining molecular docking, molecular dynamics and machine learning approaches in an active learning scheme* — [OC18, p.50]
41. Mustafa Ersoz: *Photocatalytic hydrogen evolution by metal sulfide based binary and ternary 2D/2D heterojunction photocatalysts* — [OC22, p.51]
42. Daniele Fazzi: *Modelling disorder effects in organic soft materials* — [OC5, p.52]
43. Julio Cesar Fernandes Pape Brito: *In situ spectroscopic characterization of bifunctional acid-base organic-inorganic nanoporous hybrid catalysts* — [OC28, p.53]
44. Vittorio Ferrara: *Symmetric and asymmetric multilayer electrodes for semi-transparent perovskite solar cells* — [OC109, p.54]
45. Riccardo Ferrero: *Automated design and computational investigation of derivatized cyclodextrins for drug delivery and gas adsorption* — [OC35, p.55]
46. Paolo Fichera: *Interactions between hydroxyapatite surfaces and small reactive molecules of environmental interest: a computational approach* — [OC124, p.56]
47. Valeria Finelli: *Spectroscopic investigation of photoinduced redox activity in Ce-UiO-67 metal-organic framework* — [OC54, p.57]
48. Martina Fracchia: *Understanding the stability of Ni-In catalysts for the steam reforming of acetic acid from quasi-simultaneous operando XAS-XRD and computational modelling* — [OC97, p.58]
49. Pier Luigi Gentili: *An unconventional chemical contribution to the development of quantum artificial intelligence* — [OC15, p.59]
50. Samuele Giannini: *Dissecting the nature and quantum dynamics of electronic excitations and charge carriers in opto-electronic materials* — [OC31, p.60]
51. Alberto Giribaldi: *Effect of the deposition temperature on the magnetic and thermoelectric properties of* $MnFe_2O_4$ *thin films* — [OC51, p.61]

52. Giuseppe Graziano: *On the temperature-induced collapse of smart polymers in aqueous solutions* — [OC101, p.62]
53. Enrico Greco: *Fluorescent silk fibroin nanoparticles: preparation and physico-chemical characterization* — [OC11, p.63]
54. Nicolas Grimblat: *Identifying the origins of NMR shifts from quantum alchemy* — [OC24, p.64]
55. Jennifer Gubitosa: *Realizing stimuli-responsive platforms via iCVD for delivering green-synthesized AuNPs and accelerating wound healing: a proof-on concept* — [OC104, p.65]
56. Virginia Guiotto: *Advanced characterisation of organic and inorganic fillers for* CO_2*-selective mixed matrix membranes* — [OC9, p.66]
57. Ilkay Hilal Gübbük: *Synthesis of metal doped g-*C_3N_4 *nanostructures and their use as catalysts for environmental applications* — [OC37, p.67]
58. Imren Hatay Patir: *Nanofiber-based semiconductor materials for enhanced photocatalytic hydrogen production* — [OC27, p.68]
59. Wolfgang Kautek: *Surface diagnostics and laser cleaning potentials of synthetic and historical patinas on outdoor bronzes* — [OC38, p.69]
60. Gyozo Lang: *Investigating the temperature dependence of ferrate ion formation at high-purity iron electrodes using dual dynamic voltammetry (DDV)* — [OC3, p.70]
61. Aniello Langella: *Atomistic insights into solid-state phase transition in P2 layered oxides as high energy cathodes for Na-ion batteries* — [OC70, p.71]
62. Pierluigi Lasala: *Boosting bioelectricity generation in biophotovoltaics with engineered gold nanoparticles* — [OC94, p.72]
63. Francesco Laudani: *Ion beam-induced* MoS_2 *surface modification: an XPS study of* Ar^+ *and Ar gas cluster ion beam treatments* — [OC34, p.73]
64. Raffaella Lettieri: *Reimagining wine waste: unlocking the potential of natural polymers for sustainable innovation* — [OC40, p.74]
65. Lucio Litti: *In-operando reaction kinetic monitoring by SERS in microfluidics* — [OC103, p.75]
66. Leonardo Lo Presti: *Nanoscale distortions produce mesoscale modulations in Li-doped KTa/*NbO_3 *perovskite ferroelectrics: a crystallographic study* — [OC12, p.76]
67. Silvia Lob: *Nanostructured fluids for the conservation of cultural heritage: the role of surfactant structure in cleaning efficiency* — [OC41, p.77]
68. Federico Locardi: *Green solvents for nanocrystals synthesis: a step toward environmental sustainability* — [OC82, p.78]
69. Alexander R. Lowe: *The investigation of the heat of liquid intrusion/extrusion into/from hydrophobic porous materials by high pressure calorimetry* — [OC78, p.79]
70. Lorenzo Maccarino: *Quaternary-amino functionalized swellable organically modified silica for the removal of methyl orange from water* — [OC79, p.80]
71. Pierfrancesco Maltoni: *Investigation of the magnetic properties of ionic liquid -based ferrofluids* — [OC114, p.81]
72. Gabriele Manca: *An innovative strategy for rapid synthesis of ZnO@Au nanostructures and their application in photocatalytic processes* — [OC105, p.82]
73. Andrea Marangon: *Synthesis and characterization of lignin derivate porous materials from bamboo culms (Phyllostacys Edulis) for removal of aromatic pollutants* — [OC10, p.83]

74. Assimo Maris: *Unraveling molecular structures and dynamics: the role of rotational spectroscopy and quantum simulations* — [OC86, p.84]
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PL1

ABOUT ARTIFICIAL PHOTOSYNTHESIS, NEW ELECTROCHEMISTRY, AND ARTIFICIAL ION PUMPS

ORGANIC HETEROJUNCTIONS FOR PHYSICAL CHEMISTRY

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Throughout the search for simple candidates for artificial photosynthesis and electrochemistry for the energy change, carbon nanostructures with heteroatom doping and edge functionality turned out to be unexpectedly efficient. N-doped or O-doped carbons and Carbon nitrides: all these systems are easy to make from omni-available and sustainable precursors. To the general surprise, such carbocatalysts not only outperform even noble metals and some enzymes, but also are at the same time more stable and less sensitive.

Besides introducing these materials and their physical chemistry, I will focus on “heterojunction chemistry”, namely what such structures do with apparently well-known species, such as metallic gold. I will present how the nobility of Gold can be changed in the nanospace, for the purpose of new chemical transformations, such as the room temperature ammonia synthesis or the electrochemical synthesis of formic acid from glycerol, but also for the physical effects as such.

Another exciting playground for such materials is in novel energy storage, both in supercapacitors and battery applications. If time allows, I will also present the realization of a light driven ion pump based on simple chemical components.

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UNDERSTANDING SURFACES USING PROBE MOLECULES AND IN SITU SPECTROSCOPIES

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Spectroscopic techniques represent a "Swiss Army Knife" in understanding molecules and materials, since their capability to shed light on their intimate nature, as well as over their mutual interactions. The present contribution aims to illustrate potentialities and limits of widely used spectroscopies (IR, Raman, UV-Visible and XAS) in studying zeolites and Metal organic Frameworks. Case studies will be selected in respect to the use of zeolites and MOFs as heterogeneous catalysts or selective adsorber, investigating the complex phenomena occurring at their nanostructured surfaces. These methods provide detailed insights into the structural and electronic properties of the materials, as well as their dynamic behavior under real operational conditions. Techniques such as infrared (IR) spectroscopy, Raman spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy and X-ray Absorption (XAS), just to mention some of them, enable the observation of key intermediates, reaction mechanisms, and changes in the local structure of the active sites involved in the process. In situ studies, conducted in controlled temperatures and pressure regimes, have been essential in understanding adsorption phenomena occurring at the surfaces of nanostructured materials used as selective adsorbers.

Furthermore, in the case of catalytic system, operando spectroscopies have greatly enhanced our understanding of catalyst behavior in real-time. The combination of these spectroscopic and molecular modelling approaches has been instrumental in unraveling the molecular-level interactions between catalysts and reactants, identifying reaction pathways, and guiding the design of more efficient, selective, and durable catalytic systems [1-4].

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ADVANCES IN NANOMATERIAL AND NANOSTRUCTURED MATERIAL MODIFIED ELECTRODES

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The modification of electrodes by nanomaterials with the objective of conferring electrocatalytic effects and increase sensitivity has been an important topic of materials' research with applications in fields such as energy and sensors. The synthesis and characterization tools that are now available have led to many important and useful advances. Such nanomaterials include metallic nanoparticles and carbon nanomaterials such as carbon nanotubes and graphene. Some of these will be referred to in the context of devising new electrochemical sensing and biosensing platforms.

The benefits of immobilized metal and metal oxide nanoparticles will be illustrated and how performance can be further enhanced by the deposition of electroactive redox polymers, their formation being finely tuned by changing electropolymerisation conditions, potential range and scanning speed [1-4]. Attention will also be given to performing electropolymerisation in binary (one hydrogen bond acceptor (HBA) and one hydrogen bond donor (HBD)) and ternary (one HBA and two HBD) deep eutectic solvents (DES). Deep eutectic solvents have the advantage of low toxicity and sufficient conductivity, if doped, to permit electrode reactions. The nanostructuring occurring in DES makes the electrochemical sensing behaviour different and with enhanced properties. Some merits of these sensor architectures for the detection of key analytes in the areas of health, food and the environment will be indicated and future directions for using novel materials will be discussed.

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INTERMOLECULAR PHOTOINDUCED ELECTRON TRANSFER IN BIOSYSTEMS: IMPACT OF CONFORMATIONAL TRANSITIONS AND MULTIPLE CHANNELS ON KINETICS

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Studying the kinetics of photoinduced electron transfer (ET) processes in biologically relevant systems using theoretical-computational methods remains a challenging task. Besides the inherent complexity at the electronic level, two fundamental aspects make this problem particularly difficult to address: the commonly observed non-exponential dynamics and the involvement of potentially multiple photoinduced ET channels (Figure 1). Among the hybrid quantum mechanical/classical mechanical computational approaches used for the explicit simulation of photoinduced ET kinetics, I will focus here on a specific method, namely the Perturbed Matrix Method [1,2], which has the advantage of accounting for large-scale conformational effects in ET kinetics and multiple, alternative ET pathways. I will describe its underlying physical principles and provide insights into key applications, specifically three intermolecular ET reactions in which solvent and protein conformational dynamics are key factors and where multiple ET channels may be present. I will discuss ET reactions in two flavoproteins: the riboflavin-binding protein [3] and lactate monooxygenase [4]. The first involves an ultrafast (sub-ps) ET reaction that exemplifies the "frozen-environment" picture (i.e. only a limited number of protein local motions influence the ET), while the latter occurs on the picosecond timescale and is shown to be actively coupled to environmental fluctuations. As a third application, I will discuss ET reactions occurring in the reaction center of photosystem II [5], providing an example of the role of solvation/desolvation in photoinduced ET. The non-exponential behavior observed in these case studies is shown to arise primarily from active coupling with environmental fluctuations and, to a lesser extent, from the presence of branching ET pathways.

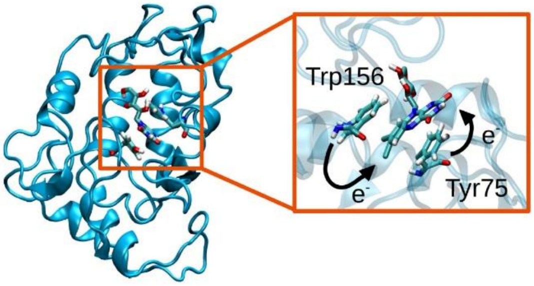

Figure 1. Structure of riboflavin binding protein and zoom of the active site cleft.

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PHYSICAL CHEMISTRY AND SOCIETY: FROM INDUSTRY TO PHYLOSOPHY AND VICEVERSA

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Physical Chemistry is a term invented in Europe, in Russia by Lomosonov in 1752. It is no coincidence that it developed in parallel with the industrial revolution, organizing in the four modern realms of Thermodynamics, Kinetics, Electrochemistry and Quantum chemistry. But from such a general point of view it allows us to look back at society, Nature and to our mode of production by clearly pointing out their criteria and limits and boundaries.

For the same reason, it is no accident that the chemist-physicist tends more than other chemists to be one engaged in social, economic and, today, ecological facts (see Fig. 1).

What have been and what are today these stimuli that our discipline brings and gives to society? And are we aware of this role and of the limitations we show in the educational and conceptual development of the discipline?

We present here some reflections on the modern role of physical chemistry in the present social, economic and energetic transition; and on the many ties and bindings (clearly revealed by a sincere analysis) which limit the cultural development of our theories.

Figure 1. Some famous chemist-physicists: Mikhail Lomosonov, Eunice Newton Footes, Agnes Pockels, Frederick Soddy, Katharine Burr Blodgett, Lise Meitner, Enzo Tiezzi, Alfonso Maria Liquori, Ylia Prigogine, Dorothy Crowfoot Hodgkin, Paul Crutzen.

This is based on a tradition of similar situations in the history of our disciplines which will be opportunely mentioned and commented.

The idea is not to make a historic review, but to reveal, through direct examples, a cultural dynamic interaction which has strongly contributed to change the society, but has also profoundly influenced the basic contents and even the principles of our science.

Physical chemistry does not directly produce new molecules, but is able to influence all the realm of chemical processes in biological, geological and astronomical conditions; for this same reason it contributed to push humankind in the present condition of “metabolic” fracture with the rest of the ecosystem, but is contemporarily the main device to solve the anthropocene conflicts.

PL3

INVERSE METHODS FOR NUCLEAR MAGNETIC RESONANCE OF NON-CRYSTALLINE MATERIALS

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Understanding the atomic-scale structure of disordered materials, such as silicate glasses, is crucial for advancing technologies in optics, ion exchange, and chemical durability. In this talk, I will present a framework for extracting quantitative, model-free probability distributions of nuclear interaction tensors from two-dimensional isotropic/anisotropic frequency correlation NMR spectra. These tensor distributions, encompassing both nuclear shielding and electric field gradient (EFG) tensors, offer a direct and detailed statistical representation of local structure, surpassing the capabilities of conventional spectral fitting of MAS spectra in glasses.

Our methodology integrates advanced linear inverse theory with statistical learning techniques, employing a hybrid approach that combines truncated singular value decomposition and smooth LASSO regularization. This approach enables robust reconstruction of three-dimensional distributions of tensor parameters from experimental spectra, which are then interpreted through quantum chemical calculations to map tensor features to specific local structural motifs.

I will demonstrate the application of this method using ^{29}Si and ^{31}P NMR spectra of network-modified silicate glasses. These case studies reveal the structural roles of modifier cations and phosphorus in determining the connectivity of the glass network, providing a quantitative structural basis for understanding the macroscopic properties of glass. The methods are implemented in the open-source Python package *MRInversion*, offering a broadly applicable framework for structural analysis in disordered materials [1].

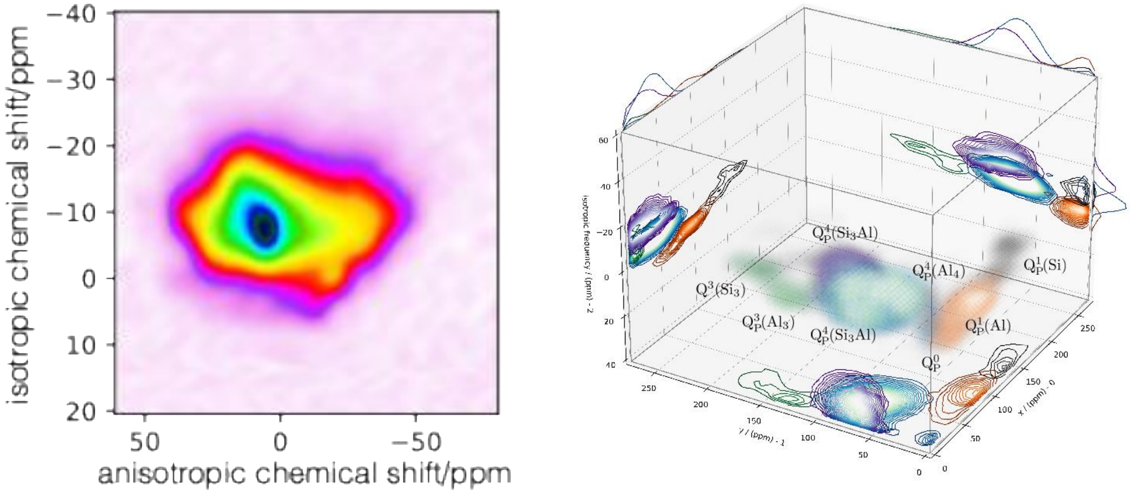

Figure 1. On the left is the 2D ^{31}P isotropic/anisotropic correlation spectrum of $20K_2O{\cdot}15Al_2O_3{\cdot}5P_2O_5{\cdot}60SiO_2$ glass, and on the right is the inverse solution to the ^{31}P magnetic shielding tensor distributions.

[1] D. J. Srivastava et al. J. Chem. Phys. 153 (2020) 134201.

PL4

BIOTHERMODYNAMICS FOR THE CHARACTERIZATION OF PROTEINS AND THEIR INTERACTIONS WITH BIOLOGICALLY IMPORTANT MOLECULES IN SOLUTION

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Biological functions in all living organisms are primarily carried out by proteins, which operate in aqueous environments. Proteins are linear polymers that fold into unique three-dimensional structures, essential for their function, although some remain intrinsically disordered under physiological conditions. Protein activity can be regulated through covalent modifications or by the reversible, noncovalent binding of small or large molecules, with interaction energies ranging up to approximately 80 kJ/mol. The native folded state of a protein is often stabilized by the specific binding of small molecules, with stability closely linked to binding affinity. In the cellular environment, proteins function within a highly regulated aqueous medium characterized by specific pH, ionic strength, salt concentration, and the presence of various biochemical molecules. Importantly, proteins cannot function in the absence of water or essential components such as cofactors and regulatory ligands.

A variety of experimental techniques are employed to assess protein stability and molecular interactions. These include spectroscopic (often fluorescence-based) and calorimetric methods. Differential Scanning Calorimetry (DSC) is a standard tool for evaluating protein stability under different conditions, while Isothermal Titration Calorimetry (ITC) quantifies binding affinity and enthalpy changes. The Microscale Thermophoresis (MST) is a momentary heating-based technique. The Fluorescent Thermal Shift Assay (TSA or Differential Scanning Fluorimetry, DSF) is a practical method for assessing protein stabilities and protein–small molecule interactions, though its use is limited by the complexity of data analysis. To address this, we developed the Thermott web server to facilitate data fitting. The Surface Plasmon Resonance (SPR) and BioLayer Interferometry (BLI) provide convenient kinetic measurements of protein-ligand interactions.

These methods enable the determination of a wide range of thermodynamic and kinetic parameters, deepening our molecular understanding of biomolecular interactions. Key parameters include Gibbs free energy (equilibrium), standard enthalpy change (heat exchange at constant pressure), and entropy (changes in molecular degrees of freedom). Further properties such as heat capacity, compressibility, expansibility, and higher-order thermodynamic derivatives can also be assessed. Binding kinetics—such as association (on-rate) and dissociation (off-rate) constants—are measurable under various conditions, including changes in temperature, pressure, pH, and salt concentration. So-called *intrinsic* [1] energies may also be helpful to account for binding-linked reactions.

Biothermodynamic characterization of protein stabilities and interactions is vital in protein-based research. In any biophysical protein experiments, for example, X-ray crystallography, it is essential to determine conditions at which the proteins will remain stable. Protein–protein interactions underpin fields such as immunology, where antibody–antigen binding is fundamental, while protein–nucleic acid interactions are central to molecular biology. New drug discovery and design benefit significantly from identifying and characterizing lead compounds for pharmaceutical development [2].

[1] V. Linkuviene et al. Quart. Rev. Biophys. 51 (2018) e10.
[2] Carbonic Anhydrase as Drug Target. D. Matulis Ed., Springer-Nature, 2019.

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SL1

COLAVER SRL: PROCESSING AND PRODUCTION OF GLASS AND QUARTZ ARTICLES FOR LABORATORIES

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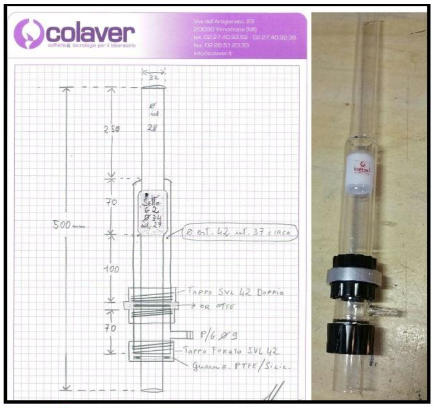

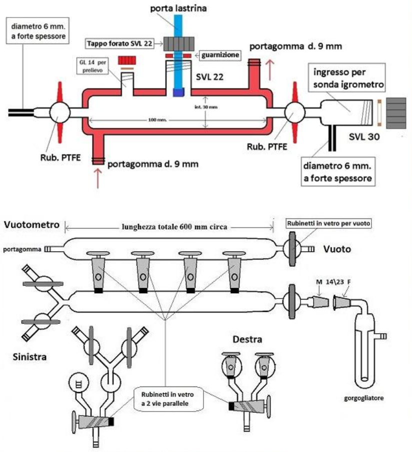

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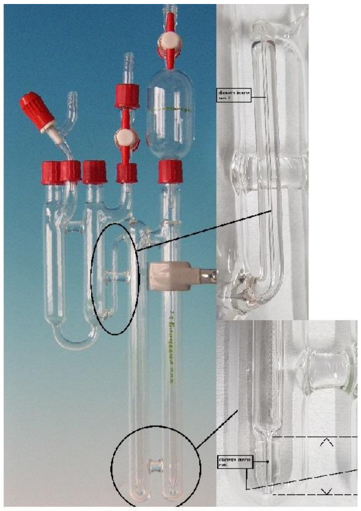

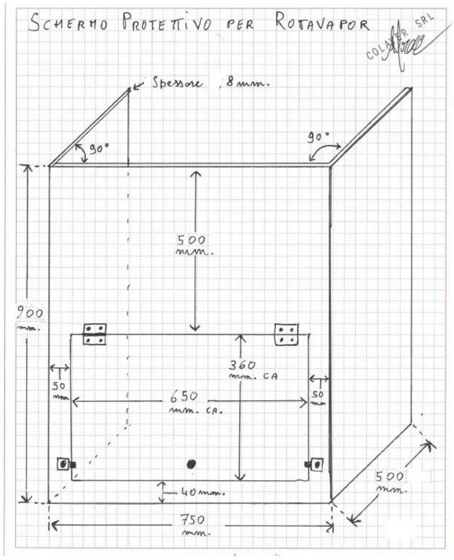

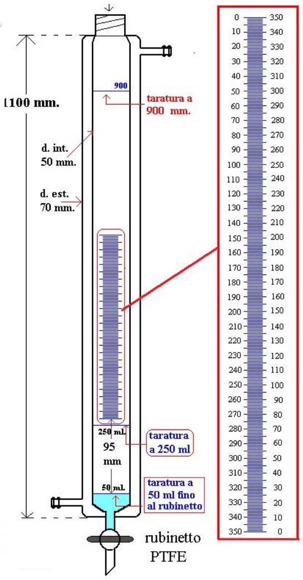

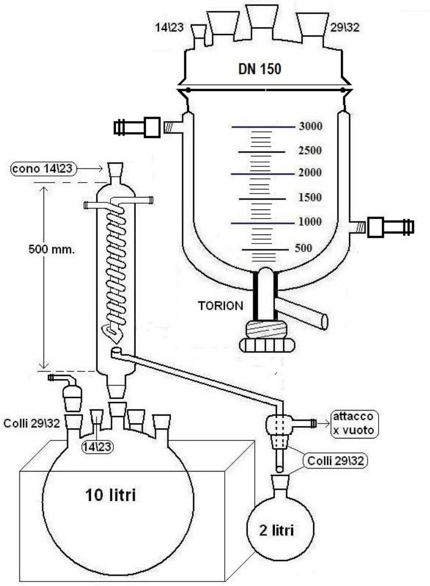

SL3

ADVANCED TECHNIQUES FOR THE PHYSICO-CHEMICAL CHARACTERIZAITON OF MATERIALS

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The relationship between stress and deformation defines the rheological properties of a material. Most films encountered in vivo and in industrial applications are viscoelastic, where this behavior is intermediate between purely viscous and purely elastic. Understanding the rheological and mechanical properties of films is a prerequisite to optimize their properties, correlate micro/nano-structure with their functions and optimize product’s stability. In this contribution we will present two techniques for the characterization of thin films, both relying on an oscillating probe interacting with a 2D sample: interfacial shear rheology and AM-FM viscoelastic mapping mode.

AM-FM Viscoelastic Mapping Mode[1,2,3] is a flexible, convenient AFM tool for nanomechanical characterization. With a range of applicability that spans a remarkable six orders of magnitude in storage modulus (from less than 1 MPa to hundreds of GPa), it is a general-purpose technique for anything from biomaterials and polymers to metals and ceramics. AM-FM Mode provides elastic information including storage modulus, Young’s modulus, contact stiffness and viscoelastic information including viscoelastic loss tangent and loss modulus.

An interfacial rheometer uses a magnetized tip positioned at the air-liquid or liquid-liquid interface that is oscillated using permanent magnets. The probe movement is recorded with a high-resolution camera and the viscoelastic properties for the film can be calculated, allowing for the study of phase changes, surface reactions, aggregation and adsorption, stability of micelles and colloids and many more.

[1] Protected by certain U.S. patents assigned to or licensed by Oxford Instruments Asylum Research, Inc., including 8,555,711, 8,448,501, 8,024,963, 7,958,563, 7,603,891, and 7,921,466.
[2] R. Garcia et al. Eur. Polym. J. 49 (2013) 1897.
[3] R. Proksch et al. Appl. Phys. Lett. 100 (2012) 073106.

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SL2

BENCHTOP MAGNETIC RESONANCES: EPR AND NMR RESEARCH ON YOUR TABLE (WITH NO CRYOGENICS)

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Benchtop solutions for NMR and EPR are quickly increasing their flexibility, due to the variety of accessories that enlarge the possibilities of analysis, without the need of any laboratory infrastructure or cooling.

Among them, there is the MultiHarmonic accessory that greatly increases the SNR of our EPR systems, and the last born multinuclear probe of the Fourier80

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OC68

EXPLORING CHIRAL SENSITIVITY OF TRUECARS SIGNAL: MONITORING ULTRAFAST ELECTRONIC COHERENCES SPAWNED BY ENANTIOMERICALLY EQUIVALENT S_0/S_1 CONICAL INTERSECTIONS IN *cis-trans* PHOTOISOMERIZATION OF A RETINAL CHROMOPHORE MODEL

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The cis-trans photoisomerization of Retinal, an achiral chromophore in isolation, can proceed via either a clockwise or counterclockwise rotation along double bond through enantiomerically equivalent CIs. However, introducing chiral perturbations, such as embedding the chromophore in a chiral environment, can break the symmetry, leading to preferential rotation and enantiomeric selectivity, which directly influences the quantum yield. Monitoring the vibronic coherences spawned upon nonadiabatic passages through each enantiomerically distinct CI along different pathways could then provide valuable insights toward chiroptical control of the final product. Theoretically, transient redistribution of ultrafast electronic coherences in attosecond Raman signals (TRUECARS) has recently been proposed [1] for the direct monitoring of the CI passage in a background-free manner. Accordingly, in this study we simulate and capture the vibronic coherences generated by the ultrafast passage through two enantiomerically distinct CIs in the 2-cis-penta-2,4-dieniminium cation (cis-PSB3), which serves as a minimal model for rPSB11. To this end, we resort to a recently developed analytical potential energy model by Olivucci et al. [2] along three key modes, namely bond-length alternation (BLA), torsion (Tors), and hydrogen-out-of-plane (HOOP) wagging. We perform nonadiabatic vibronic wavepacket dynamics to compute the electronic coherence required to simulate the TRUECARS signal. Our results show that for a wavepacket initially excited at cis geometry, the coherence between diabatic and adiabatic states is exactly null, while sizable electronic coherences, governed by the cis region of the configurations, emerge when starting the propagation from a distorted geometry or selectively tracking clockwise vs counterclockwise torsional motion (Figure 1). To assess the robustness of these electronic coherences in a more realistic system with additional degrees of freedom, we added a set of harmonic displaced (bath) modes to the initial 3D model. We then performed nonadiabatic wavepacket dynamics using ML-MCTDH method to investigate their impact on the coherences and the signal. The results show that coherences are quenched rapidly over longer timescales, while less affected at the first 100 fs, which governs by the cis region of the configurations, where change due to the bath modes is smaller.

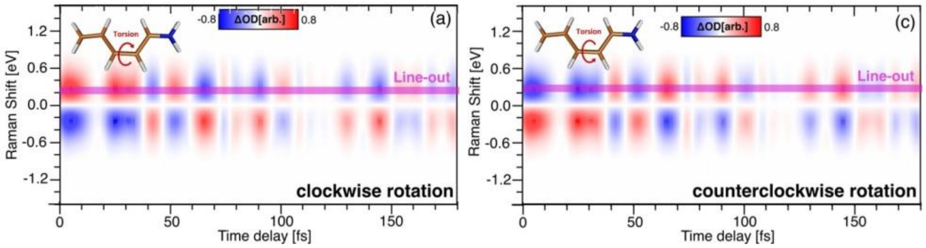

Figure 1. The TRUECARS signals simulated along the enantiomerically equivalent clockwise (a) and counterclockwise (b) photoisomerization paths of the cis-PSB3 model.

[1] M. Kowalewski et al. Phys. Rev. Lett. 115 (2015) 193003.
[2] E. Marsili et al. J. Chem. Theory Comput. 16 (2020) 6032.

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OC88

STUDY OF TiO_2-BASED PHOTOCATALYSTS COUPLED WITH MAGNETIC ZEOLITES AND CARBON NANOMATERIALS FOR H_2 PRODUCTION

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The exploitation of solar light as a renewable and clean energy source seems to be the most promising approach to comply with the development objectives for a sustainable future, as it has already sustained life on Earth for a very long time and it can still be exploited for many of modern society's needs. Alongside, H_2 represents a cost-effective and environmentally friendly option as energy vector, which produces only water by combustion, that can be further harvested by sunlight-driven photocatalytic processes, including reforming in the aqueous-phase of different biomasses [1].

To this end, titanium dioxide-based materials were synthesized, characterized, and tested: specifically, a three-component photocatalysts was developed starting from the coupling of nanosized-anatase TiO_2 with carbon-based nanomaterials and porous zeolites. Composite photocatalysts were prepared via soft-chemistry sol-gel route; in this stage, carbon nanomaterials obtained by the treatment of different concentrated starch solutions, are introduced into the titanium dioxide lattice in different ratios (V/V); the gel is then treated under hydrothermal conditions for 3 hours at 150°C, also in the presence of different zeolite ratios, to make the carbon-doped TiO_2 crystallize over the supporting porous material and then address the photocatalytic activity according to the composition. The used zeolites were also synthesized starting from raw materials deriving from both commercial reagents or from waste recovery (such as metal oxides recovered from different fly ashes and rice husk ashes), for which a life cycle assessment is planned, and then transformed into porous structures using a simple and fast ultrasonic method. The composite photocatalyst should have important visible light absorption features, as well as a proper electronic structure that can enhance the lifetime of the charge carriers, together with positive support and porosity characteristics [2].

Composites were investigated in the preliminary photocatalytic tests, under simulated solar light (500 W/m^2, 4h), for lab-scale H_2 production, in the presence of 0.1 M glucose as a probe biomass-derived sacrificial agent, and 0.5 wt% Pt as the conventional co-catalyst. The H_2 evolved and accumulated in the photoreactor headspace was determined by gas chromatography coupled with a thermal conductivity detector, and the results were reported in terms of hydrogen evolution rate "HER", calculated as µmoles of H_2 per gram of catalyst per hour ($\mu mol\ g^{-1}\ h^{-1}$). Eventually, rice husk will also be used as an insoluble feedstock biomass to be processed by photo-reforming to obtain hydrogen, thus increasing the sustainability of the overall process.

[1] C. Y. Toe et al. Energy Environ. Sci. 14 (2021) 1140.
[2] G. Zhang et al. Micropor. Mesopor. Mater. 225 (2018) 61.

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OC57

LATTICE DYNAMICS AND POLAR DOMAIN STRUCTURE OF GIANT-REFRACTION $K_{0.997}Li_{0.003}Ta_{0.64}Nb_{0.36}O_3$ SOLID SOLUTION

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Ferroelectricity in ABO_3 perovskites is generally attributed to off-center displacement of B ions with respect to their coordination environment, eventually clustering into coherently polarized nanoregions (PNR) below the Curie point T_C [1,2]. Although this mechanism has been supported for decades by indirect experimental evidence, to this day little is known about the local structure of the PNR, as well as their relative arrangement at the micrometer scale. In this work, we investigate ferroelectricity in a Li-doped perovskite solid solution $K_{0.997}Li_{0.003}Ta_{0.64}Nb_{0.36}O_3$ (KLTN) displaying giant broadband refraction (n>25) below T_C, where a supercrystal with large-scale periodicity (~5 µm) is observed [3], as illustrated in Fig. 1. Density functional theory calculations performed on the parent structures - ferroelectric $KNbO_3$ and paraelectric $KTaO_3$ – help to rationalize the interplay between Li, Ta and Nb displacements observed in the solid solution through X-ray diffraction (XRD) measurements. In parallel, molecular dynamics simulations calibrated on the same XRD data investigate the atomic structure at higher length scales (~10-100 nm), where the PNR emerge. Observations from *ab-initio* and classical simulations are then combined in order to interpret the temperature-dependent lattice dynamics of KLTN, leading from the room-temperature paraelectric phase to the below-T_c ferroelectric phase. These results provide a basis to rationalize the structural origin of the remarkable optical properties of KLTN.

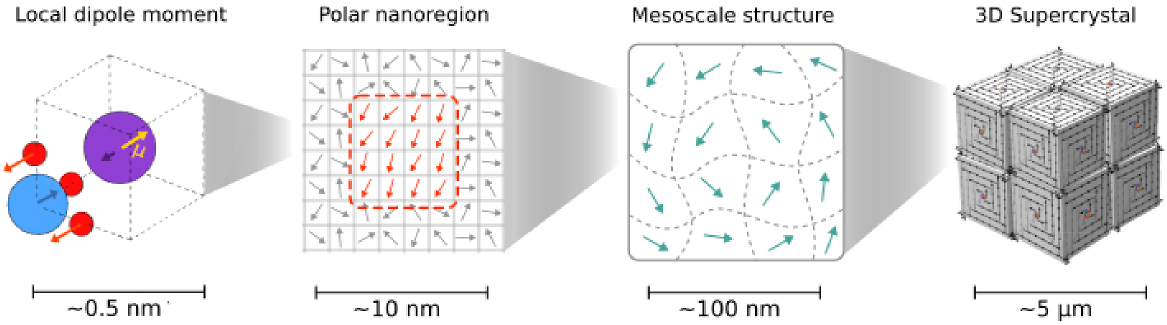

Figure 1. Illustration of the plausible structure of the KLTN solid solution below the Curie point, at different length scales.

[1] V. Polinger et al. Phys. Rev. B 98 (2018) 214102.
[2] M. S. Mark et al. Phys. Rev. Lett. 116 (2016) 207602.
[3] L. Lo Presti et al. Phys. Rev. B 102 (2020) 214110.

OC43

HIERARCHICAL ZEOLITES FROM *TOP-DOWN* APPROACH: A SYSTEMATIC INVESTIGATION OF THEIR STRUCTURAL AND ADSORPTION PROPERTIES

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Hierarchical zeolites, which exhibit a distinctive structure characterized by interconnected micropores and mesopores, are versatile materials that can overcome the typical issues related to microporous materials, including poor mass transfer, hindered diffusion, and strict selectivity of resulting products. One possible route to obtain hierarchical porous materials is through *top-down* approaches, in which secondary porosity is introduced via post-synthetic modification of a pre-existing microporous matrix. [1,2] In this contribution, a *top-down* method was employed to obtain hierarchical porous materials with different properties. In detail: two commercial zeolites, HZSM5 and HUSY (both with SiO_2/Al_2O_3 = 80) with a MFI and FAU structure respectively, and a natural clinoptilolite (HCLI, Si/Al = 5) with HEU structure were desilicated using NaOH solutions at varying concentrations, to evaluate the treatment efficiency. The synthesized hierarchical architectures were characterized by multi-technique approach using XRD, N_2 physisorption at 77K, TGA and FTIR spectroscopy of adsorbed probe molecules, to assess the nature, strength and accessibility of the acid sites (Figure 1A,A'). The obtained hierarchical zeolites were evaluated for their ability to recover Cu^{2+} and Co^{2+} ions from aqueous solutions by using UV-Vis spectroscopy. Selectivity tests were also carried out to determine the materials' affinity for the target ions. The three investigated zeolites exhibited distinct behaviors, based on their different physicochemical properties (Figure 1B). HZSM5 demonstrated the highest adsorption capacity but showed no specific affinity for either metal ion, in contrast to HUSY and HCLI, which displayed a clear preference for Co^{2+} (Figure 1B). Notably, the desilication treatment significantly enhanced the adsorption efficiency of the studied materials.

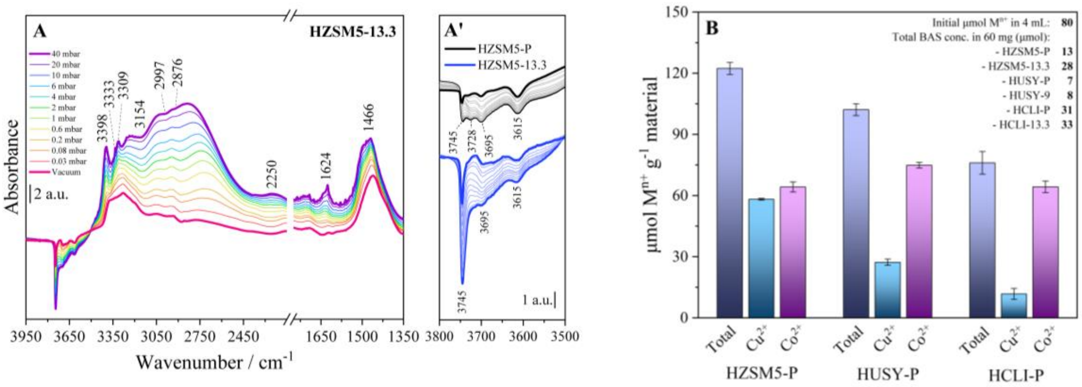

Figure 1. FTIR of NH_3 adsorbed and hierarchical HZSM5 at room temperature (A); comparison of HZSM5 spectra before and after desalination in the OH stretching region (A'); amount of Mn^+ captured by the studied zeolites from aqueous solution after 24 hours, expressed as μmol g^{-1}

Dr. Gioele Ancora holds a PhD career grant supported by Next Generation EU – MUR.

[1] M. Hartmann, Angew. Chem. Int. Ed. 43 (2004) 5880.
[2] S. Mitchell et al. Nat. Commun. 6 (2015) 8633.

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OC102

CO_2 ELECTROREDUCTION AND GLYCEROL OXIDATION ELECTROCATALYSTS FABRICATED BY ELECTRODEPOSITION

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Carbon dioxide reduction reaction (CO2RR) is a key technology for the chemical industry in a highly electrified energy scenario. To achieve its economic feasibility, it is necessary to reduce the electrolyzer operating voltage. To this end, replacing the sluggish anodic oxygen evolution reaction (OER) with the glycerol oxidation reaction (GOR) is an interesting approach that also offers the opportunity to upcycle a low-value product.

Besides the need to develop efficient and selective catalysts, the fabrication routes should be easily scalable. In this context, we present electrodeposition as an effective and versatile tool to obtain thin film layers of electrocatalysts on metal foams and microporous layers of gas diffusion electrodes (GDE).

In this contribution, it will be presented the recent efforts of the group in the development of coupled systems. On one hand, AuCu, CuIn alloys were successfully deposited on GDEs and tested in continuous flow towards the CO2RR employing different electrolytes. The results show that the presence of halides in the catholyte can avoid the undesirable hydrogen evolution reaction and favor the formation of carbon monoxide or formic acid, an effect that is enhanced by the use of binary alloys. On the other hand, NiCo layered double hydroxides and AuIn alloys were deposited on nickel foams to perform the electroxidation of glycerol, with an electrode potential reduction of 0.2 to 0.5 V with respect to the OER reaction. Results show a strong dependence of the operating conditions in the product distribution, being feasible to obtain C3 products (DHA or lactic acid) under continuous flow of the electrolyte. [1] Finally, both half reactions have been coupled in a continuous flow reactor at operating current densities up to 200 mA cm^{-2}.

Acknowledgements: This work has been funded by project CO2GLY (PID2022-138491OB-C33) funded by MICIU/AEI /10.13039/501100011033 and by FEDER, UE. M.A. thanks Pla de Doctorats Industrials de la SUR de la Generalitat de Catalunya (2021DI20) and M.M. thanks Ajuts Joan Oró per a la contractació de personal investigador predoctoral en formació (FI) (2024 FI-1 00421), both granted by Agència de Gestió d’Ajuts Universitaris i de Recerca (AGAUR).

[1] K. Fernández-Caso et al. Chem. Eng. J. 480 (2024) 147908

OC44 DEEP LEARNING FOR SPECTRAL DATA MODELLING IN CULTURAL HERITAGE

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The advent of deep learning has revolutionized data analysis and modeling across scientific disciplines, enabling unprecedented accuracy and efficiency in complex data interpretation. In the field of cultural heritage, deep learning has recently emerged as a powerful tool for analyzing spectral data, facilitating material identification, classification, and predictive modeling [1]. This approach is particularly valuable for non-destructive techniques such as Raman spectroscopy and X-ray fluorescence (XRF), which are widely used in the study of historical artifacts. However, these techniques are often applied using portable instruments, which typically have lower performance compared to laboratory-based equipment. This research presents case studies demonstrating how deep learning can significantly enhance the extraction of chemical information from spectral data in cultural heritage research. In one study, a neural network was employed to classify and interpret Raman spectra from pigments used in street art, with a focus on the Berlin Wall's graffiti layers. The model successfully predicted the composition of pigment mixtures, despite Raman spectroscopy traditionally being considered unsuitable for quantitative measurements [2]. Another study applied deep learning to the XRF spectral characterization of archaeological metals, including bronze arrowheads and silver coins, to detect alloying patterns and reveal key chemical features. The results highlight the potential of deep learning models to refine material classification and enhance provenance studies. By integrating artificial intelligence into spectral data processing, this presentation underscores the transformative role of deep learning in modeling chemical information. The findings demonstrate how AI-driven methodologies can enhance material identification, improve analytical precision, and open new opportunities for spectroscopic analysis, offering deeper insights into historical artifacts.

Acknowledgements: Project MML-ARCH - "Metodologie di machine learning applicate all'archeometria: una nuova frontiera per l'interpretazione materica dei Beni Culturali", Programma "CHANGES Cultural Heritage Active iNnovation for Sustainable Society" CUP B53C22003890006 - Codice Identificativo PE_00000020, finanziato dall'Unione Europea – Next Generation EU sui fondi PNRR MUR – M4C2 – Investimento 1.3 "Partenariati estesi a Università, centri di ricerca, imprese e finanziamento progetti di ricerca" Avviso pubblico per la presentazione di Proposte di intervento per la creazione di "Partenariati estesi alle università, ai centri di ricerca, alle aziende per il finanziamento di progetti di ricerca di base".

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OC30

CATALYSIS OF HYDROGEN EVOLUTION REACTION USING BIO-INSPIRED WC-BASED CATALYSTS IN BIPHASIC REACTIONS

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The hydrogen evolution reaction (HER) at liquid/liquid interfaces, which share similar properties with biological membranes, stands out due to its significant advantages over alternative HER processes, such as reusability and the elimination of preliminary steps like the cleaning of solid electrodes. Furthermore, recent research has accelerated efforts to design effective electrocatalysts for HER and to develop alternative catalysts to precious metals like Pt, which, despite their high efficiency, lead to substantial costs. Among transition metal carbides, tungsten carbide (WC) exhibits unique surface reactivity and catalytic properties similar to Pt and other noble metals. In addition to these characteristics, WC is considered an ideal electrocatalyst substrate for HER due to its high conductivity, broad pH compatibility, good anti-toxicity, low cost, and electrochemical stability. However, despite these advantages, several factors limit the application of WC-based catalysts, including their large particle sizes, low specific surface areas, and poor morphology control, which affect their hydrogen adsorption-desorption properties. Studies aiming to overcome these drawbacks have reported that the combination of two or more components can optimize hydrogen adsorption-desorption capabilities, thereby achieving the desired electrochemical HER activity. Also, hybridization of different components can enhance HER catalyst performance through synergistic effects such as electronic modulation, interface stabilization, and atomic regulation. Inspired by the active centers that facilitate catalytic activity in biological systems, the development of catalysts for energy conversion applications represents a promising approach. In this study, the HER activity of WC/NiCo catalysts, designed using transition metals inspired by hydrogenase enzymes, was investigated at biphasic systems, which are notable for their similarity to biological membranes. Optical, electrochemical, and chromatographic analyses were conducted to evaluate their performance. The synergistic effect of Ni and Co with WC, along with the increased specific surface area, was found to enhance catalytic activity in HERs compared to pristine WC catalysts.

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OC56

NONEQUILIBRIUM THERMODYNAMICS OF NON-IDEAL REACTION-DIFFUSION SYSTEMS: IMPLICATIONS FOR ACTIVE SELF-ORGANIZATION

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We develop a framework describing the dynamics and thermodynamics of open non-ideal reaction-diffusion systems, which embodies Flory-Huggins theories of mixtures and chemical reaction network theories [1]. Our theory elucidates the mechanisms underpinning the emergence of self-organized dissipative structures in these systems. It evaluates the dissipation needed to sustain and control them, discriminating the contributions from each reaction and diffusion process with spatial resolution. It also reveals the role of the reaction network in powering and shaping these structures. We identify particular classes of networks in which diffusion processes always equilibrate within the structures, while dissipation occurs solely due to chemical reactions. The spatial configurations resulting from these processes can be derived by minimizing a kinetic potential, contrasting with the minimization of the thermodynamic free energy in passive systems. This framework opens the way to investigating the energetic cost of phenomena such as liquid-liquid phase separation, coacervation, and the formation of biomolecular condensates.

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OC93

Zn_2SiO_4:Eu^{3+} AS SMART MULTICOLOR VISIBLE EMITTER

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Lighting is a major source of energy demand, and even if significant progress has been made for substituting incandescent lamps with new and more efficient devices, increasing use of lighting drove up total energy consumption, especially in emerging areas. Lighting plays an important role even in CO_2 production, contributing to climate change [2]. With the purpose of finding a solution to these issues, inorganic solid-state materials earn a chance to be one of the most promising alternatives to produce high efficiency devices.

Depending on the nature of their luminescence, inorganic phosphors can be divided into two groups: metal-activator based, and non-activator based phosphors. In the first case, the emission is due to dopants, transition-metal or rare-earth ions, in the crystal lattice of an inorganic host matrix. In the latter, instead, the emission comes from different types of crystal defects, typical of each material, without adding external elements [3]. These two pathways to reach luminescence in inorganic materials are usually considered separately, but the combination of them leads to more functional materials, with tunable optical properties [4]. In this work we synthesized, by a simple hydrothermal procedure, different zinc silicate phosphors, changing the Zn to Si ratio in the synthesis, and adding a fixed concentration of Eu^{3+} acting as dopant. Depending on the synthetic conditions, we are able to tune the optical properties of these materials, reaching multicolor emission by changing the excitation wavelength (Figure 1). Directly exciting the lanthanide, its emission in between 550 nm – 720 nm prevails over the contribution of the defects; the latter, below 550 nm, is the main contribution when the excitation is centered on the defect's energy levels. This multimodal behavior can be adjusted by thermal annealing. Each contribution to the total emission of the phosphors has a characteristic decay time, so this opens the possibility to change the chromaticity of the material in a different time range.

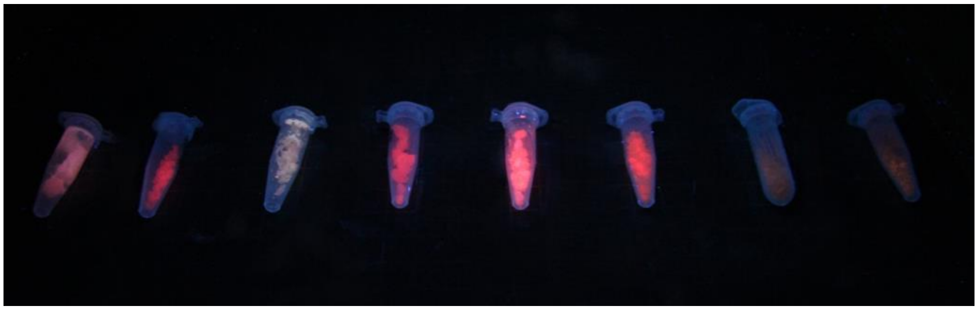

Figure 1. Multicolor emission in Eu^{3+}- doped silicates.

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OC55

BIOCOMPATIBLE HYDROGELS LOADED WITH *BRASSICACEAE* EXTRACTS FOR THE CONTROLLED DISINFECTION OF AGRICULTURAL SOILS

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Biofumigation [1,2] was proposed as an alternative to the use of toxic fumigants such as metam sodium [3] for the disinfection of agricultural soils, in view of the biocidal effect of isothiocyanates (ITCs) released by some vegetal species, like *Brassicaceae*. However, biofumigation also presents limitations; thus, an advanced and viable alternative could be the use of controlled-release systems, i.e., porous carriers, mesoporous particles, or gelled polymer networks. In the present work, we explore the use of biocompatible hydrogels, based on sodium alginate and sodium carboxymethylcellulose, conveniently loaded with *Brassicaceae* extracts for this purpose. The extract was characterized by means of HPLC-MS, showing its high content in glucosinolates, especially glucoraphanin, a secondary metabolite produced by several species of this family. Glucoraphanin is a precursor to sulforaphane, an isothiocyanate with well-known biocidal properties towards several soil-borne phytopathogens [4,5]. The physicochemical properties of the synthesized gels were investigated by means of Attenuated Total Reflectance-Fourier Transform Infrared spectroscopy (ATR-FTIR), Thermogravimetric analyses (TGA), Differential Scanning Calorimetry (DSC), rheometry, and Scanning Electron Microscope (SEM), both in the presence and in the absence of the loaded extract. Loading and release kinetics (in water) were studied by means of HPLC-DAD, and the Weibull model was employed to interpret the results. It was found that both hydrogels are able to effectively confine the *Brassicaceae* extract's active principle, slowly releasing it in an aqueous environment. The biodegradable nature of these polymers grants that the gel is eventually completely disrupted, ensuring a gradual but complete release of glucosinolates in the treated soil. These systems surely are interesting tools to contrast harmful microorganisms, in view of the biocidal properties of glucosinolates, and their potential goes beyond their use in agriculture, as they could be applied as antifouling or antimicrobial agents in cultural heritage cleaning or other fields.

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OC26

FLUORINATED NANOSTRUCTURES AS BIOIMAGING TOOLS AND DELIVERY AGENTS

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This work addresses the current need for novel sensitive, robust, and selective diagnostic tools for non-invasive *in vivo* imaging, which are able to improve the medical practice through earlier diagnosis of disease, implementation of targeted therapies, and localization of diseased tissues. Our approach is based on the development of sustainable fluorinated probes enabling ^{19}F-MRI, as a complementary tool, to be coupled with other diagnostic imaging techniques such as ^{1}H-MRI, Raman and fluorescence imaging, in order to overcome their present shortcomings. This talk reports about a unique fluorinated imaging agent (PERFECTA) bearing 36 equivalent ^{19}F atoms and therefore showing a single, intense ^{19}F-NMR signal. Biocompatible nanoparticles loaded with PERFECTA demonstrated excellent cellular compatibility and spectral properties (relaxation times and sensitivity) adequate for in vivo ^{19}F-MRI use [1,2]. In this presentation PERFECTA ability to work as multiscale and multimodal probe will be shown as represented in Figure 1 [3]. Moreover, effects of fluorination on self-assembly of PERFECTA amphiphilic derivatives will be also presented as well as their biological interactions and response also in the perspective to use them in precision medicine [4].

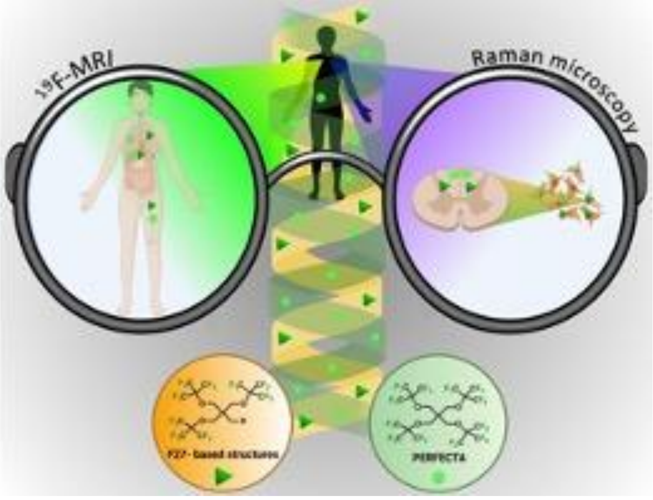

Figure 1. Representation of PERFECTA imaging applications at multiscale level from whole body by ^{19}F-MRI to cells and tissues by Raman microscopy.

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OC62

FUSOGENIC PNIPAM-STABILIZED LIPID NANOPARTICLES FOR ENHANCED AINTICANCER DRUG DELIVERY

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One of the most effective strategies in nanomedicine is the solubilisation of therapeutic agents within nanovectors to enhance their efficacy and prolong their circulation time in the body after administration. Among these, lipid-based nanocarriers remain the most suitable due to their biocompatibility and similarity to plasma membranes, as demonstrated by lipid-based vaccines for mRNA delivery against COVID-19. In recent years, however, increasing attention has been devoted to the design of more efficient drug delivery systems. In this context, a new class of complex lipid-based nanocarriers, known as cubosomes, has emerged as particularly promising candidates due to their exceptional properties, including high stability and enhanced drug-loading capacity. Herein, we developed a new class of lipid nanocarriers based on the lipid glycerol monooleate (GMO) using a novel polymeric stabiliser, the block copolymer poly(N,N-dimethylacrylamide)-poly(N-isopropylacrylamide) (PDMA-b-PNIPAM). This stabiliser not only imparts steric stability to the lipid nanocarriers but also improves the interaction with biomimetic membranes and confers thermoresponsive properties under physiological conditions compared to traditional Pluronic F127-based formulations.[1] Although many strategic features characterise these nanostructures, none of these cubic formulations have yet been approved by the Food and Drug Administration (FDA). In order to address their fate in the biological environment and thus achieve future therapeutic application as drug delivery systems (DDS), we extended the study of this new class of PNIPAM-stabilised nanoparticles to two human cancer cell types through a series of in vitro studies. In particular, using scanning electron microscopy (SEM), confocal laser scanning microscopy (CLSM), and flow cytometry (Figure 1) we underscored the primary role of the PNIPAM-based stabiliser in both the internalisation and chemotherapeutic efficacy of the lipid nanocarrier encapsulating the anticancer drug camptothecin (CPT), confirming that PDMA-b-PNIPAM-stabilised cubosomes constitute promising candidates for chemotherapeutic drug delivery.[2]

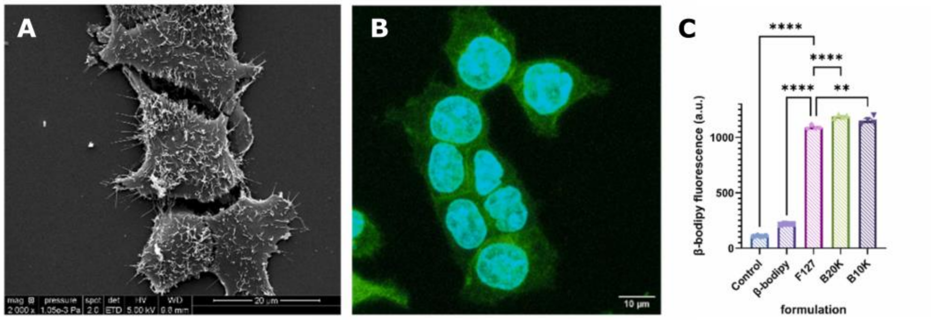

Figure 1. Scanning Electron Microscopy image (SEM) (A), Confocal Laser Scanning Microscopy image (B), and quantification by flow cytometry (C) of HCT-116 cells after exposure to lipid nanoparticles. Readapted from [2]

[1] A. Balestri et al. Colloids Surf. B. Biointerfaces 220 (2022) 112884.
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OC20

SOLID STATE SOLVATION: A FRESH VIEW

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The design of efficient organic electronic devices, including OLEDs and OPV cells, relies on the choice and optimization of a functional dye embedded in a solid matrix. The properties of the dye are non-trivially affected by the local environment, and the understanding of solid-state solvation (SSS), i.e. how the local surroundings affect the properties of the active dye in the solid state, if properly mastered, is crucial to optimize the device performance. However, while the effects of low-viscosity solvents are well-known, SSS is still a less investigated and controversial topic. In this work, we exploited solvatochromic dyes as microscopic polarity probes to investigate the dielectric and dynamical response of several amorphous matrices typically used in OLED fabrication (Figure 1). Micro-Raman spectroscopy was proposed to easily estimate the static behavior of the matrices, obtaining a reliable polarity scale. Conversely, steady-state fluorescence spectra depend in a non-trivial way on both the matrix polarity and its dynamics. The extensive analysis of time-resolved spectra collected over a wide time range (15 fs – 15 ns), supported by theoretical work, allowed to fully characterize the relaxation dynamics of a few matrices of interest for OLED applications. The proposed approach can be extended to any amorphous material and represents a step forward towards the comprehension of SSS and its exploitation for the engineering of materials for optoelectronic devices.[1]

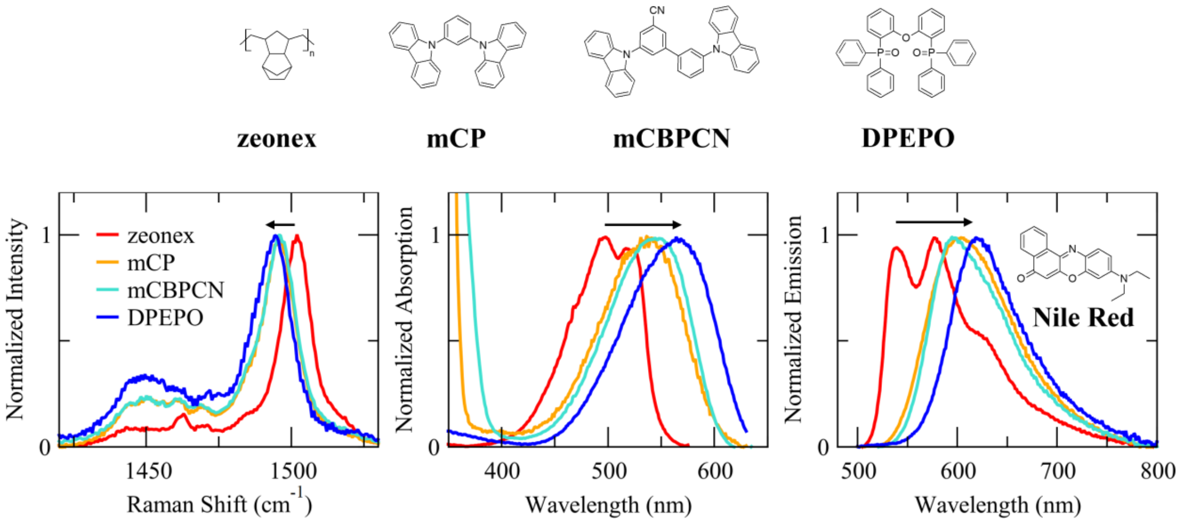

Figure 1. Raman, absorption and emission spectra of a polar dye (Nile Red) in different matrices.

[1] B. Bardi et al. Mater. Horiz. 10 (2023) 4172.

OC115

HYDROGEN PRODUCTION THROUGH THERMAL DEGRADATION OF CONFINED AMMONIA BORANE

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The development of highly efficient materials for chemical hydrogen storage is one of the great challenges for driving the hydrogen economy to a major breakthrough. The safety of hydrogen tanks and the energy required for compression to high pressure have drastically slowed down the spread of the hydrogen-based mobility. Several alternatives have been proposed to overcome these problems using inorganic or organic carriers. Among all the available species, ammonia borane (AB) is one of the most interesting compounds with a theoretical gravimetric hydrogen storage capacity of up to 19.6 wt % [1]. The most challenging and attractive AB dehydrogenation route is the solid-state thermal-induced dehydrogenation. Nevertheless, this reaction is complex, involves several pathways and mechanisms that could be promoted or suppressed by the presence of additives. The solid-state dehydrogenation kinetic of AB under thermal stimuli is widely investigated by directly mixing AB with dehydrogenation catalysts [2] or by confinement into a porous matrix [3].

Nevertheless, an interesting process is the preparation on an unstable AB with a tuned the degradative pathways by adding a chemical species.

In our work, we proposed a new route to modify the thermochemical behaviour of AB by solid state encapsuling it tailored polymeric matrix. We diffusely studied these systems using TGA-IR, DSC and IR and Raman spectroscopy producing a solid interpretation based on kinetic and thermodynamic parameters of the chemical pathways.

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OC49 WATER REMEDIATION FROM HEAVY METALS AND ORGANIC POLLUTANTS USING CELLULOSE-DERIVED ADSORBENTS

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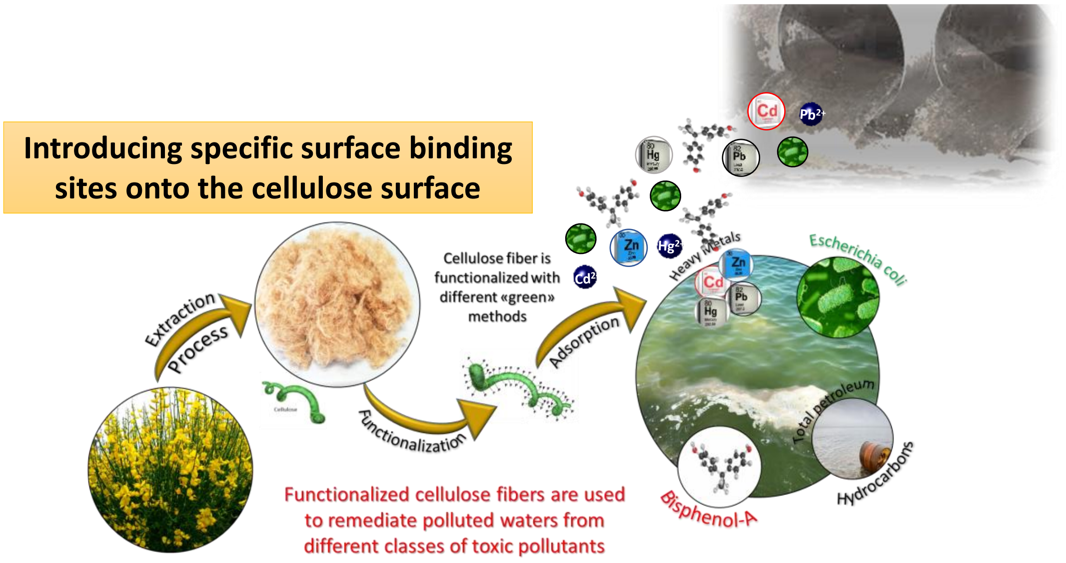

Figure 1. Schematic representation of cellulose extraction from vegetables, its surface functionalization to develop selective and efficient adsorbent materials

Adsorption is one of the most straightforward and efficient methods for removal of pollutants from water [1]. Due to its huge mechanical properties and its abundance as waste material, cellulose can be exploited as a platform for the development of advanced adsorbents. Indeed, despite its relatively low surface area compared to conventional adsorbent materials (activated carbons, porous organic polymers, covalent/metal organic frameworks, etc.), the possibility to easily functionalize its surface renders this natural material very attractive for the technology of water remediation, e.g. to develop stable permeable reactive barriers to be used in dynamic conditions [2]. Here we show that ad hoc surface grafting of cellulose, can be used to tune its surface properties (hydrophilic vs. hydrophobic), leading to cellulose-based adsorbent materials which retain most of the useful properties of pristine cellulose but exhibiting improved removal performances, such as high adsorption capacity and selectivity, for the removal of both organic pollutants [3-5] and heavy metal ions [2, 6-7].

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[2] F. E. Arias Arias et al. Chemosphere 180 (2017) 11.
[3] A. Tursi et al. Chemosphere 201 (2018) 530.
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OC69

THE INTERPLAY OF KEY PARAMETERS IN THE TRANSPORT PROCESS OF SMALL SYNTHETIC CHLORIDE CARRIERS

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The study of small chloride ion transporters has attracted considerable attention as a promising alternative therapy to conventional drugs for cystic fibrosis [1,2]. Chloride ion homeostasis is critical for several cellular functions, and dysfunction in the protein channels responsible for chloride transport - caused by genetic mutations - can vary widely among patients. While traditional therapies target specific mutations, an alternative approach using small synthetic transporters that bypass the faulty protein could offer a broadly applicable solution. In recent years, extensive research on the transport capabilities of different molecular classes has led to the identification of several promising candidates [3–6]. However, the complex interplay of different physicochemical features governing different stages of the transport process remains poorly understood, making it difficult to establish clear molecular design principles.

To address this, chloride release assays [7] were performed by using vesicle dispersions on different molecular classes, including squaramides, thioureas and tambjamines, among others. Transport performance was assessed by using different lipid bilayers, namely, 100%$_{\text{mol}}$ POPC, POPC:cholesterol 70:30, POPC:POPG 75:25, and POPC:POPG 25:75. This experimental approach provided valuable insights into the transporter behavior, opening the route to a detailed comparison of the impact of different molecular properties on the overall transport efficiency. The analysis of the experimental chloride release curves is performed through the non-linear least-squares fitting of theoretical data obtained with numerical simulations. The underlying mathematical model was initially designed for the simplest case of a non-electrogenic uniport mechanism [8] but currently being extended to explicitly include additional important contributions, such as the osmotic pressure and the possible volume variation, counter-ion transport and membrane potential, beside membrane partitioning, passive diffusion and adduct formation equilibria. The goal is to develop a robust algorithm capable of fitting experimental curves, representing an analytical tool, on the one hand, for data interpretation and to dissect the weight of the different stages on the whole transport process, and a predictive tool, on the other, to guide the synthesis of new optimized transporters.

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OC83

SELF-ASSEMBLY AND BIOLOGICAL PROPERTIES OF HIGHLY FLUORINATED OLIGONUCLEOTIDE AMPHIPHILES

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Nucleic acids offer significant advantages over small-molecule drugs due to their high specificity and adaptability to a wide range of disease phenotypes [1]. However, their instability in biological media and rapid clearance limit their applicability [1], requiring nanocarriers to overcome these challenges [2]. Among these, spherical nucleic acids (SNAs) have emerged as powerful tools, particularly when self-assembled from DNA amphiphiles [3]. Yet, this non-covalent strategy has drawbacks, notably the disassembly of SNAs upon contact with serum proteins in complex biological media [4].
In this study, we developed highly fluorinated DNA amphiphiles that readily self-assemble into SNAs with tunable stability profiles in biological media. These amphiphiles feature innovative branched fluorinated moieties [5], which potentially offer improved biodegradability compared to their linear counterparts. Depending on fluorination degree, the self-assembled SNAs exhibit excellent serum stability and efficiently deliver nucleic acid therapeutics for gene silencing applications. These systems demonstrate great potential as promising candidates for nucleic acid-based therapies [6].

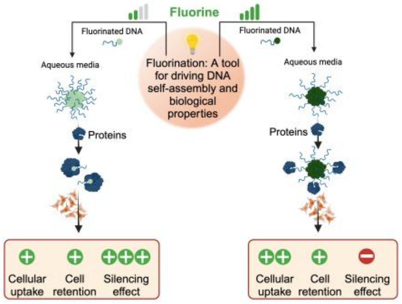

Figure 1. Schematic representation of how fluorination can be leveraged to drive nucleic acid self-assembly and fine-tune SNAs interaction with proteins, as well as their gene-silencing properties.

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OC110 ELECTROLYTE GATED ORGANIC TANSISTORS FOR THE DETECTION OF BIOMARKERS FOR PERSONALIZED MEDICINE

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Electrolyte gated organic transistors (EGOTs) have emerged in the last decade as a solid alternative to optical devices for the twofold aim of investigating fundamental aspects of biomolecular recognition processes and of detecting and possibly quantifying biomolecular targets even in complex samples such as bodily fluids [1]. EGOTs combine the advantages of organic electronic devices (e.g. the possibility of economically- and environmentally-sustainable fabrication on flexible substrates and the well demonstrated biocompatibility) with those offered by the electrolyte gating scheme, above all the possibility to be operated at voltages <1V, enabled by the high capacitance of the electrical double layers forming at both the gate/electrolyte and channel/electrolyte interfaces.
I will present some of the latest application of this technology to the detection of different biomarkers of medical relevance ranging from small molecules to proteins to extracellular vesicles [2,3], highlighting the crucial role played by the functionalization of device interface to endow the device with the necessary selectivity to enable its robust operation. The analysis of the response of these devices to the presence of the target biomarker in the electrolyte solution has also been reinforced by our recently proposed model that unifies the view of interfacial capacitive coupling of electrolyte-gated organic field-effect transistors (EGOFETs) with the volumetric capacitive coupling in organic electrochemical transistors (OECTs) [4].

Acknowledgements: The research leading to these results has received funding from the European Union – NextGenerationEU through the Italian Ministry of University and Research under PNRR – M4C2-I1.3 Project PE_00000019 “HEAL ITALIA” to Carlo Augusto Bortolotti (CUP E93C22001860006).

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OC90

LASER-MODIFIED MoS_2 STRUCTURES FOR IMPROVED SEMICONDUCTOR SERS SENSING

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Molybdenum disulfide (MoS_2) is a widely studied 2D material with growing interest in photocatalysis, optoelectronics, and sensing applications. In chemical sensing, semiconductor-based Surface-Enhanced Raman Spectroscopy (SERS) has attracted significant attention for overcoming some limitations of noble metal nanostructures. A key challenge in using MoS_2 for SERS is enhancing the chemical mechanism (CM), primarily driven by charge transfer phenomena. Recent advancements in sensitivity have been reported for defective MoS_2 nanosheets and complex structures like MoS_2 nanoflowers [1, 2]. Hierarchical MoS_2-based nanostructures offer a promising solution, providing stable structures with high chemical sensitivity.

In this work, MoS_2 nanosheets were modified by pulsed laser irradiation in aqueous/ethanolic dispersion. This simple, eco-friendly approach induces significant structural changes, producing highly defective MoS_2 layers self-assembled in hierarchical architectures using a Nd:YAG nanosecond pulsed laser. These structures were characterized by UV and PL spectroscopy, and their morphology was analyzed using scanning transmission electron microscopy (STEM) (Figure 1) and atomic force microscopy (AFM). SERS properties were studied using 4-mercaptobenzoic acid (4-MBA) as probe molecule, revealing enhanced signal intensities on laser-modified structures. Sensitivity varied with shape and composition, linked to factors such as (a) the formation of the 1T MoS_2 phase, (b) the high surface area of the produced structures, and (c) laser-induced defects.

X-ray photoelectron spectroscopy (XPS) analysis confirmed an increase in defect density, observing MoS_{2-x} and oxide species, highlighting the successful introduction of defects into the material. This strategy opens new possibilities for designing semiconductor materials for SERS-based sensing applications.

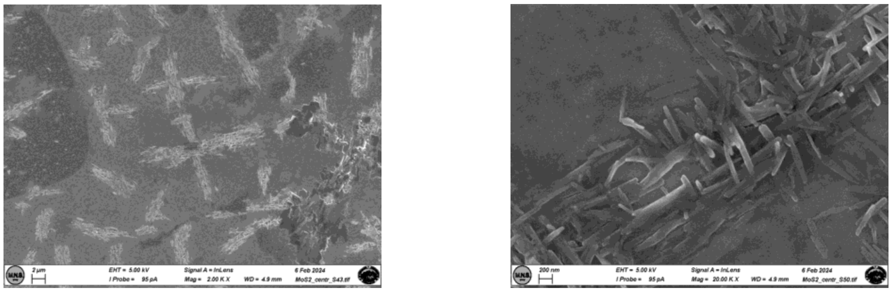

Figure 1. STEM images of MoS_2 laser-modified hierarchical structures at different magnifications

Acknowledgements: European Union (NextGeneration EU), through the MUR PNRR project SAMOTHRACE (ECS00000022). PON project Bionanotech Research and Innovation Tower (BRIT)-University of Catania. PRIN PNRR 2022-ELATED. PRIN 2022 – LANCIA.

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OC96

FINE-TUNING AMORPHOUS MAGNESIUM CALCIUM PHOSPHATE PARTICLES: HOW POLYACRYLIC ACID PREVENTS AGGREGATION AND CRYSTALLIZATION

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Amorphous magnesium-calcium phosphate (AMCP) nanoparticles represent a promising platform for biomedical applications [1,2]. However, their intrinsic tendency to aggregate into micrometric clusters significantly hampers their functionality, limiting their stability and dispersibility—key factors for efficient drug delivery. Therefore, precise control over their nanoscale dimensions is essential to enhance their performance [3].

A powerful strategy to regulate AMCP size and stability against crystallization involves the incorporation of stabilizing polymers, such as polyacrylic acid (PAA), which can mitigate aggregation while modulating the physicochemical properties of the nanoparticles. In this study, we systematically investigate the interplay between polyacrylic acid and magnesium content in shaping AMCP characteristics, focusing on the impact of varying calcium-to-magnesium (Ca/Mg) ratios and PAA molecular weight (Mw) on particle size, redispersibility, stability of the amorphous phase, and pH-dependent solubility.

Our findings reveal that PAA serves as an exceptional stabilizing agent, significantly reducing nanoparticles aggregation and enhancing dispersibility. The Ca/Mg ratio and PAA Mw play a pivotal role in dictating particle size and stability, underscoring their critical influence on nanoparticle design. Notably, PAA incorporation not only delayed thermal crystallization but also conferred resistance to dissolution in acidic environments, reinforcing the potential of AMCPs for pH-responsive drug delivery applications. Furthermore, a higher magnesium content was found to reduce the size of the obtained nanoparticles and to enhance the stability of the amorphous phase, while PAA effectively inhibited the transformation of AMCP into hydroxyapatite under physiological conditions, ensuring long-term structural integrity.

To elucidate these mechanisms, we employed a comprehensive suite of techniques, including dynamic light scattering (DLS), transmission electron microscopy (TEM), Fourier-transform infrared spectroscopy (FT-IR), and thermogravimetric analysis (TGA). This study paves the way for unlocking new possibilities for next-generation, smart drug delivery systems.

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OC121 OLEIC ACID-INDUCED DISSOLUTION OF SEMICONDUCTOR NANOCRYSTALS

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Semiconductor nanocrystals (NCs) have found widespread applications in optoelectronic devices such as light-emitting diodes, photovoltaics, and lasers, as well as in biological and medical applications due to their tunable optical properties and high stability. [1-2] However, the incorporation of toxic heavy metals like Cd, Pb, and Hg into NCs raises significant environmental and health concerns, particularly related to their disposal. [3] While efforts to reduce NC toxicity have focused on synthetic modifications such as tailoring their morphology, composition, and shell coatings, post-synthetic degradation strategies remain underexplored. [4]

This study investigates the potential of oleic acid (OA), a bio-based fatty acid known for its ability to form stable complexes with heavy metal ions through its carboxylic ends, to induce controlled dissolution of NCs (Figure 1). Morphological changes of NCs upon exposure to oleic acid were characterized using UV-Vis spectroscopy, small-angle X-ray scattering (SAXS), and transmission electron microscopy (TEM). The results demonstrate an effective dissolution of heavy metal-based NCs and highlight the broad applicability of this method across various shapes and compositions, including CdSe, PbS quantum dots, and CdTe nanorods. This study introduces an innovative bio-based strategy for dissolving heavy-metal NCs after their use, offering a sustainable solution for the disposal and recycling of NC-based devices.

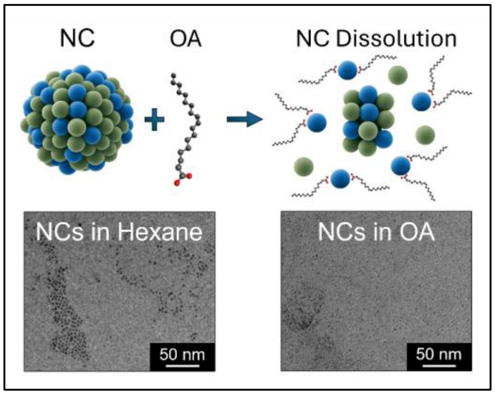

Figure 1. Schematic representation of NCs dissolution assisted by oleic acid and TEM results before and after oleic acid exposure.

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OC46

PHYSICO-CHEMICAL PROPERTIES OF TERNARY SLAG CEMENT WITH LOW CLINKER AND HIGH LIMESTONE FILLER CONTENT WITH SUPERPLASTICIZERS

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Using supplementary cementitious materials (SCMs) as cement replacement is a common practice to reduce carbon dioxide (CO_2) emissions and minimize the carbon footprint of global cement production, which accounts for 8% of all anthropogenic greenhouse gas emissions. [1]

This study focuses on the physico-chemical properties and hydration reactions of low-carbon ternary blended cement (OPC), ground granulated blast furnace slag (GGBS), and limestone. Organic additives, known as superplasticizers (SPs), are added to reduce the water content in the mixture while maintaining suitable rheological properties. There are different generations of superplasticizers, and in this study, polycarboxylate ether (PCE) polymers are used. These polymers adsorb onto the surface of cement grains, preventing particle flocculation. When mixed with water, anhydrous cement undergoes a series of exothermic reactions known as hydration reactions. OPC and GGBS react similarly with water but at different rates, leading to the formation of hydrated products. The combination of hydrated phases leads to the formation of a complex cement matrix. The inclusion of limestone and GGBS inside the mixture can lead to the formation of additional phases, particularly the AFm phase. [1]

Water consumption during the hydration process is studied using differential scanning calorimetry (DSC) analysis (Figure 1). A typical DSC run involves heating and cooling the sample. Water reacts and is consumed during hydration, and its quantity can be measured using the Free Water Index (FWI).

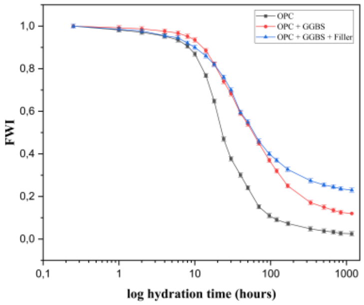

Figure 1. Free water index vs hydration time of three different cement samples.

Other physico-chemical analyses required stopping the hydration of the sample. Different types of hydration stoppages exist, and in this study, two soft drying methods are compared: freeze drying and exchange solvent with isopropanol. Different hydration stoppage methods result in varying degrees of pore structure and labile phase preservation, particularly for phases like carboaluminates and ettringite. This research provides important insights into the hydration stoppage methods, contributing to preserving various hydrated phases in ternary systems.

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OC8

POLY(3-HEXYLTHIOPHENE)-BASED SMART BIOINTERFACES FOR BIOMEDICAL APPLICATIONS

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Conductive polymers have emerged in recent years as promising materials in the field of bioelectronics and tissue engineering due to their interesting mixed ionic-electronic conductivity, biocompatibility, and tunable physico-chemical properties. In this work we present different studies based on conductive polymers, with a focus on bare P3HT and P3HT-based blends, to interface with cells for biomedical applications (Figure 1). The increase in the electrical conductivity of P3HT-based blend, is very interesting for the possible integration with biological systems, facilitating efficient signal transduction between devices and cells, making it an ideal candidate for bioelectronic interfaces [1]. In our work we focus the attention on the characterization of morphological, nanomechanical and physico-chemical properties of the surfaces. Moreover, the adsorption study of extracellular matrix proteins has been performed to estimate the first interactions with biological environment, since it could drive the cell response. Finally, the biocompatibility with different cell lines, neuronal and mesenchymal, has been investigated to test the cell viability, proliferation, and differentiation via the expression of specific markers. The very promising results highlight the polymer capability to modulate cellular behaviour through electrical, mechanical, and interfacial properties and induce osteogenic differentiation even in absence of specific growth medium and differentiation factors [2]. This study paves the way to further study for potential applications of this substrate in the field of biomaterials.

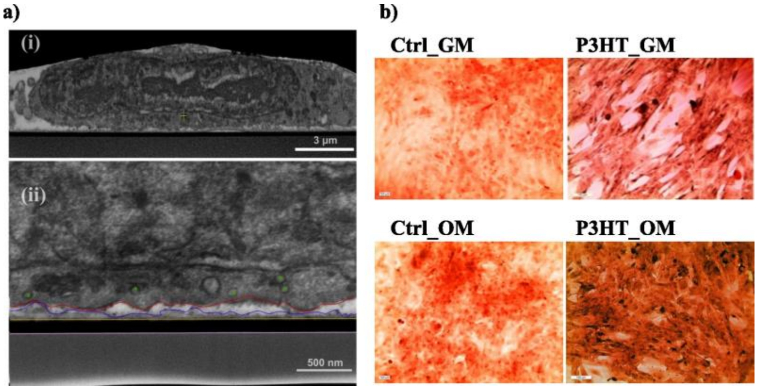

Figure 1. a) FIB/SEM of the P3HT/HT22 cells (i) and P3HT-MWCNT/HT22 cells (ii) interfaces, b) Alizarin Red S staining for calcium mineralization of differentiated osteoblasts from mesenchymal stem cells

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OC52

A PHYSICOCHEMICAL APPROACH TO HYDROXYAPATITE EXTRACTION FROM ASHES: LINKING PROCESSING PARAMETERS TO FUNCTIONAL PROPERTIES

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Converting waste ashes into functional materials aligns with circular economy principles while offering innovative solutions for several applications, such as catalysis and environmental remediation. At the same time, it represents an intriguing challenge that requires a targeted focus on the intricate physical chemistry governing the transformation process and determining the bulk and surface properties of the extracted materials.

This study presents a systematic exploration of hydroxyapatites ($Ca_{10}(PO_4)_6(OH)_2$, HAP) [1] derived from waste-to-energy ash. HAP materials were obtained via a three-step extraction process: (i) dissolution, (ii) crystallization, and (iii) maturation. Four distinct hydroxyapatite samples, labeled HAP-1, HAP-2, HAP-3, and HAP-4, were synthesized by varying key extraction parameters (e.g., concentration of precipitating agent, addition rate, etc.) to examine their impact on the structural, morphological, and surface properties of the resulting materials. XRPD revealed that all the samples exhibited reflections corresponding to the hexagonal structure of hydroxyapatite (JCPDS 00-09-0432) as the sole crystalline phase. HAP-1 and HAP-2 showed higher crystallinity compared to HAP-3 and HAP-4, which contained a greater amorphous fraction. HR-TEM of all samples revealed the typical HAP needle-shaped morphology, with highly crystalline domains for HAP-1 and HAP-2.

EDX analyses revealed minor elemental substitutions (Si, Al, Fe, Mg, Na), which could influence crystallinity and surface reactivity. Additionally, N_2 physisorption measurements confirmed variations in porosity and surface area, with the more amorphous samples exhibiting higher surface areas. Surface acid-base properties were analyzed through liquid-solid phase titrations and adsorption microcalorimetry. All samples exhibited the characteristic amphoteric nature of synthetic HAP surfaces. [2] The most amorphous samples exhibited the highest number of both acid and base sites. Microcalorimetry provided insights into both the number and strength distribution of these sites through the adsorption of NH_3 and SO_2 probes. Figure 1 highlights the results, which show a predominant basicity in all samples. The strength of the basic sites was notably higher than that of the acidic sites. In conclusion, we demonstrated how controlled synthesis parameters modify HAP properties, enhancing their suitability for applications such as heterogeneous catalysis and pollutant adsorption, as illustrated by specific examples.

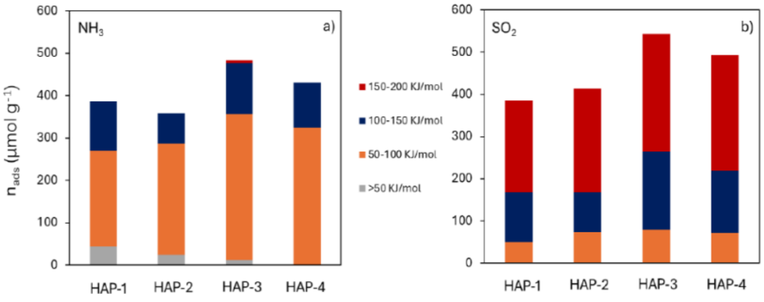

Figure 1. Energy distribution of acid and basic sites in HAP samples, as determined by a) NH_3 and b) SO_2 adsorption microcalorimetry, respectively.

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OC2

OXIDES-STABILIZED PICKERING EMULSIONS: INFLUENCE OF SURFACE PROPERTIES, IN-SITU FUNCTIONALIZATION, AND STIMULI-INDUCED RESPONSIVENESS

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Pickering emulsions are gaining significant interest as a superior alternative to conventional surfactant-stabilized emulsions, offering promising applications across various fields, including medicine, pharmaceuticals, cosmetics, the food industry, and cultural heritage preservation [1,2]. In this study, we investigate the role of oxide surface properties in the stabilization of Pickering emulsions, specifically focusing on ZnO and TiO_2 nanoparticles as solid emulsifiers – chosen for their broad range of applications arising from their UV-blocking, photocatalytic and antibacterial properties. The resulting emulsions display excellent stability over time and against temperature variations, mechanical stress and increased ionic strength. We explore the interplay between the oxide surface features and in situ functionalization with fatty acids in determining key emulsion characteristics, including type, droplet size, stability, and the responsiveness to external stimuli (acidification by mineral and organic acids, UV and sunlight irradiation, addition of multivalent cations and CO_2 bubbling) [3]. The switching behavior of oxides-stabilized Pickering emulsions can be controlled by various stimuli, with reversibility achieved through pH adjustment, gas bubbling, or darkness. While stable emulsions can be recovered after multiple cycles, irreversible destabilization occurs with excess acid or multivalent cations. The inversion mechanism is attributed to surface charge-mediated flocculation rather than wetting changes [4]. Our work offers valuable insights for enhancing the design of sustainable, surfactant-free emulsions that can be optimized for practical applications, such as stable UV protection or controlled destabilization in photocatalytic processes.

Acknowledgements: We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title: UPcycling SOOT for sustainable nanocomposites-based wearable sensors (UP - SOOT) – CUP G53D23003000006 - Grant Assignment Decree No. 958 adopted on 30/06/2023 by MUR.

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OC39

OPTICAL AND CHIROPTICAL LINEAR RESPONSE PROPERTIES OF MATERIALS

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Accurate simulations of linear response properties are important for the rational design of materials used in a variety of technological applications, including electronics, quantum technology, and catalysis. Although band gaps are often used as a proxy for electronic excitations, direct calculations of excitation energies and polarizabilities are desirable as they provide more accurate data and more information about the electronic response of the material. In this contribution, we present the implementation of electric dipole-electric dipole (DD), and mixed electric dipole-magnetic dipole (DM) and electric dipole-electric quadrupole (DQ) polarizabilities for periodic systems at density functional theory level with periodic boundary conditions (DFT-PBC) employing Gaussian-type atomic orbitals (GTOs) as basis set.[1,2,3] The DD polarizability provides information about electronic excitations, while the DM-DQ polarizabilities allow the calculation of the optical rotation (OR) in chiral crystals. First, we discuss various technical aspects of the calculations, e.g., the dependence on basis set size, role of exact exchange, convergence with reciprocal space discretization, and choice of gauge. Then, we compare simulations with experimental data. This approach can open new avenues to study the electronic properties of materials with the same accurate tools available for molecules.

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OC50

POLYMER BEHAVIOR IN AQUEOUS SOLUTION ACROSS THE LOWER CRITICAL SOLUTION TEMPERATURE: INSIGHTS FROM MOLECULAR DYNAMICS SIMULATION

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The thermoresponsiveness of polymer hydrogels and microgels, exploited for tissue engineering, bio-separation, and drug delivery, originates from the de-mixing process of the aqueous solution occurring at a Lower Critical Solution Temperature (LCST). Focusing on this process, we reproduce by atomistic molecular dynamics simulations the polymer solution behavior, across the LCST and at infinite dilution, for the amphiphilic synthetic macromolecules poly(N-isopropylmethacrylamide), PNIPMAM, and poly(2-isopropyl-2-oxazoline), PIPOX, in satisfactory agreement with experiments. The molecular characteristics of the two systems are compared to those of the aqueous solution of poly(N-isopropylacrylamide), PNIPAM, historically the most investigated thermoresponsive polymer, whose phase behavior in water has been effectively described by us by means of the same computing technique [1]. Simulation findings allow to interpret differences in solution properties of these polymers (Figure 1), highlighting the major responsible factors. Whilst recognizing the crucial role of hydrophobicity in LCST behavior, this investigation shows how the conformational features of individual molecules determine their temperature response [2].

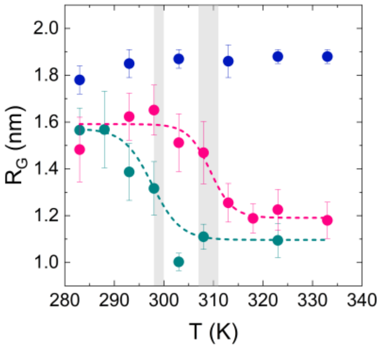

Figure 1. Temperature behavior of the radius of gyration, R_G, for the investigated polymers in water.

Acknowledgments: Financial support by Progetto Co-MGELS funded by the European Union-NextGeneration EU under the National Recovery and Resilience Plan (PNRR) Mission 4 “Istruzione e Ricerca” - Component C2 - Investment 1.1 - "Fondo PRIN", Project code PRIN2022PAYLXW Sector PE11, CUP B53D23008890006 is acknowledged. The CINECA award, under the ISCRA initiative, is acknowledged for the availability of high-performance computing resources and support.

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OC19 TOWARDS THE PREDICTION OF NOVEL AND MORE EFFICIENT DYE CANDIDATES FOR INDOOR DYE-SENSITIZED SOLAR CELLS VIA A COMBINED MACHINE LEARNING AND DENSITY FUNCTIONAL THEORY STRATEGY

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Dye-sensitized solar cells (DSSCs) have emerged as one of the technologies of choice for indoor applications and for powering Internet of Things (IoT) devices due to their outstanding ability to capture ambient illumination and convert it into electricity [1]. In this field, significant research efforts have been made to develop new organic dyes capable of absorbing a wide range of artificial light emissions at varying intensities [2,3]. However, the traditional research process is often expensive and time-consuming. In this context, we developed a two-stage approach by combining Machine Learning (ML) techniques with Density Functional Theory (DFT) methods to develop novel organic dye candidates for indoor applications and predict their power conversion efficiency (PCE) under different indoor light sources and intensities [4]. Additionally, the synthetic accessibility (SAscore) of the dye candidates has been evaluated. The developed protocol allowed us to identify three promising dye candidates for indoor DSSCs with PCE > 29% under different artificial illumination conditions. By comparing these data with the experimental PCE values from literature dyes under indoor conditions, we could assume that the three identified dye candidates could yield experimental PCE values comparable to or even exceeding current findings in the literature. Our results demonstrate that the developed ML-DFT protocol represents an effective strategy to accelerate the discovery of novel and potentially more efficient organic dyes for indoor DSSCs. Current efforts are focused on the synthesis of the most promising dye candidates to adopt an iterative framework where the model could be continuously updated through validated data, which could contribute to enhancing the efficiency of the developed ML-DFT protocol.

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OC75

NATURAL GUMS-BASED MATERIALS FOR ADVANCED TECHNOLOGICAL APPLICATIONS: ANTI-COUNTERFEITING AND THERMOCHEMICAL ENERGY STORAGE

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In recent years, natural polysaccharide gums have gained significant attention due to their ability to absorb large amounts of water while maintaining structural integrity [1,2]. This property can indeed be exploited to develop advanced materials and technologies in various sectors [1,2]. Here we explore the possibility of utilizing natural polysaccharide gums both for thermal energy storage and for developing functional hydrogels for anti-counterfeiting. A variety of natural polysaccharide gums, such as tara (Figure 1a), guar, Konjac, and Xanthan, were characterized using thermal (TGA, DSC), dynamic-mechanical (frequency sweep), and imaging speckle techniques.

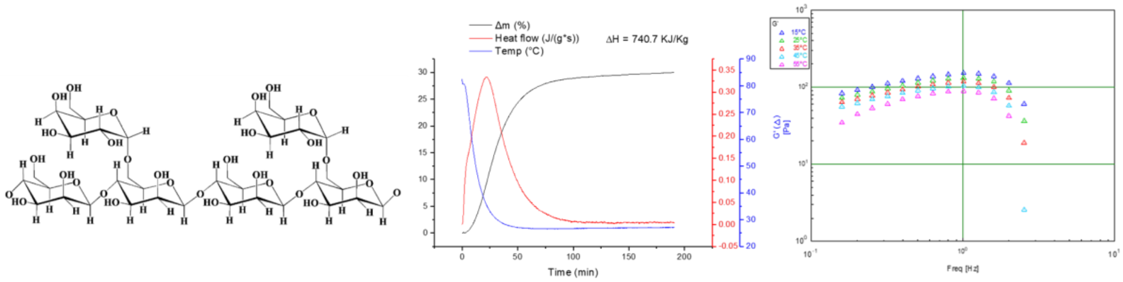

Figure 1. a) Chemical structures of Tara gum, b) Representative results of Setaram TGA, c) Representative results of dynamic-mechanical experiments.

A thorough thermal characterization of the natural gums shows high heat storage capacities between 600 and 750 kJ kg^{-1} in the low-intermediate temperature range (up to 80 °C) (Figure 1b). These materials are cost-effective, non-toxic, and widely available, making them suitable for large-scale applications in thermochemical energy storage. The polysaccharide gums were also used to prepare hydrogels incorporating varying amounts of cellulose citrate [3]. The incorporation of cellulose into gum matrices significantly altered their thermal properties, with distinct changes observed in thermal transition temperatures and decomposition profiles. Rheological analysis revealed that all hydrogels displayed strong gel behavior, with guar-based hydrogels showing the most structured network (Figure 1c). The addition of cellulose improved the properties of xanthan-based hydrogels, while weakening the guar and tara systems. Imaging speckle was used to assess the optical properties of the materials, which can also be applied in traceability and authentication systems. This study highlights the versatility and potential of natural polysaccharide-based materials in various advanced technological fields.

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OC117 PHYSICO-CHEMICAL CHARACTERIZATION OF BIOBASED MATERIALS WITH ACTIVE BIOFILLERS OBTAINED VIA SOLVENT-CASTING AND EXTRUSION METHODS

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In recent years, biodegradable polymers have gained significant attention due to their capacity to break down into non-toxic, environmentally friendly materials. Nevertheless, natural polymers have intrinsic drawbacks that limit their application for the production of bioplastic material. Strategic blending of different biopolymers can be used to enhance mechanical strength, thermal stability, electrical properties and hydrophobicity. In this context, a blend composed of chitosan, starch and PVA (polyvinyl alcohol) has been produced and characterized due to the excellent miscibility of the components. Two processing techniques were explored and compared to obtain the novel materials: solvent casting, commonly used in laboratory-scale applications, and extrusion, a method widely employed in industrial production. The resulting prototypes were characterized in terms of their mechanical (Young modulus and tensile stress at break), structural (Fourier Transform Infrared Spectroscopy FT-IR), and thermal properties (Differential Scanning Calorimetry DSC), emphasizing the key differences between the two production methods. Furthermore, active biofillers based on lignin were characterized and incorporated into the blends to confer new properties to the material. [3] This study offers valuable insights into the scale-up process for innovative and biodegradable materials.

Acknowledgements: This project was funded by National infrastructure METROFOOD-IT (PNRR).

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TENSIMETRIC DETERMINATION OF ACTIVITY AND PARTIAL MIXING PROPERTIES OF UREA IN TYPE III DEEP EUTECTIC SOLVENTS

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In recent years, deep eutectic solvents (DESs) have gained increasing attention as a "green" alternative to conventional organic solvents thanks to their remarkable proprieties, including low vapor pressure, non-flammability, good thermal stability, and tunability.[1] These liquids were defined by Abranches et al. as "a eutectic solvent whose components present enthalpic-driven negative deviations from thermodynamic ideality".[2] Current research primarily focuses on the intermolecular forces taking place in these liquids, in particular hydrogen bonding, to explain the stabilization of the solution phase compared to the pure components that eventually results in anomalously lower eutectic temperatures. However, this approach usually overlooks the role of entropic contributions in the stabilization of the liquid phase. The investigation of DESs' fundamental thermodynamic properties is still in its early stages, despite the fact that understanding key mixing properties, such as Gibbs energies, enthalpies, and entropies, would provide deeper insight into the nature of the "deep" eutectic behavior. Moreover, gaining knowledge of these properties is essential for predicting DES performances in practical applications.[3] Among DESs, the most extensively studied are the so-called "Type III", formed by a molecular and an ionic component. A well-known example is reline, composed of urea as the molecular component and choline chloride as the ionic counterpart. Although vapor pressure measurements are one of the most direct methods to measure the activity of a component in a solution and its partial mixing properties, to the best of our knowledge, only two vapor pressure determinations of reline are available in the literature.[4,5]By analyzing these data it comes out that they lead to contradictory and physically inconsistent results in terms of activity coefficient of urea. In addiction apparently, no vapor pressure data based on effusion close-to-equilibrium conditions are available in the literature. To fill this gap on the thermodynamic description of this prototypical DES, we undertook a series of experiments through Knudsen effusion mass spectrometry and Knudsen effusion mass loss experiments in the temperature range 320-360K near the eutectic composition. These experiments allowed us to evaluate the urea activity as a function of temperature and the urea partial mixing properties, as it was demonstrated that in the explored temperature range the vapor contains only gaseous urea. To quantify deviations from the ideal behavior, the results are compared to Raoultian ideal behavior, considering the enthalpic and entropic contributions. Moreover, to gain structural insights into the liquid phase, we performed Classical MD simulations to establish a correlation between structural organization and deviations from ideality. Finally, we are attempting to determine the thermodynamic quantities of mixing of reline through the thermodynamic integration (TI) method, aiming to compare the computational results with the experimental data.[6]

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OC107

THE STEREOCHEMICAL EFFECT IN DRIVING THE AGGREGATION BEHAVIOUR OF PORPHYRIN-CHOLIC ACID DERIVATIVES

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Understanding how the property of 'chirality' can be read and transferred from a molecular to a supramolecular level is an intriguing topic, widely investigated and debated nowadays to explain the symmetry breaking at the origin of life. Porphyrins are ubiquitous dye molecules able to read the chiral information, featuring a versatile and multifaceted chemistry, mainly due to their π-conjugated skeleton. Their structure confers them the ability to aggregate in supramolecular architectures [1], *via* a J- or H- type aggregation pattern [2], easily detectable by their spectroscopic features. In our recent work [3], we synthesized new porphyrin-cholic acid derivatives and studied their peculiar self-assembly in aqueous environments, revealing significant chiral features (strong bisignated bands) dependent on the solvent composition. The porphyrin unit exploited a C3-β covalent bond with the C3 position of the cholic acid chiral molecule, responsible for the extrinsic chirality given to the conjugates. Here, we have attempted a different synthetic strategy, leading to the C3-α analogues. Combining spectroscopic techniques (CD, UV-Vis and Fluorescence), a completely different behaviour in the transmission of the chiral information of the novel synthesized stereoisomers emerged. SEM and TEM microscopy showed that the opposite stereochemistry at the C3 covalent bond infers a striking different ability of self-assembly in aqueous environments, resulting in drastic changes of the supramolecular morphology (from elongated to spherical hollow objects, as reported in Fig. 1). To deeply investigate the stereochemical effect on driving the aggregation of the title porphyrin-cholic acid derivatives, a theoretical study based on molecular dynamics simulations was carried out. Modelling the aggregates as ellipsoids rotating in a solvent box, a different degree of the aggregates sphericity was identified as parameter to explain the aggregation behaviour of the C3-α and C3-β aggregates. From this theoretical-experimental study, a direct correlation between molecular structure, aggregation behaviour and chiral induction was proposed. A rational analysis was obtained for the molecular actors able to self-organize from the bottom to the nano- and meso-scale, in a stereochemistry-dependent way, constructing distinct supramolecular structures, with specific chiral features and potential applicability as smart chiral sensing materials or as hosting structures for drug-delivery systems.

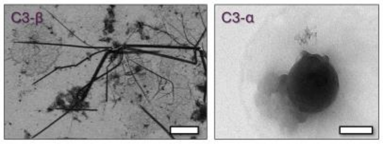

Figure 1.: (left) SEM image of elongated structures from C3-β molecules aggregation (size bar of 10 µm); (right) TEM image of spherical vesicular objects from C3-α molecules aggregation (size bar of 100 nm).

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OC77 PHYSICOCHEMICAL STUDIES OF MODIFIED APTAMERS TARGETING EPHRIN RECEPTOR TYROSINE KINASE A2 (EphA2) IN GLIOBLASTOMA STEM CELLS

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DNA and RNA aptamers are short synthetic nucleic acids able to adopt distinctive three-dimensional structures. These structures allow aptamers to bind, with high affinity and specificity, to a wide variety of molecular targets, including small molecules, proteins, nucleic acids, as well as cells, tissues, and organisms [1]. While DNA aptamers are widely studied, the remarkable therapeutic potential of the RNA aptamers should be highlighted. Like DNA aptamers, RNA aptamers can be identified through *in vitro* selection techniques, such as SELEX (Systematic Evolution of Ligands by Exponential Enrichment) [2].

In 2019, Condorelli's group identified an RNA aptamer namely A40s, a 30-mer oligonucleotide, capable of binding the cell surface of human glioblastoma stem cells (GSCs) through direct recognition of the ephrin type-A receptor 2 (EphA2) [3,4]. Building on these preliminary findings, the physicochemical properties of the aptamer A40s were analyzed using several biophysical techniques. Furthermore, various modified analogues of A40s were designed and synthesized to develop aptamers with enhanced thermal stability, increased nuclease resistance in serum, and improved binding efficiency to EphA2 compared to A40s. The results indicate that some of the modified aptamers displayed higher thermal stability than the parent oligonucleotide, thus proving that the selected modifications allow a marked improvement of the aptamer thermal stability, paving the way for the development of novel systems characteristics suitable appropriate for future clinical applications.

Acknowledgements: CN00000041 National Center for Gene 'Therapy and Drugs based on RNA Technology', funded by European Union-NextGenerationEU and financed by PNRR MUR-M4C2-Investimento 1.4-CUP UNINA: E63C22000940007

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CORRELATED QM/MM CALCULATIONS FOR THE DETERMINATION OF SPECTRAL PROPERTIES OF BIOMIMETIC PHOTOSWITCHES IN SOLUTION

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The accurate study of molecular systems in realistic environments is vital to the understanding of key light driven ultrafast processes occurring both in nature and in the context of photo-pharmacology. To this end, electron correlation effects and an atomistic description of the environment must be included in the computational methodology when simulating spectral properties of such systems [1].

Multiscale QM/MM modeling [2,3] achieves this goal by treating the solute with a high-level QM correlated method, and the solvent molecules as polarizable classical multipoles, retaining their atomistic detail while reducing the computational costs.

In this work, molecules of biomimetic interest [4,5] are studied using a recently proposed polarizable method [6] based on the coupling between CASSCF and the fluctuating charges (FQ) [7] approach. This high level of theory grants an accurate characterization of ground and excited state wavefunctions and, thus, spectra determination. Excitation energies are computed for several different snapshots sampled from a classical molecular dynamics simulation in order to take into account solvent conformation effects, and averaged over to recover the final signal [8,9].

The selection of the active space and its maintenance throughout the snapshot ensemble is also a demanding task requiring careful consideration.

Acknowledgments: This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101169312.

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OC89

BIOMOLECULE ADSORPTION ON SMART SWITCHABLE GERMANIUM SURFACES

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Smart surfaces that are responsive to electrochemical triggers and change in hydrophobicity offer exciting possibilities for applications in microfluidics, separation systems, biosensors and analytics. When coupled with spectroscopy, they act as an analytical tool to observe the reaction and provide a deeper understanding of the dynamics occurring during the adsorption of proteins onto the smart surfaces. [1,2]

The main focus of this research work is on controlling adsorption of proteins by switching between hydrophobic –H terminated surface and hydrophilic –OH terminated surface of germanium (100) crystal which is induced through an applied electrode potential [3]. The adsorption of different proteins – albumin and lysozyme – is studied in deuterated phosphate buffer solution (pH 7.4) *in situ* using an electrochemical cell combined with polarized attenuated total reflection infrared (ATR-IR) spectroscopy (Figure 1). These proteins differ in regards to their size, charge and unfolding tendencies which gives an insight into the effect of these properties on the adsorption dynamics of proteins. Changes in the conformational structure of the protein structure are observed along with partially reversible adsorption while switching between the hydrophobicity of the surface. Our work studying adsorption control of proteins on smart surfaces will further contribute in understanding and designing bioanalytical tools which are simple in application and easy to control.

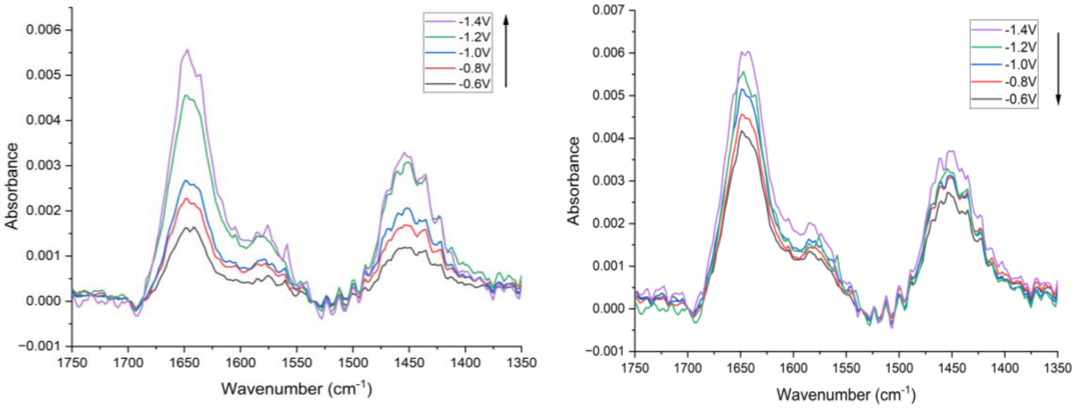

Figure 1. Potential dependent in-situ p-polarized ATR-IR spectra of the protein lysozyme showing partially reversible adsorption process on germanium (100) surface.

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OC112

DESIGN AND DEVELOPMENT OF NOVEL NANOCOMPOSITE ANION EXCHANGE MEMBRANES FOR FUEL CELLS AND ELECTROLYSERS

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Anion exchange membranes (AEMs) are considered promising candidates for several electrochemical energy conversion and storage (EECS) devices including fuel cells and electrolysers. The alkaline working conditions empower faster electrochemical reaction kinetics, allowing for the use of low-cost non-precious metal catalysts, contrary to well-known proton exchange membranes (PEMs) [1]. However, current AEMs still exhibit low conductivity and poor alkaline stability, limiting the development of AEM-based EECS devices [2]. Thus, researchers are working on enhancing membranes' composition, morphology and nanostructure to improve the AEMs performance, durability, and reliability.

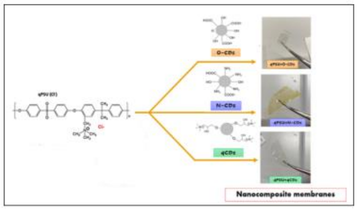

Figure 1. A schematic representation of nanocomposite membranes based on qPSU and variously functionalized CDs.

Here, novel nanocomposite anion exchange membranes have been prepared by introducing carbon dots (CDs), a new class of carbon nanoparticles consisting of a grafitic core and an easy-to-functionalize surface, into quaternary ammonium-functionalized polysulfone (qPSU).
For this study, CDs with various functionalization, i.e., O-CDs, N-CDs and qCDs, (Figure 1) have been synthetized using a low cost, eco-friendly and scalable synthetic approach. In order to understand how CDs can affect membranes properties, a complete analysis of their morphology structure, physico-chemical properties and electrochemical performance has been provided. In this regard, NMR spectroscopy played an important role in suppling crucial insights into the molecular dynamics of water molecules. This was achieved through direct measurements of the self-diffusion coefficient (PFG NMR method) and relaxation times (T_1) values. Moreover, Electrochemical Impedance Spectroscopy (EIS) supplied a description of membranes ionic conductivity. Characterizations results obtained have proved that the presence and also the type of CDs strongly influence membranes properties.

Acknowledgments: This work was supported by the Ministero degli Affari Esteri e della Cooperazione Internazionale (MAECI) within the framework of the Italian-German joint research initiative "Green Hydrogen Research: A Collaboration to Empower Tomorrow's Energy", under the project DURALYS (DURAble, Scalable, and Recyclable Components and Cell Designs for Next Generation Alkaline Exchange Membrane Water Electrolysis).

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UNVEILING THE MESOSCALE ASSEMBLY OF GOLD NANOPARTICLES ON SOFT TEMPLATES VIA NANOPLASMONIC ISOSBESTIC POINTS

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The controlled clustering of plasmonic nanoparticles (NPs) generates unique optical properties through the coupling of localized surface plasmon resonances (LSPR) of individual NPs. This phenomenon can be achieved with lower synthetic efforts, using spontaneous assembly onto soft templates in liquid media, such as liposomes [1], lipid NPs [2], polymeric NPs [3], and biological vesicles [4]. The structure of NPs assemblies originates from thermodynamic equilibrium, and the LSPR variation induced by clustering can yield information on the physicochemical properties of the templating agent, including concentration, nanomechanics, and purity from biological contaminants [4,5]. However, monitoring how the assembly mesostructure determines final optical properties remains a critical challenge to inform the design of advanced plasmonic materials [6,7]. Here, we introduce "nanoplasmonic isosbestics" as optical descriptors of the mesoscale organization of gold nanoparticles (AuNPs) on soft templates. Unlike isosbestic points in molecular spectroscopy, which describe chemical equilibria, our numerical simulations demonstrate that nanoplasmonic isosbestics emerge from the coexistence of individual AuNPs and AuNP clusters where the interparticle spacing controls the isosbestic wavelength. By templating AuNPs assembly onto synthetic free-standing lipid bilayers with tunable membrane rigidity, we experimentally achieve precise control over interparticle spacing and prove that it is mirrored by univocal modulation of the isosbestic wavelength. In addition, from an analytical perspective, we show that isosbestic points can fingerprint key template's properties, such as the stiffness of the free-standing bilayers, enabling non-invasive optical probing. As a proof-of-concept, we apply this approach to profile the stiffness of biologically relevant templates, i.e., Extracellular Vesicles (EVs). For the first time, we demonstrate a direct correlation between interparticle spacing and isosbestic behavior, providing fundamental understanding of structure-function relationship in plasmonic systems. These findings position plasmonic isosbestic points as descriptors to reveal mesoscale organization in nanoplasmonic structures and introduce a new strategy for optically characterizing soft materials.

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OC59

INVESTIGATION OF TETRABUTYLAMMONIUM-BASED DEEP EUTECTIC SOLVENTS: THE INFLUENCE OF COUNTER-IONS AND H-BOND DONOR ON THE FORMATION OF LIQUID PHASE

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Deep Eutectic Solvents (DESs) and Eutectic Solvents (ESs) are a class of materials known for their tunable properties and lower environmental impact, with their physicochemical properties being strongly determined by the chemical components that make them up. Among these, mixtures of quaternary ammonium salts, specifically tetrabutylammonium (TBA) derivatives, combined with hydrogen bonds donors (HBDs), yield eutectic systems with melting points significantly lower than those of their pure constituents. DESs, in particular, exhibit a notable melting point depression compared to the ideal mixture due to the formation of strong intermolecular interactions, primarily hydrogen bonding. The magnitude of this deviation is dictated by the nature and strength of these interactions, as well as the spatial arrangement of the components. In our study, we explored new low-hydrophilicity solvents by investigating TBA-based eutectic mixtures incorporating a variety of anions, including bromide, acetate, and triflate. These anions were selected for their diverse size, structural attributes, and acid-base properties. The TBA salts were combined with various HBDs, such as long-chain alcohols, carboxylic acids, and imidazoles with different ring substitutions. We conducted comprehensive analysis using infrared spectroscopy across the far and mid-infrared ranges, also utilizing advanced facilities like the SOLEIL Synchrotron in Paris. The experimental findings were further interpreted using quantum chemical (DFT) and classical molecular dynamics simulations. Additionally, the thermal properties and experimental phase diagrams of the mixtures were examined by means of differential scanning calorimetry (DSC). Thermogravimetric measurements (TGA) were used to determine the thermal stability of the pure components and their mixtures. A key observation is that the degree of deviation from ideality is strongly dependent on the specific hydrogen bond donor (HBD) used. For example, systems incorporating 1-octanol and octanoic acid show minimal deviations, while those with imidazoles exhibit more pronounced shifts. This underscores the critical role of hydrogen bond donation and acceptance in determining the thermophysical properties of potential DES systems. Both spectroscopic and computational analyses confirm the presence of strong hydrogen bonds in all investigated systems. Furthermore, van der Waals interactions between the TBA chains and HBDs contribute additional stabilization, shaping the overall behavior of these eutectic mixtures.

OC13

ANALYSIS OF THE DYNAMICS OF PHOTOGENERATED CARRIERS AT THE $MAPbBr_3/SrTiO_3$ INTERFACE WITH IR SYNCHROTRON RADIATION: A STUDY FOR HYBRID PHOTOVOLTAICS

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Within the field of research on photovoltaics (PV), the class of hybrid organic-inorganic perovskites (HOIPs) represents the protagonist of a fast-pace progress. This is due to the high efficiency of HOIP-based PV devices achievable at low-cost with features of lightweight, mechanical flexibility and optical modulability. [1] The interest of researchers on HOIP like the tri-halides of methylammonium and lead, is motivated by the combination of long lifetime of the photogenerated charge carriers in HOIP (of the order of several microseconds) and corresponding long diffusion lengths (of the order of several microns). [2]

In this contribution it will be presented a study on the dynamics of the photogenerated carriers at interfaces of interest in photovoltaics like those formed by $CH_3NH_3PbBr_3$ thin films (thickness < 300 nm) spin-coated onto $SrTiO_3$ substrate, employing the infrared (IR) synchrotron radiation of the AILES beamline of SOLEIL (wavenumber range: 400-3000 cm^{-1}) as probe-beam. The linear polarization of the probe-beam and the adoption of grazing-angle incidence (72°) setup allow the verification of the Berreman effect [3] (BE) at the frequencies of the longitudinal optical (LO) phonons of the substrate (at ca. 860 cm^{-1}) at the $CH_3NH_3PbBr_3/SrTiO_3$ interface when the HOIP is excited at the above bandgap energy of 2.3 eV (out-of-equilibrium experiment). BE consists in the shift of the IR absorption at the frequencies of LO phonons of the substrate due to the formation of a quasi 2-dimensional electron system at the interface due to above-bandgap excitation of the $CH_3NH_3PbBr_3$ film. The resulting optically induced metallization of $CH_3NH_3PbBr_3$ manifests as variations in the LO phonon frequency of the substrate, which are experimentally probed with transverse magnetic (TM)-polarized reflectivity at grazing angle. The analysis of these optical data in terms of ellipsometric parameters at various temperatures gives insight into the dynamics of the photogenerated charge carriers and allows for the estimate of three relevant parameters: (i) the thickness of the quasi two-dimensional electron gas; (ii) the corresponding charge density; (iii) the mobility of the photogenerated charge carriers at the interface under investigation.

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OC18

COMBINING MOLECULAR DOCKING, MOLECULAR DYNAMICS AND MACHINE LEARNING APPROACHES IN AN ACTIVE LEARNING SCHEME

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Molecular dynamics (MD) simulations are an integral and well-used tool in drug discovery especially in identifying new candidate molecules. With the increase in the virtual molecule library sizes, it becomes challenging to apply structure-based approaches like molecular docking and MD. Machine learning (ML) approaches could be helpful in this respect and can be combined with these structure-based approaches. In fact, docking and ML methods are combined to explore a larger chemical space of molecule libraries [1]. However, docking by itself could be limited in identifying true positives in terms of suggested molecules being effective against their targets Hence, MD studies are generally applied for top-scoring molecules to assess the stability of the ligand in the binding pocket. Though, it is also possible that some promising molecules could be eliminated due to their initial binding modes not being favorable and hence having not promising docking score. But this could be because of sampling issue or even docking programs allowing close contacts. For these reasons, we previously started applying an approach in which short MD simulations (1 to 5 ns) for each of the molecules docked to the target protein and performed binding energy calculations (simpler ones such as MM/GBSA) and then selected the compounds based on their average binding scores [2]. However, applying short MD simulations approach for large number of molecules is computationally demanding. Hence, ML approaches were used in which certain number of molecules from a large virtual library are randomly selected and docked into the target binding site followed by short MD and binding energy score calculation. Then ML models are built and trained using these MD data. The binding energies of remaining molecules in the library are predicted using the ML models. The molecules with high predicted scores were then docked into the binding site, short MD simulations and binding energy calculations performed. The results for these molecules are added as training data for ML models. These cycles are repeated until models cannot be optimized statistically. From the last round, the best scoring molecules could now be selected for further studies. The aim here is to generate workflow for this active learning approach. As a test case, FTO (Fat mass and obesity associated) protein, a RNA demethylation enzyme is considered.

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OC22 PHOTOCATALYTIC HYDROGEN EVOLUTION BY METAL SULFYDE BASED BINARY AND TERNARY 2D/2D HETEROJUNCTION PHOTOCATALYSTS

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Photocatalytic water splitting using semiconductor-based materials has emerged as a promising strategy for hydrogen production, offering a sustainable energy alternative. The development of efficient photocatalysts with strong visible-light absorption and effective charge separation is crucial for enhancing hydrogen evolution reaction (HER) performance. Despite extensive research, achieving all desired photocatalytic properties within a single semiconductor remains a significant challenge. To overcome this limitation, heterojunction structures have been engineered by integrating various two-dimensional (2D) materials, such as molybdenum sulfide, carbon nitride, black phosphorus, and borophene. These 2D/2D heterojunctions facilitate improved charge carrier separation, tunable band alignment, and enhanced light-matter interactions, thereby optimizing photocatalytic efficiency. In this study, molybdenum-based binary and ternary 2D/2D heterojunctions comprising tungsten sulfide, molybdenum sulfide, carbon nitride, and black phosphorus were synthesized and analyzed for photocatalytic HER applications. The heterojunctions exhibited both type-I and type-II band alignments, leading to significantly enhanced photocatalytic activity. Furthermore, the incorporation of nickel (Ni) and cobalt (Co) into the ternary heterojunctions resulted in a remarkable increase in HER performance, with hydrogen evolution rates. These findings demonstrate the potential of tailored 2D/2D heterojunctions in advancing photocatalytic hydrogen production and highlight the impact of transition metal modification on charge transfer dynamics.

OC5

MODELLING DISORDER EFFECTS IN ORGANIC SOFT MATERIALS

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π-conjugated soft materials enable disruptive technologies such as organic photovoltaics, transistors, thermoelectrics, bioelectronics and batteries [1]. Tremendous progress in the synthesis, processing and characterization of organic electronic semiconductors has been achieved over the past decades, however fundamental *structure-properties functions* remain elusive yet [2]. Amongst those, are solid state *charge* and *ion transport*, representing complex multiscale phenomena developing in *space* (from the molecular- up to the mesoscopic-scale) and *time* (from ultrafast to continuous state) domains [3]. In this contribution, I will report case-studies of organic conjugated soft materials where the interplay between molecular structure, supramolecular organization, inter-molecular interactions and thermal effects governs the solid-state phase transitions, the electronic and the ionic transport properties (Figure 1) [4-6]. Density functional theory and force-field based molecular dynamics of both crystalline and amorphous materials will be critically discussed, by emphasising the impact of static and dynamic disorder effects on governing the properties of organic functional materials.

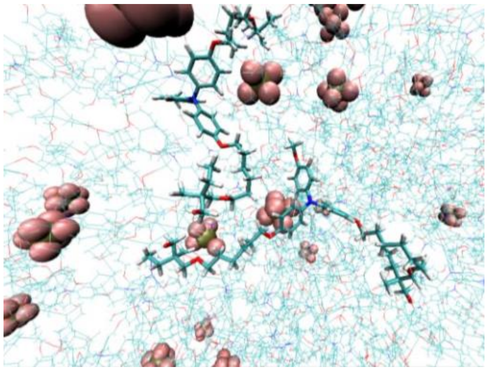

Figure 1. Atomistic simulations of an organic cathode based on cross-linked polymer interacting with PF_6^- ions.

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OC28

IN SITU SPECTROSCOPIC CHARACTERIZATION OF BIFUNCTIONAL ACID-BASE ORGANIC-INORGANIC NANOPOROUS HYBRID CATALYSTS

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Organic-inorganic porous hybrid materials, resulting from the integration of inorganic frameworks with organic functional groups, are highly appealing for the development of high-performance and multifunctional heterogeneous catalysts. In this study, we present the synthesis and characterization of silica-based ordered mesoporous bifunctional hybrids incorporating both acidic and basic active sites. A green approach was employed using 2-methyltetrahydrofuran (MeTHF) as a solvent instead of toluene to graft the basic site (3-aminopropyl)triethoxysilane (APTS) and the acid-site precursor (3-mercaptopropyl)trimethoxysilane (MPTS) onto the surface silanols of ordered mesoporous silica nanoparticles (MSNs) [1]. The thiol groups were subsequently oxidized to sulfonic acids ($-SO_3H$), introducing acidic functionalities into the hybrid material. The characterization of multifunctional hybrid materials requires advanced experimental techniques capable of elucidating organic-inorganic interactions to optimize the spatial separation of catalytic sites and prevent their mutual neutralization. To address this challenge, an integrated analytical approach combining Fourier-transform infrared (FTIR) spectroscopy, multinuclear magic-angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy, X-ray powder diffraction (XRPD), volumetric analysis, and thermogravimetric analysis (TGA) was carried out. Given the simultaneous presence of acidic and basic active sites, it was crucial to investigate their mutual interactions and their individual nature and strength. This was achieved by adsorbing probe molecules with distinct acid or base properties and analysing their interactions via FTIR and multinuclear MAS NMR spectroscopies [2]. Specifically, ammonia (NH_3) adsorption confirmed the presence of sulfonic acid groups, demonstrating their Brønsted acidity through the protonation of ammonia. Meanwhile, carbon dioxide (CO_2) adsorption revealed that a fraction of the basic sites remained intact even after oxidation, indicating that the oxidation process did not entirely eliminate the surface basic functional groups. These findings highlight the coexistence of acidic and basic sites within the hybrid material, providing valuable insights into its chemical behaviour and potential applications in catalysis, particularly in cascade reactions. The ability to finely tune and characterize such bifunctional surfaces paves the way for the development of advanced heterogeneous catalysts with tailored acid-base properties.

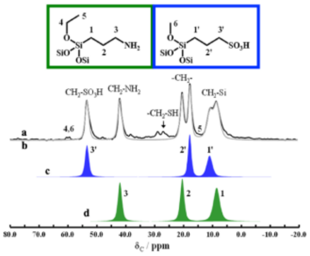

Figure 1.^{13}C CPMAS NMR spectrum of pristine bifunctional hybrid catalyst.

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OC109 SYMMETRIC AND ASYMMETRIC MULTILAYER ELECTRODES FOR SEMI-TRANSPARENT PEROVSKITE SOLAR CELLS

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Semi-transparent perovskite solar cells (ST-PSCs) are currently attracting due to their ability to generate energy while maintaining optical transparency, making them ideal for applications such as building-integrated photovoltaics (BIPV) and tandem solar cells. [1] The efficiency of ST-PSCs is influenced by the electrical and optical properties of their components. Conventional metallic thin film electrodes reduce transparency, limiting overall device transparency. [2] To address this, dielectric/metal/dielectric (D/M/D) multilayer structures have been explored as a promising alternative, balancing electrical conductivity and light transmission. [3] The design of D/M/D electrodes is based on the physicochemical principles related to the modulation of the light absorption due to the surface plasmons of the metal, highly sensitive to the refractive index of the dielectric at the interface, and on the multiple light refractions within D/M/D the multilayer, which reduce optical losses.[4] As properly controlled, these processes lead to an enhancement of the electrode's transparency in the visible range. Thus, innovative D/M/D electrodes using nickel as the metallic layer, enclosed inbetween dielectric layers, can apply as top electrode in ST-PSCs. Nickel was chosen due to its abundance and low cost. For comparative analysis, gold-based structures were also evaluated. Both symmetric and asymmetric D/M/Ds were fabricated, by using MoO_x and WO_x as dielectrics to assess differences between symmetric and asymmetric systems. The electrodes, including MoO_x/Ni/MoO_x, MoO_x/Au/MoO_x, and WO_x-based variants, were deposited via thermal evaporation, and characterized through UV-Vis-NIR spectroscopy, sheet resistance measurements and depth-profiling X-ray photoelectron spectroscopy (XPS). Experimental results highlight the potential of D/M/D electrodes for ST-PSCs, as a cost-effective and efficient solution. Gold-based systems exhibited superior performance, while nickel electrodes proved to be a possible economically alternative. Moreover, asymmetric D/M/D structures showed improved optical transmittance compared to symmetric configurations, underscoring their potential for next-generation transparent photovoltaic technologies.

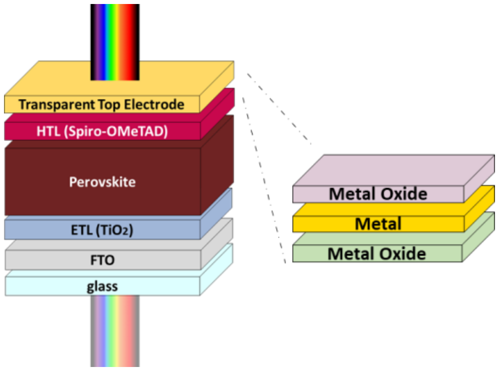

Figure 1. ST-PSC scheme with a detailed view of the D/M/D multilayer applied as transparent top electrode.

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OC35

AUTOMATED DESIGN AND COMPUTATIONAL INVESTIGATION OF DERIVATIZED CYCLODEXTRINS FOR DRUG DELIVERY AND GAS ADSORPTION

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Cyclodextrins (CDs) are cyclic oligosaccharides composed of α-D-glucopyranose monomers linked by α-(1,4) glycosidic bonds, forming a non-symmetric toroidal structure that results in a truncated hollow cone shape [1]. Due to their ability to form inclusion complexes with a wide variety of substrates, including pharmacologically active compounds, metal cations, and vitamins, CDs have attracted significant interest in Drug Delivery Systems (DDS) and environmental applications. In DDSs, CDs are employed in their native monomeric form, derivatized versions (e.g., methyl and hydroxypropyl modifications), and crosslinked nanosponge (NS) structures [2,3].

With the increasing use of derivatized CDs, we have developed and implemented an automated multistep procedure for selectively modeling methylated and hydroxypropylated CDs [4,5]. We generated derivatized CD structures with a fixed degree of functionalization employing the "stk" Python module [6]. The resulting structures undergo an initial geometry optimization at the GFN2 level to determine their energetic ranking [7]. Subsequently, lower-energy structures are re-optimized using the composite r^2SCAN-3c method, providing a more accurate representation of the derivatized CDs [8]. This automated procedure ensures the efficient production of derivatized CD models that closely resemble the actual synthetic material, with the ultimate goal of applying them to the study of encapsulation of therapeutic agents, like melatonin and other drugs. This approach enables the high-throughput generation of CD derivatives, allowing for the exploration of a wide range of functionalized CDs for various applications in drug delivery, the environmental sector.

This optimized procedure has been applied to create a library of native and derivatized CD-complexes with drugs such as melatonin, curcumin, caffeine and vemurafenib. Using automated optimization workflows, we systematically explored the inclusion complexes towards these molecules, providing ranked set of CDs tailored for each drug. Additionally, the automated process has been applied to encapsulate therapeutic and poisonous gases, such as CO_2, CO, SO_2, H_2S, H_2 and CH_4, within CDs. This enables a comprehensive exploration of CD-gas interactions, including solvent effects and the formation of stable complexes. In addition, the calculations of kinetic parameters as k_{on} and k_{off} of each chemical equilibrium could help to shed light on the release models of previously cited guests. By generating a dataset of potential CD hosts, this work aims to pave the way for the development of a machine learning algorithm capable of identifying the optimal host-guest match in CD chemistry.

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OC124

INTERACTIONS BETWEEN HYDROXYAPATITE SURFACES AND SMALL REACTIVE MOLECULES OF ENVIRONMENTAL INTEREST: A COMPUTATIONAL APPROACH

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In recent years, hydroxyapatite (HA, $Ca_{10}(PO_4)_6(OH)_2$) has emerged as a highly promising mineral in green chemistry due to its feasible synthesis from waste materials. [1] Its key properties, such as thermal and chemical stability, tunable acid-base characteristics, non-toxicity, great adsorption capacities, and ion-exchange capability, make it an attractive support for eco-friendly catalysts in heterogeneous catalysis aimed at the abatement of various classes of pollutants. [2] Therefore, the nature and strength of the interactions between molecules and the catalyst surface, in terms of energy, are crucial to determining the reaction outcome. In this regard, computational methods have become increasingly accurate in studying such interactions, [3] enabling guided approaches to catalyst design and development. This process has been further accelerated over the past decades due to the rapid advancement in computing power. [4]

In this contribution, a periodic quantum mechanical (QM) approach has been employed to characterize the interactions between small reactive molecules and the most stable hydroxyapatite surfaces. Besides HA in its pure form, copper-substituted models will also be considered. In fact, it is known that calcium ions can be replaced by various metal ions, including transition metals, to enhance HA's catalytic activity and performance while maintaining its overall structure. [5]

More specifically, results will be presented on the interaction of formaldehyde, a benchmark volatile organic compound, with the HA (001), (010) (both stoichiometric and non-stoichiometric), and (101) facets, in both pure and Cu-substituted hydroxyapatite. Changes in geometrical parameters, energetic properties (i.e., binding energy and enthalpy), and vibrational features will be analysed to establish a preliminary framework for computational investigations on the oxidative decomposition of pollutants in environmental remediation.

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OC54 SPECTROSCOPIC INVESTIGATION OF PHOTOINDUCED REDOX ACTIVITY IN Ce-UiO-67 METAL-ORGANIC FRAMEWORK

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Catalytic activity driven by energy sources alternative to bare heating is a topic of increasing relevance. Electro- and photo-catalytic methods, in fact, allow for superior selectivity with lower energy consumption, as compared to conventional approaches. Nonetheless, these methods still exhibit lower conversion rates compared to thermal ones, highlighting the need for the development of novel catalysts tailored to specific processes. Among several proposed materials, Ce-based metal-organic frameworks (MOFs) are theoretically suitable for many processes, as their electronic properties can be finely tuned by rationally designing them.[1] A few applied examples demonstrated optimal performances in several reactions involving partial oxidation of light hydrocarbons, though a detailed description of the correlation of Ce and its redox behaviour with reactivity is still limited.[2, 3]

Ce-UiO-67 MOF was synthesized [4] and preliminary characterized by standard physico-chemical methods. This material proved to be active in the allylic partial oxidation of cyclohexene and was tested accordingly, in both thermal and photochemical conditions. To better investigate the redox behaviour of Ce sites, an *in situ* X-ray absorption spectroscopy (XAS) study at Ce $M_{4,5}$-edges was performed at the APE-HE beamline of Elettra Sincrotrone Trieste, evaluating the fraction of Ce^{4+}/Ce^{3+} depending on temperature, chemical feed composition and illumination (with a 405 nm solid state laser, 40 mW nominal output power).

The XAS investigation was initially conducted under thermal conditions (heating from 25 to 150 °C) by varying the gas phase conditions from inert (He), to reducing (H_2) to oxidizing (O_2). Under these conditions, we observed a very limited interconversion of Ce^{4+}/Ce^{3+} species at the highest temperature, as well as in combination with the substrate (cyclohexene). Conversely, a large amount of Ce^{3+} formed under illumination when cyclohexene is contacted with Ce-UiO-67. This suggests that Ce^{3+} can be stabilized via activation of the substrate. Further, reactivity with the oxidant and impacts on catalytic performances will be discussed.

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OC97

UNDERSTANDING THE STABILITY OF Ni-In CATALYSTS FOR STEAM REFORMING OF ACETIC ACID FROM QUASI-SIMULTANEOUS OPERANDO XAS-XRD AND COMPUTATIONAL MODELLING

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Steam reforming of oxygenated molecules derived from bio-oils presents a promising alternative to conventional methane reforming for hydrogen production. However, the process currently suffers from stability issues that hinder its potential to become a commercially viable industrial process [1]. Only expensive noble metal-based catalysts have shown satisfactory stability, whereas base metals, like nickel, experience rapid and severe deactivation. Indium is a well-known stability promoter for high-temperature dry reforming reactions, but its application to other reforming processes for hydrogen production, particularly those involving oxygenated compounds, remains unexplored, despite the latter's well-known susceptibility to fast deactivation. Furthermore, the stabilization mechanism remains poorly understood, with most of the limited insights gained from ex-situ characterizations only.

Here, we present an In-modified Ni-based catalyst supported on a Mg-Al-In mixed oxide, evaluated in the steam reforming of acetic acid. The catalyst demonstrated stable activity for over 24 hours at 700 °C, yielding twice the hydrogen productivity compared to the In-free catalyst, which exhibited poor stability. In order to understand the reasons behind its exceptional stability, we performed an operando quasi-simultaneous X-ray absorption-X-ray diffraction (XAS-XRD) experiment, assisted by computational modelling, while replicating the catalytic tests [2]. Catalysts with varying In content were reduced in H_2 up to 700°C. After purging the system, an aqueous solution of acetic acid was introduced to initiate the reaction, and the gas flow was analyzed using an online mass spectrometer. The operando experiment was performed by automatically switching between XRD and XAS, collecting spectra Ni and In K-edges. A complete round of XRD and XAS data collection took about 12 minutes. The results show that upon reduction, the surface of the Ni nanoparticles becomes enriched with In, as confirmed by TEM-EDS, leading to the formation of a Ni_3In-like shell and Ni_3In carbide particles. The presence of In in the surface layers competes with carbon insertion, effectively protecting the Ni particles from coke deposition. As the reaction proceeds, the intermetallic phase is consumed resulting in the formation of Ni nanoparticles that are more stable, although less active, than those of the unpromoted catalyst. This may be due to a different faceting, resulting from the Ni-In dealloying, which again disfavors coke formation.

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OC15

AN UNCONVENTIONAL CHEMICAL CONTRIBUTION TO THE DEVELOPMENT OF QUANTUM ARTIFICIAL INTELLIGENCE

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Humanity is spurred to face global challenges and promote a sustainable future. Facing global challenges means dealing with Complex Systems [1,2]. However, we encounter many difficulties in understanding and predicting the behaviour of Complex Systems due to Epistemological Complexity [3]. A deeper comprehension and a more satisfying prediction of Complex Systems require that we face Computational Complexity and formulate universally valid and effective algorithms for recognizing variable patterns. In this regard, a promising research line is Natural Computing [3]. Within Natural Computing, two computing strategies look particularly alluring: Quantum Computing (QC) and Artificial Intelligence (AI). Their combination has sparked the birth of Quantum Artificial Intelligence (QAI) [4].

Chemistry can contribute to Quantum Artificial Intelligence by devising innovative materials for quantum computing [5] and developing Chemical AI [6-8]. Chemical AI refers to using Molecular, Supramolecular and Systems Chemistry in liquid solutions to mimic some performances of biological intelligence. All the molecules abide by the quantum-mechanical laws. Hence, in principle, any chemical system can be exploited to encode and process qubits. However, it is well-known that decoherent phenomena hinder quantum computation, and extreme conditions are usually required to protect and manipulate qubits. CAI proposes an alternative strategy that exploits thermalized quantum mixed states rather than qubits. Quantum mixed states can be generated by micro-heterogeneous chemical systems, which are thermalized with the surrounding micro-environment. They can be manipulated through physicochemical inputs and characterized by fitting their exponential kinetics through the Maximum Entropy Method [9]. Mixed states are used to implement chemical fuzzy sets [10]. The amount of information encoded by these chemical fuzzy sets can be easily compressed and decompressed [11]. Mixtures of properly selected chemical fuzzy sets granulate the physicochemical variables and allow the imitation of the performances of human sensory systems. The mimicry of the fuzziness of human color vision through a mixture of direct photochromic compounds extended vision in the UV [12,13].

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OC31 DISSECTING THE NATURE AND QUANTUM DYNAMICS OF ELECTRONIC EXCITATIONS AND CHARGE CARRIERS IN OPTO-ELECTRONIC MATERIALS

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The field of organic opto-electronics has expanded rapidly in recent years. Organic photovoltaic devices (OPVs) for light-to-charge conversion and organic field-effect transistors (OFETs) for charge transport are among the most prominent organic technologies. Driven largely by synthetic trial-and-error improvements, a new generation of highly light-absorbing organic semiconductors, known as non-fullerene acceptors (NFAs), has pushed solar conversion efficiencies toward 20%, enabling strong charge generation [1]. Meanwhile, highly conducting molecular organic crystals and polymers have enabled large charge carrier mobilities [2].

Key processes such as light absorption, charge generation and electronic transport are central to these technologies. However, their fundamental understanding remains limited due to challenges in studying relevant time and length scales as well as realistic morphologies of the materials. Quantum phenomena, driven by electronic and excitonic interactions between molecular components, influence both optical properties [3,4] and electronic transport [5,6]. Establishing structure-property relationships and elucidating the nature and dynamics of electronic excitations and charge transfer could provide critical insights for further efficiency improvements.

Here, I will discuss how first-principles-based model Hamiltonians [3,4], combined with quantum dynamics simulations [5,6]—accounting for non-adiabatic effects and electron-nuclear coupling—can provide this understanding. I will show how excitonic interactions between localized Frenkel-like excitations modify spectral absorption upon aggregation in NFA systems (like Y6 and m-4TICO) [3,4] and how intermolecular charge transfer states, in some cases, contribute to spectral changes going from the solution of these materials to their solid-state morphologies. These charge transfer states facilitate charge separation and generation of free charge carriers. I will demonstrate that once separated, photogenerated charges in crystalline samples of organic materials do not travel via simple hopping or as fully delocalized waves, as previously assumed for similar systems. Instead, they behave as quantum particles undergoing diffusive jumps over several lattice spacings (nanometers) at a time [6]. Computed exciton diffusion length [5] and charge mobilities [6] align well with experimental estimates. Based on these insights, I will propose strategies to leverage solid-state packing effects for intelligent material design, aiming to enhance performance of devices.

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OC51

EFFECT OF THE DEPOSITION TEMPERATURE ON THE MAGNETIC AND THERMOELECTRIC PROPERTIES OF $MnFe_2O_4$ THIN FILMS

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Manganese spinel ferrite ($MnFe_2O_4$) has been extensively studied as a magnetic material. However, its thermoelectric properties haven't been studied thoroughly yet. A theoretical study identified some ferrites with spinel type structure as promising thermoelectric materials, thanks to their high Seebeck coefficient [1]. Multifunctional materials with thermoelectric properties are valuable options for the development of energy harvesting devices, since they are useful in the perspective of supporting the transition to greener energy sources [2]. $MnFe_2O_4$ has been deposited as a thin film *via* pulsed laser deposition (PLD), varying the deposition temperature to study its influence on the structural, thermoelectric and magnetic properties of the samples. X-ray diffraction patterns showed an increasing crystallinity and stronger orientation along the [311] direction of the structure as a function of increasing temperature. The thin films, whose thickness was found out to be ~180 nm, showed uniaxial magnetic anisotropy in the in-plane direction, confirming the polycrystallinity of the samples; the values of M_r/M_s and H_c are lower in the cross-plane direction, as typically observed for thin films. Thermoelectric properties of manganese ferrite thin films have been investigated for the first time: the Seebeck coefficient is negative and rather constant from 40°C to 340°C, with values ranging from -3 μV/K to -180 μV/K through the series, while the electrical conductivity increases with temperature from 0.001 S/cm to about 0.01 S/cm. These values vary hugely depending on the deposition temperature, with a maximum calculated power factor of 0.07 $\mu W/(m \cdot K^2)$ at 340°C in the sample deposited at 200°C. These results are promising for the development of multifunctional materials with both magnetic and energy harvesting properties that can be tailored by different deposition conditions.

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OC101 ON THE TEMPERATURE-INDUCED COLLAPSE OF SMART POLYMERS IN AQUEOUS SOLUTIONS

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It has been found that several water-soluble polymers, such as poly(N-isopropylacrylamide) [1], poly(N-vinylcaprolactam) [2], polypropylene-oxide [3], undergo a temperature-induced coil-to-globule collapse transition in water and aqueous solutions. In all cases the collapse proves to be reversible and endothermic (DSC measurements are not equivocal on this point), demonstrating that the driving force is of entropic origin. In several cases T(collapse) is around 30 °C, and so the thermo-responsiveness of such polymers has been recognized as very interesting and promising for the development of drug carriers in the human body.

Polymer chains lose conformational entropy upon collapse; this implies that the entropy gain driving the collapse has to come from water molecules. There is a marked difference in solvent-excluded volume among the swollen conformations constituting the coil macro-state and the compact ones constituting the globule macro-state. This situation resembles that holding for the unfolded and folded conformations of globular proteins [4]. A decrease in solvent-excluded volume leads to an increase in the volume accessible to water molecules, and thus to an increase in their translational entropy. Using classic scaled particle theory, and simple geometric models of the coil and globule macro-states, it is possible to show that the large increase in water translational entropy, driving polymer collapse, stems from the very large number density of water that, in turn, has its origin in the strength of H-bonds and the small size of water molecules [5-7].

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OC11

FLUORESCENT SILK FIBROIN NANOPARTICLES: PREPARATION AND PHYSICO-CHEMICAL CHARACTERIZATION

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Fluorescent silk fibroin (SF) nanoparticles (F-SFNs) have gained significant attention in recent years due to their unique properties and potential applications in nanomedicine. SF, derived from the natural protein found in silkworm cocoons, has long been recognized for its mechanical strength, biocompatibility, and biodegradability. Furthermore, the possibility of obtaining SF in the form of nanoparticles through a reproducible and relatively simple desolvation method has further expanded their utility, including biomedical applications [1]. Two main approaches can be applied for the preparation of F-SFNs: the first and most widely used in the literature involves the labeling of pre-formed SFNs [2]. The second and less widespread approach involves the labeling of the SF as obtained after the degumming phase and then proceeding to the production of the nanoparticles using fluorescent fibroin. In this contribution, the second approach was followed by using fluorescein isothiocyanate (FITC) for SF labeling, capable of reacting with the free amino groups of Lys residues of fibroin to form a thiourea bond.

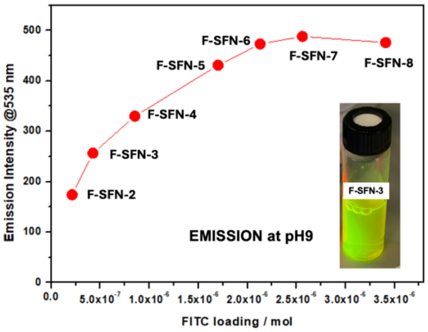

Figure 1 Emission of F-SFNs suspensions (0.25 ml ml^{-1}) at pH 9 as a function of FITC loading.

A set of F-SNFs was prepared with increasing amounts of FITC to identify the optimal loading in terms of maximizing fluorescence properties without interfering with the nanoparticle formation process (Figure 1). To identify whether FITC labeling interferes with the nanoparticle formation process, all prepared samples were characterized from a morphological-structural and dimensional point of view by FT-IR spectroscopy, scanning electron microscopy (FE-SEM), and Nanoparticles Tracking Analysis (NTA). The photophysical properties of all the nanoparticles produced were studied by means of UV-Vis absorption and emission electron spectroscopies as a function of pH and solvent polarity and compared with the properties of the fluorophore in solution in order to highlight any protective/shielding effects exerted by the nanoparticles against the fluorophore.
The multi-technique characterization allowed highlighting the effect of synthesis parameters on the morphological and physical-chemical properties of the resulting fluorescent silk fibroin nanoparticles, evidencing the possibility of finely tuning the fluorescence properties by a proper synthetic approach, making them suitable for uptake studies, which were carried out in mesenchymal stem cells.

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OC24

IDENTIFYING THE ORIGINS OF NMR SHIFTS FROM QUANTUM ALCHEMY

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Calculation of chemical shifts (σ) of large dataset using DFT calculations can turn to be an expensive task. Black box models, although successful, [1] do not provide physical insight, but rather require careful analysis of predictions to improve their explainability.

An alternative approach is Quantum Alchemy (QA): this approach continuously transforms one molecule into another at the quantum mechanical (QM) level, by treating nuclear charges (Z) as continuous variables of the molecular Hamiltonian [2]. This means that instead of thousands of independent QM calculations, the same results can be obtained by interpolating from a reference system using a Taylor series expansion of Z variations.

In this work, employing the DELTA50 database [3], we use physically interpretable response functions as predictive model using QA. This approach allowed us to understand the physical origins of chemical shifts calculations. Perturbation of Z and dielectric constant (ε) were independently studied to understand the response for different molecular systems and different solvents, respectively (Figure 1).

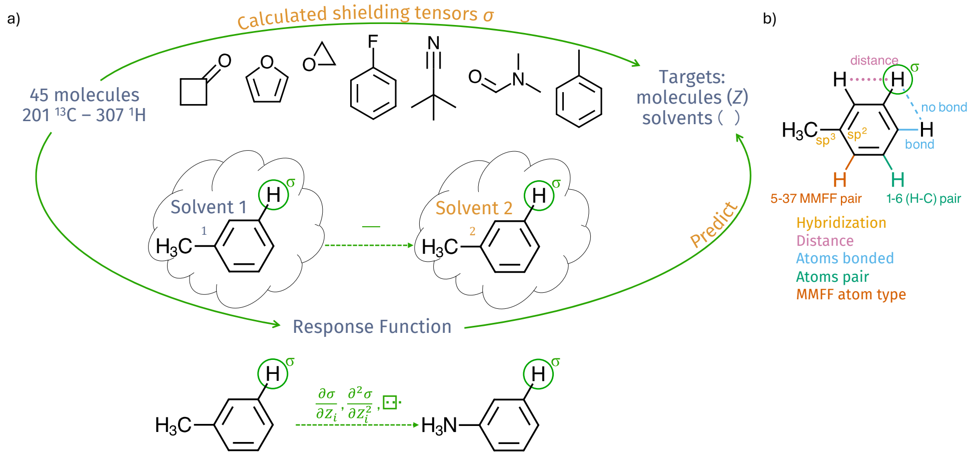

Figure 1. a) Representative workflow of this work. b) Analyzed features.

Our results revealed that both ^{1}H and ^{13}C have a smooth and regular response to Z and ε perturbations. They suggest that for ^{1}H chemical shifts, truncating the Taylor series at the second order, the median error is 0.058. For ^{13}C chemical shifts, the median of the second order Taylor series is unreliable, with a value of 1.350. Interestingly, considering only the scenario where the perturbation and the calculated nucleus is further than 1.54Å (over 70% of calculations), a median of 0.631 is achieved. The inclusion of third order allows to describe also those short distance scenarios, with a median of 0.471. The study of the solvent response function revealed that all solvents can be described by modifying only the ε while using Chloroform as base solvent.

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OC104 REALIZING STIMULI-RESPONSIVE PLATFORMS VIA iCVD FOR DELIVERING GREEN-SYNTHESIZED AuNPs AND ACCELERATING WOUND HEALING: A PROOF-ON CONCEPT

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Chronic wounds result from the failure of the normal wound healing process, and pH has a key role during it. Indeed, it could be considered a useful and simple tool to quickly recognize a nonhealing wound. [1] Furthermore, the wounds' pH can influence susceptibility to infection, antimicrobial activity, modulate the by-product generation, and influence biochemical process. Open wounds characteristically have neutral or alkaline pH ranging from 6.5 to 8.5, while that of chronic wounds ranging from 7.2 to 8.9. [2] Targeting the pH and making the wound environment acidic could be beneficial for the healing process, discouraging the overgrowth of bacteria. Thus, looking for smart delivery systems for releasing therapeutic agents having effectiveness in healing chronic wounds, is a challenge today. For pursuing this aim, a pH-responsive polymeric hydrogel constituted by Methacrylic acid (MAA), crosslinked by Diethylenglykol-divinylether (DEGDVE), and Ethylene glycol dimethylacrylate (EGDMA) as primer, was realized for delivering Green-synthesized and properly functionalized AuNPs via initiated chemical vapor deposition (iCVD) technique. Three AuNPs typologies synthesized by using natural extracts such as Snail Slime (AuNPs-SS), *Punica granatum* juice (AuNPs-PGJ), and a water-based polyphenolic extract from grape pomace (AuNPs-GWE) were selected as new potential healers, and deposited via drop casting onto three different substrates: conventional micro cover glass, silica wafer, and a commercial latex-free elastic dressing retention tape made of a soft, non-woven flexible fabric. [3-5] With the aim of assessing if the AuNPs release was affected by the hydrogel coating, different coating thicknesses were realized. The uncoated and coated samples were characterized by optical microscope and spectroscopic ellipsometry for assessing the morphology and the polymer coating thickness, respectively. Preliminary assessments about the release of AuNPs from the hydrogel coating were accomplished in Simulated Wound Fluid (SWF) medium prepared at three different pH values, 6.5, 7.5, and 8.5, and buffer solutions at pH 5.0, 7.0, and 8.0. Work is in progress for investigating the kinetic aspects of the release process in the selected media and testing the AuNPs effectiveness by determining the % of wound closure, after assessing their biocompatibility.

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OC9

ADVANCED CHARACTERISATION OF ORGANIC AND INORGANIC FILLERS FOR CO_2-SELECTIVE MIXED MATRIX MEMBRANES

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To address climate change, Carbon Capture Utilization and Storage (CCUS) technologies play a crucial role in reducing CO_2 emissions. Membrane-based separation is an attractive approach due to its efficiency, scalability, and low carbon footprint. The DAM4CO$_2$ EIC-Pathfinder project focuses on developing innovative Mixed Matrix Membranes (MMMs) for CO_2 separation and photoconversion into hydrocarbons. [1]

Traditional MMMs incorporate inorganic fillers like Metal Organic Frameworks (MOFs), but interface defects often reduce their performance. Issues such as poor compatibility, aggregation, and large particle size hinder gas transport efficiency. [2] To overcome these limitations, DAM4CO$_2$ explores the use of Polymers of Intrinsic Microporosity (PIMs) as alternative organic fillers, aiming to enhance interfacial compatibility. [3] The project synthesizes novel MOFs and PIMs using non-critical raw materials, optimizing their morphology for dispersion in MMMs. In particular, the primary fillers studied and compared are PIMs containing different halogen anions and modified Zn-based UTSA-16 MOFs, selected for their potential to enhance CO_2 selectivity and membrane stability.

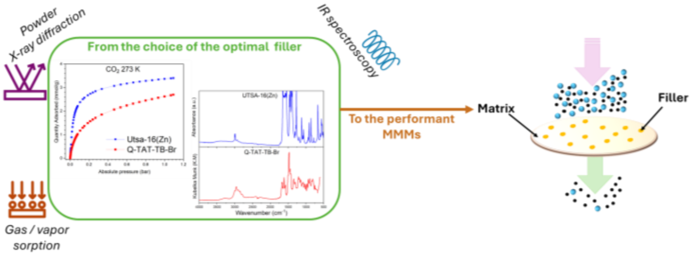

Figure 1. Characterization-driven selection of the optimal filler for high-performance MMMs.

Advanced characterization (PXRD, FT-IR, and volumetric isotherms) evaluates CO_2 selectivity against CH_4 and N_2. The most promising fillers are then integrated into a soluble PIM matrix (e.g., PIM-1, DAT-TB) for further analyses.

Comprehensive characterization identifies optimal fillers to produce defect-free MMMs, enhancing CO_2 separation. The project also assesses membrane scalability and real-condition performances, paving the way for simultaneous CO_2 separation and photoconversion into renewable fuels.

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OC37

SYNTHESIS OF METAL DOPED g-C_3N_4 NANOSTRUCTURES AND THEIR USE AS CATALYSTS FOR ENVIRONMENTAL APPLICATIONS

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A large amount of dyes is produced worldwide every year and it is known how serious and global health and environmental problems are caused by the release of its by-products into nature. According to the World Health Organization (WHO) reports, environmental pollutants found in soil, air and water cause 25% of diseases that impair human health [1]. In this study, metallic composite containing graphitic carbon nitride (g-C_3N_4) was synthesized to be used as a catalyst in the catalytic degradation of synthetic dyes with sodium borohydride ($NaBH_4$). Copper metal, which is cheaply available, was selected as the metal and copper immobilized form of graphite carbon nitride (CuO@g-C_3N_4) as catalyst was synthesized using simple one-step heat treatment [2]. The synthesis method of the nanocomposite is shown in Figure 1.

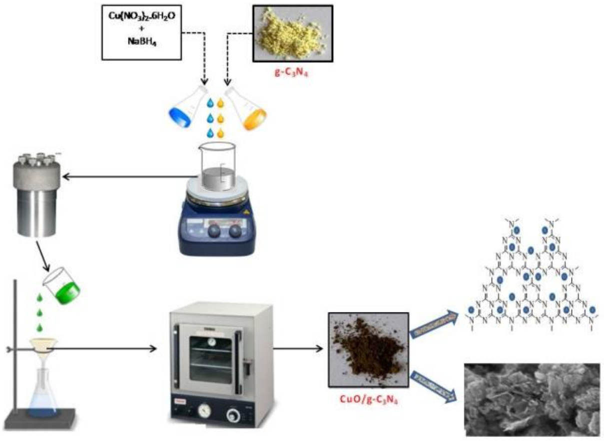

Figure 1. Illustration of synthesis procedure for g-C_3N_4 decorated CuO composite

The synthesized CuO@g-C_3N_4 was characterized by Fourier Transform Infrared Spectroscopy, X-ray Diffraction, Scanning Electron Microscopy, Electron Scattering analysis [3]. Degradation experiments of the synthetic dye were carried out in the presence of $NaBH_4$ used as a reducing agent and the degradation times were monitored by UV-Vis Spectrophotometer (UV-Vis). The catalytic activity of the prepared composite was tested in a wide spectrum at room temperature in aqueous medium. Chemical catalytic activity, effect factors and kinetics of CuO@g-C_3N_4 nanocomposites for dyes were investigated. The results showed that CuO@g-C_3N_4 nanocomposites can be used as a highly effective chemical catalyst to degrade dye contaminants.

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OC27 NANOFIBER-BASED SEMICONDUCTOR MATERIALS FOR ENHANCED PHOTOCATALYTIC HYDROGEN PRODUCTION

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Photocatalytic hydrogen production by splitting water using sunlight is one of the prominent research areas in recent years due to the abundant availability of solar energy and its clean and renewable energy source. In order to increase the efficiency of H_2 production using solar energy, there is a need for further research on photocatalytic materials that are specific to hydrogen evolution reaction (HER), stable, and have high catalytic activity. Nanomaterials are widely investigated as promising materials for photocatalytic hydrogen production due to their properties such as large surface area, high catalytic active sites and light absorption. Among various forms of photocatalytic nanomaterials, nanofiber-based semiconductor materials show great potential for HER compared to other nanostructured materials due to their unique physicochemical, optical, and electrochemical properties. Metal oxide and sulfide nanofibers were prepared by electrospinning process and characterized by different techniques such as SEM, TEM, XRD, UV–Vis and CV. Photocatalytic HER under visible light irradiation was investigated using nanofiber structures as catalyst, triethanolamine as electron donor. Nanofiber structures showed approximately 2-times higher photocatalytic activity compared to bulk forms. Moreover, photocatalytic HER activities of nanofibers were enhanced by using biopolymers template. Lastly, CeO_2 and Yb_2O_3 nanofibers displayed increasing photocatalytic HER activity when biopolymers added to the reaction media, which are act as electron transfer mediator between electron donor solution and catalysts. Studies have shown that nanofiber structures help to improve the photocatalytic H_2 production performance of conventional semiconductor materials.

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OC38

SURFACE DIAGNOSTICS AND LASER CLEANING POTENTIALS OF SYNTHETIC AND HISTORICAL PATINAS ON OUTDOOR BRONZES

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Environmental influences that lead to the formation of patina layers have altered considerably due to changes in atmospheric emissions over the past decades. Brochantite, $Cu_4(OH)_6SO_4$, has been the most stable patina phase in a neutral and moderately acidic, humid and, in particular, industrial environment containing SO_2. As industrial emissions have become cleaner with lower SO_2 content, Cu and its alloys cannot 'naturally' turn green anymore as in the early industrial era due to pollution. In this situation, analyses of various patina phases on historical copper roofing sheets from the Belvedere Palace, built 1723 by Prince Eugene of Savoy [1], and on representative memorials such as that of Emperor Josef II (Vienna, 1807), King Gustav II Adolf (Gothenburg, 1854), archduchess Maria Theresia (Vienna, 1887), Minin and Pozharsky, Moscow, Red Square, 1818), and on the Quadrigas (1885) atop the Austrian parliament in Vienna [2] provided insight into the mechanisms of long-term corrosion of outdoor cultural heritage objects. Alloy composition and metal microstructure analyses of the artefacts shed light into casting details and the resulting patina layers. Brochantite was often found as the main mineral component of the patina. The stratigraphy showed distributions of Cu, Sn, S, Cl, etc.. Areas that have been exposed to rain exhibited mostly brochantite ($Cu_4(OH)_6SO_4$), and atakamite ($Cu_2(OH)_3Cl$).

A synthesis for artificial brochantite patina layers was applied to the entire tambour copper panelling of the Otto Wagner Church in Steinhof, Vienna [3] and also to test coupons for laser diagnostics and cleaning experiments [1]. Patina powder samples were analysed using XRD and light microscopy. Alloy and patina analyses were performed with atomic absorption spectral analysis, SEM, EDX on polished sections, colourimetry, metallographical stratigraphy, and laser-induced breakdown spectroscopy depth profiling (Nd:YAG laser, 4 ns, 266 nm).

A selective cleaning approach of patinas may consider low-pressure water, degreasing, Nylon brushes, scalpels, vibrating and rotating tools, blasting, chemicals, but also photonic procedures, such as laser cleaning. This has already become an established treatment for a range of artefacts, including stone, ceramics, paintings, and metals, i.e. Cu, Fe, Ag and Au [4,5]. A careful selection of the laser wavelength, pulse duration and operating conditions is then crucial for the laser cleaning success [1,6-12].

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OC3

INVESTIGATING THE TEMPERATURE DEPENDENCE OF FERRATE ION FORMATION AT HIGH-PURITY IRON ELECTRODES USING DUAL DYNAMIC VOLTAMMETRY (DDV)

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Electrochemical method is one of the most common for ferrate ion (FeO_4^{2-}) production. During the electrochemical ferrate ion production an iron-containing sacrificial electrode is oxidized in a highly alkaline medium [1]. At the relevant potential region, intensive oxygen evolution decreases the current efficiency and makes the exact determination of the amount of ferrate ions produced problematic. Furthermore, due to the low stability of ferrate ions and the usual ferrate determination method (based on sampling), the characterization of ferrate ions is uncertain and has low time resolution.

Electrochemical synthesis of ferrate ions from high-purity iron electrode was performed in a 45 % (m/m) aqueous NaOH solution. The synthesis process was investigated using Dual Dynamic Voltammetry (DDV), which involves applying dynamic potential programs simultaneously to the disk and ring electrodes of a Rotating Ring–Disk Electrode (RRDE) setup [2,3]. This method enables the real-time determination of the quantity of ferrate ions formed at the electrode with high precision and time resolution. During the measurement the parasitic oxygen evolution can be formally separated from the ferrate ion formation [4,5]. The effect of temperature on ferrate ion formation between 15 °C and 45 °C was investigated, and the optimal potential range and temperature for maximizing the ferrate ion production and current efficiency were determined.

The findings indicate that ferrate ion production increases with temperature within the investigated temperature range. Regarding the potential, an optimal potential exists at each temperature where ferrate ion formation occurs at the highest possible rate (limited by other factors). This optimal potential decreases as temperature rises. The current efficiency shows a similar trend across all temperatures with respect to the potential, and the maximum current efficiency was also determined for each temperature.

Acknowledgements: the publication was created as part of the Momentum Program of the Hungarian Academy of Sciences (grant LP2022–18/2022) and in the frame of the 2018-1.1.2-KFI-2018-00123 project, implemented with the support provided by the National Research, Development and Innovation Fund of Hungary, financed under the 2018-1.1.2-KFI funding scheme. The authors thankfully acknowledge financial support from the National Research, Development, and Innovation Office (NKFIH) of Hungary (grants K129210 and FK135375).

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OC70 ATOMISTIC INSIGHTS INTO SOLID-STATE PHASE TRANSITION IN P2 LAYERED OXIDES AS HIGH ENERGY CATHODES FOR Na-ION BATTERIES

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Layered Transition Metal Oxides (Na_xTMO_2) are the most promising high-energy cathode materials for Na-ion batteries. Their structure consists of TMO_2-octahedra 2D slabs sandwiched between Na layers, wherein the arrangement and packing of oxide layers define distinct material morphologies such as P2- and O3- structures. [1] While mixed transition metal oxides in this class of cathodes have shown very good electrochemical performances their long-term stability remains a challenge. [1,2] This instability is often attributed to solid-state phase transitions during Na^+ insertion and extraction cycles, leading to structural collapse and significant capacity loss. [1,2] Understanding and controlling these structural transformations is therefore of outmost importance to improve the electrochemical performance of layered oxides. Employing the variable cell nudged elastic band (VC-NEB) [3] method combined with state-of-the-art density functional theory (DFT) calculations, [4,5] we address the prototypical case of P2 $\leftrightarrow$ P2'/OP4 transitions in Na_xMnO_2 material and its Ni-doped variant (Figure 1). We reveal the key P2-to-OP4/O2 and P2-to-P2' transitions that occur across various sodiation levels, involving substantial rearrangements around the transition metal sites, with tetrahedral transition states accountable for energy barriers. Our analysis of bond length and angle distortions highlights that shear deformations are pivotal in triggering P-to-O gliding at low sodium levels. Based on these insights, our structural distortion metrics offer a straightforward and computationally efficient descriptor to evaluate structural integrity for these layered oxides, enabling the design of NIBs with improved stability and extended lifespan.

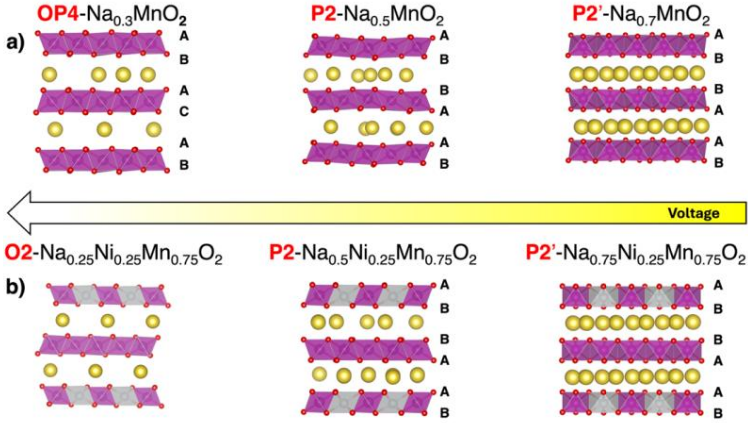

Figure 1. Schematic diagram of a) Na_xMnO_2 and b) Ni-doped Na_xMnO_2 phases evolution upon battery functioning.

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OC94

BOOSTING BIOELECTRICITY GENERATION IN BIOPHOTOVOLTAICS WITH ENGINEERED GOLD NANOPARTICLES

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To achieve a more sustainable and environmentally friendly future, innovative technologies are required to meet the increasing demand for renewable energy generation. [1, 2] The use of intact microbial cells as biocatalysts for the development of bioelectrochemical systems has found several applications in recent years, going from localized power generation [3] to (self-powered) biosensing [4] and bioelectrosynthesis of high-value products. [5] In this context, biophotovoltaics (BPVs) emerge as promising biohybrid electrochemical systems, integrating metabolically active photosynthetic bacteria with electrodes to generate bioelectricity in the presence of light. [6] Despite their potential, BPVs face challenges related to low stability and efficiency, [5] limiting their large-scale application. Nanomaterials, due to their unique physicochemical properties, offer a viable strategy to enhance BPV performance, [1] improving both extracellular electron transfer (EET) and light-harvesting efficiency. Metal nanoparticles (NPs), in particular, can act as light absorbers to boost photon capture and as conductive intermediates to facilitate charge transfer between bacterial cells and electrode surfaces. Despite the proven efficacy of NPs in facilitating charge transfer at the cell-electrode interface, the mechanisms regulating NP-bacteria interaction and the localization of the NPs within the bacterial cells remained underexplored. Herein, we investigate the modification with water dispersible and rationally surface designed Au NPs, bearing specific surface properties, of metabolically active photosynthetic purple bacterial cells (*Rhodobacter capsulatus* DSMZ 152*, R. capsulatus*) monitoring the effect of surface functionalization on the EET process at the biotic-abiotic interface. The NPs are designed to be small enough and have tailored surface properties to purposely and suitably interact with bacteria while not resulting cytotoxic. Electrochemical characterization demonstrates improved photoelectrochemical conversion and enhanced transport efficiency of photogenerated charges when using NPs-modified bacteria as photoanode.

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OC34

ION BEAM-INDUCED MoS_2 SURFACE MODIFICATION: AN XPS STUDY OF Ar^+ AND Ar GAS CLUSTER ION BEAM TREATMENTS

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Two-Dimensional (2D) materials are a class of crystals structured as sub-nanometer sheets with no dangling bonds on the basal plane. Molybdenum Disulfide MoS_2 is the second most studied 2D material after graphene [1]. The material's electrical and chemical properties can be tuned by creating defects in the material. The most studied type of defect due to its ease of formation is the sulfur vacancy, usually found to be a p-dopant [2] and increase of chemical reactivity of the surface as the defect presents increased chemical reactivity [3]. One way of creating such vacancies is ion beam exposure. It provides a precise and spatially resolved possibility of creating defects on the material's surface due to preferential sputtering of sulfur [4]. XPS studies of ion beam exposure effects on MoS2 have previously been featured in several publications which showed molybdenum (IV) to reduce to an oxidation state whose nature is not yet precisely defined [5,6,7]. As the nature of the treated surface is still not fully understood our study aims to gain further understanding through more in-depth investigation of ion beam treatment. We compare freshly cleaved surfaces of MoS_2 crystals (molybdenite) and CVD deposited MoS_2 monolayers using Ar^+ ion beam at 500 eV and 1 keV to induce preferential sputtering of sulfur and follow the evolution of molybdenum's chemical environment by recording the Mo 3d region using XPS (Figure 1). In addition, we investigate the effects of Gas Cluster Ion Beams with clusters Ar^+_{2500} at 20 keV energy and Ar^+_{1000} at 2.5 keV energy, respectively, to understand how a different energy transfer may affect the surface transformation for monomer compared to gas cluster ion beams [8]. The surface properties are then investigated further through monitoring of the reactivity by exposing the sample to ambient conditions and follow the re-oxidation process in air. The results allow for a better understanding of the surface modifications and a preliminary model for the effects of Ar ions on MoS_2 is proposed which might contribute to a more precise tailoring of MoS_2 (electronic) properties in the future.

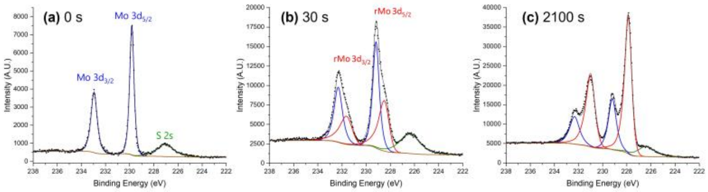

Figure 1 – Molybdenite surface: evolution of Molybdenum 3d spectrum after exposure to 500 eV Ar^+ ions time: (a) 0 s, (b) 30 s, (c) 2100 s. A new reduced molybdenum species (rMo) appears and grows along with increasing ion dose.

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OC40

REIMAGINING WINE WASTE: UNLOCKING THE POTENTIAL OF NATURAL POLYMERS FOR SUSTAINABLE INNOVATION

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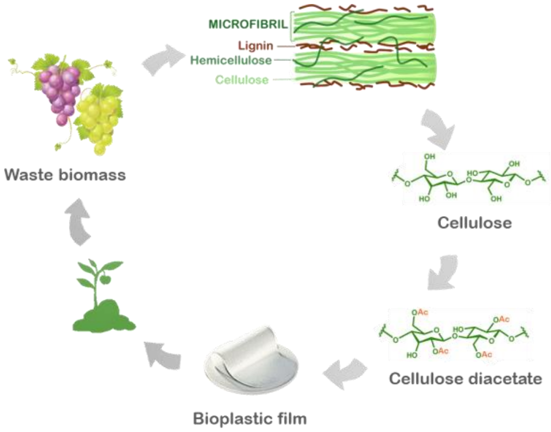
The wine industry generates a considerable amount of waste, such as grape seeds, stalks, and vine shoots, which are often undervalued. It is estimated that 100 tons of wine worldwide result in approximately 39 tons of waste [1], and traditional disposal practices, such as the incineration of pruning waste, significantly contribute to environmental impact. [2] An alternative approach to reducing environmental pollution is to utilize these low-cost wastes, which are still rich in valuable compounds, and change their destination from "waste" to "byproducts", that can be recovered and used for further applications. Specifically, wine waste biomass contains useful components such as cellulose and lignin, biopolymers that can represent a new raw material for the synthesis of biomaterials. In the present work, an eco-sustainable approach is proposed for the valorization of wine shoots. With the aim of improving the sustainability of the entire process and minimizing waste, the two main natural polymers contained in the biomass have been extracted, also employing a green pretreatment of the matrix before polymers separation. The extraction process has been optimized to obtain cellulose and lignin with adequate purity and good yields. The characteristics of the extracted products were continuously monitored in order to adjust the experimental conditions and achieve products with desirable properties. Fourier transform infrared (FT-IR) spectroscopy and Ultraviolet-visible (UV-Vis) absorption spectroscopy were used to analyze the chemical structure of the products. Differential scanning calorimetry (DSC) was employed to determine thermal events, providing information on characteristic temperatures (glass transition, crystallization, melting temperature), as well as on the purity of the polymers. Thermogravimetric analysis (TGA) was used to assess thermal stability and decomposition temperature. The properties of the extracted polymers make them promising base materials for potential applications in the development of biobased and biodegradable active materials, biocomposites, and drug delivery systems. In particular, the extracted cellulose was used as a basic material for sustainable packaging applications. Cellulose acetate films were synthesized, and their structural features, mechanical and thermal properties, and biodegradability in soil were studied.



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OC103 IN-OPERANDO REACTION KINETIC MONITORING BY SERS IN MICROFLUIDICS

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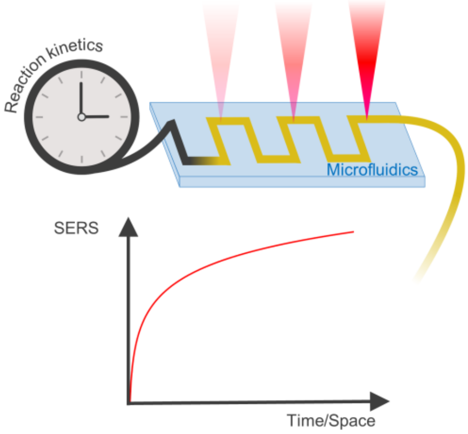
The study of kinetics and reaction mechanisms is fundamental in the chemical sciences, and various optical, magnetic and electrochemical techniques are used today. Microfluidics offers the unique opportunity of achieving accurate control over the reagent mixture, but appropriate strategies must be incorporated to track the reactive environment. It is herein presented a microfluidic device in which the entire length of the channel serves as an efficient SERS substrate, which is used to monitor laminar flows and species diffusion, as well as the second order reaction kinetic.

The chip involves an Aluminum foil inkjet-printed with an AuNP ink obtained by laser ablation synthesis, resulting in a rough film of 200nm in thickness. The same is patterned according to microfluidic side walls obtained from a 500µm brass foil, closed at the top with a glass coverslip. The ability to follow laminar flaws and species diffusion was addressed by Nile Blue and Crystal Violet dyes, while the reactive mixture between the cofactor pyridoxal 5'-phosphate (PLP) and a modified aniline was used for kinetic monitoring. micro-Raman maps were acquired along the whole channel length, namely on the centimeters scale.

The chip followed the constrains given by the PLP-aniline reaction. It needs 60 min at ambient/physiological conditions. A serpentine with cross section of 2x0.5mm, and total length of 115mm was adopted to cover the reaction time under a 1.5µL/min flow. SERS-EF was estimated as high as 105 using pMBA. The non-reactive dyes were run through the chip and the channel mapped at a lateral spatial resolution of 250µm, highlighting the diffusion and mixing of the two. The whole channel length was mapped at 500µm lateral resolution for the PLP-aniline reaction. The SERS second order kinetic well resemble H-NMR experiments.

The methods and the technology herein presented constitute a fundamental preliminary example of the great potential of the synergy between microfluidic and SERS-monitoring of a reactive environment. This approach circumvents the issues related to SERS memory effect that affect measurements in batch.



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OC12

NANOSCALE DISTORTIONS PRODUCE MESOSCALE MODULATIONS IN Li-DOPED KTa/NbO$_3$ PEROVSKITE FERROELECTRICS: A CRYSTALLOGRAPHIC STUDY

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Tantalate-niobate solid solutions are perovskite-type crystalline ferroelectrics with groundbreaking optical properties, like giant broadband refraction (n>25) across the entire visible and near infrared spectrum [1]. At the Curie point, a coherent ordered 3D mesoscale structure emerges, which could be rationalized as a ferroelectric supercrystal [2] composed by topological large-scale defects that self-organize into a hypervortex structure [3]. Here, we report on an accurate multi-T single crystal X-ray study on the Li-doped tantalate-niobate system $K_{0.997}Li_{0.003}Ta_{0.64}Nb_{0.36}O_3$ in the 300-90 K range of T, at steps of 3 K. Three first-order structural phase transitions occur, which break the $Pm\bar{3}m$ symmetry of the parent RT structure and induce uniaxial polarization within the unit cell, where Nb and Ta are displaced in opposite directions and Li is most probably off-centered (Figure 1). The transitions are confirmed by independent calorimetric and dielectric spectroscopy measurements. Classical simulations complement experimental data and offer hints on possible paths leading to the emergence of complex structures at higher (10^1–10^2 nm) length scales. The results provide a substantial step forward toward the understanding of large-scale polarization in these materials, with potential applications in miniaturized circuitry and nonlinear optics.

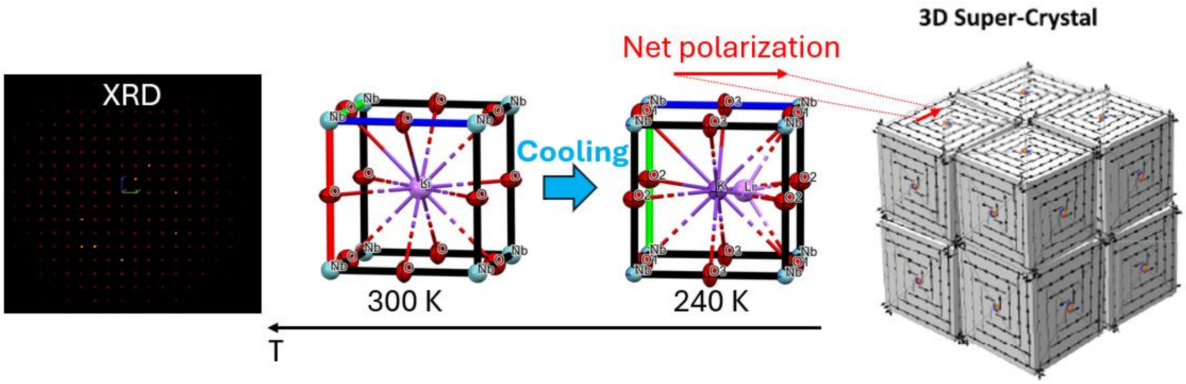

Figure 1. Structural models from multi-T single-crystal X-ray diffraction demonstrate that symmetry breaking induces net atomic polarization in $K_{0.997}Li_{0.003}Ta_{0.64}Nb_{0.36}O_3$. Below the Curie temperature, polarized domains self-organize into a 3D hypervortex mesoscale supercrystal.

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OC41

NANOSTRUCTURED FLUIDS FOR THE CONSERVATION OF CULTURAL HERITAGE: THE ROLE OF SURFACTANT STRUCTURE IN CLEANING EFFICIENCY

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Over the last decades, soft matter and colloids science have been providing fundamental contributions to the conservation and preservation of Cultural Heritage (CH), developing advanced materials [1]. In particular, nanostructured fluids (NSFs) are gaining recognition as an innovative and environmentally friendly solutions for cleaning artworks in CH conservation [2]. This study explores the use of oxy-pentadeca(oxyethylene) dodecanoate (PD)-based surfactants in NSFs for the selective removal of polymeric coatings, such as Paraloid B72, from delicate surfaces [3]. We examine how variations in the surfactant's molecular structure, specifically the capping group length, influence cleaning efficiency and dewetting behavior. Using a combination of advanced characterization techniques, including infra-red spectroscopy (FTIR), and fluorescence correlation spectroscopy (FCS), confocal laser scanning microscopy (CLSM), and small angle X-ray scattering (SAXS), we demonstrate that surfactants with propyl and ethyl capping groups outperform those with methyl and isopropyl capping, resulting in superior micelle dispersion and cleaning efficacy, particularly when applied in gels, enhancing the removal process kinetics (Figure 1). The diffusion coefficient of PD-propyl in gel is increased compared to its value in solution, and higher than the PD-methyl one, explaining the better cleaning results obtained.

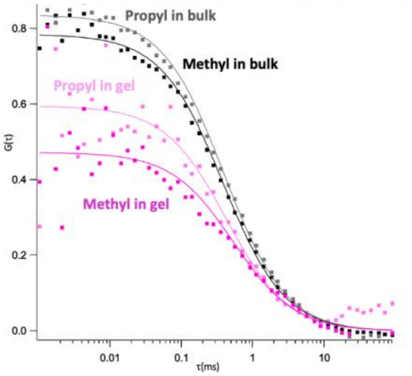

Figure 1. G(t) curves obtained by FCS, of the MEK-based NSF in bulk versus in gel, for PD-methyl and PD-propyl with their corresponding fittings.to obtain diffusion coefficient (D)

These surfactants facilitated the removal of polymer films from fresco-type substrates without damaging the underlying material. The findings reveal the critical role of surfactant design in enhancing the effectiveness of NSF-based cleaning systems, offering a sustainable and efficient approach to art conservation. Beyond cultural heritage, these surfactant systems have potential applications in various industries, including detergency and cosmetics. This research sets the foundation for developing safer, more efficient cleaning agents for both art conservation and broader industrial use (detergency, drug delivery, cosmetics, etc.).

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OC82

GREEN SOLVENTS FOR NANOCRYSTALS SYNTHESIS: A STEP TOWARD ENVIRONMENTAL SUSTAINABILITY

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Nanocrystal-based technologies are becoming increasingly essential for developing high-performance devices [1]. As a result, substantial research efforts have been dedicated to enhancing the performance of these materials while considering their environmental impact. Typically, these efforts focus on replacing toxic materials in final products, such as developing double perovskites to address the issue of lead contamination [2]. However, the production of nanocrystals, particularly through colloidal synthesis, often relies on petroleum-derived solvents [3].

In our work, we exploited hot-injection methods to obtain perovskite nanocrystals with different morphology and stoichiometry by the substitution of the classical solvent, i.e. 1-octadecene (ODE), with more environmentally friendly molecules. Exploiting the caesium lead halide perovskite nanocubes ($CsPbX_3$ NCs, X = Cl, Br, I) as reference material we studied the use of limonene as alternative *green* solvent (Figure 1a). The results showed that the NCs retained their optical and morphological properties; moreover, the solvent can be recovered from the reaction waste and re-used for new synthesis. Life Cycle Assessment (LCA) on the entire process demonstrated a lower CO_2 footprint from reaction employed limonene instead of ODE. Additionally, we demonstrated the possibility to expand the synthesis to other morphology, such as caesium lead bromide perovskite nanoplatelets (Figure 1b). Finally, we tested also the green solvent α- and β-pinene, not only for the synthesis of lead-based materials but also for the lead-free double-perovskites nanocrystals, confirming the potentiality to achieve a *green* synthesis for environmentally friendly material (Figure 1c).

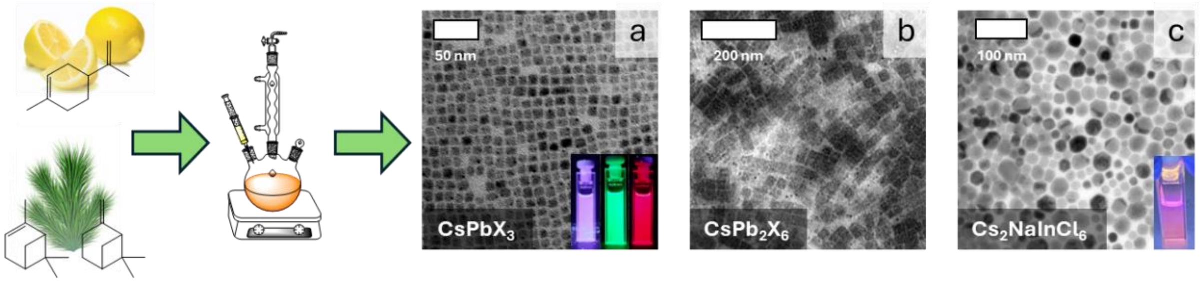

Figure 1. Limonene or pinene (alfa or beta) are employed as solvent into hot-injection method to synthetize (a) $CsPbX_3$ (X = Cl, Br, I) nanocubes, (b) $CsPb_2X_6$ nanoplatelets and (c) $Cs_2NaInCl_6$ nanoparticles.

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OC78

THE INVESTIGATION OF THE HEAT OF LIQUID INTRUSION/EXTRUSION INTO/FROM HYDROPHOBIC POROUS MATERIALS BY HIGH PRESSURE CALORIMETRY

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The heat evolved from the process of driving liquid water into and out of a porous hydrophobic matrix is a fascinating process. To measure this heat required elaborate differential scanning calorimetric equipment which controls the rate of pressurization. The associated components are also necessary to resist pressure beyond the pressure limit in order to create a stable calorimetric baseline. This talk will present the scanning transitiometry technique which is used to determine the liquid heat of water intruding into and from ZIF-8 [1]. As part of this presentation the experimental technique and the challenges around the experimental design will be presented with experimental data demonstrating that the intrusion process is exothermic and extrusion process is endothermic at 25°C. As well we show that using this technique the heat of intrusion can be manipulated by change the parameters of temperatures, aqueous environment [2,3] and crystal size [4] can be adjusted to not only effect the magnitude of the heat of intrusion value but also change the thermodynamic sign. Manipulation of these parameters provide the tools for designing thermal energy storage, energy recover or energy dissipation system which rely on mechanical work to operate [5].

Acknowledgements: This project leading to this application has received funding from the European Union’s Horizon 2020 research and innovation programme under Grant Agreement No. 101017858.

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OC79 QUATERNARY-AMINO FUNCTIONALIZED SWELLABLE ORGANICALLY MODIFIED SILICA FOR THE REMOVAL OF METHYL ORANGE FROM WATER

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Organic dyes, prevalently found as textile industries effluents, pose significant environmental risks due to their carcinogenic and mutagenic properties. Among the different classes of dyes, those containing azo groups, such as methyl orange (MO), collect increasing concerns. Their contamination of freshwater necessitates effective remediation strategies to protect human health and aquatic ecosystems. In this respect, adsorption methods offer a promising solution for efficient and cost-effective dye removal [1]. Different solids can be used for adsorption purposes, including synthetic zeolites, clays, silicas, titania particles, nanocomposites, polymer resins, various biomass-based adsorbents, activated carbons and hybrid materials [2]. Swellable Organically Modified Silicas (SOMS) are hybrid materials obtained by sol-gel process using bis(trimethoxysilylethyl)benzene (BTEB) as the silica source [2]. SOMS are able to swell in organic solvents such as ethanol, acetonitrile, and acetone and this can improve adsorption capabilities. SOMS can also be functionalized with a positive quaternary amine silane (TMA), to impart a positive charge to the final material (referred to as QA-SOMS) [3-4]. SOMS and QA-SOMS with different TMA:BTEB ratios were prepared and characterized by a multi-technique approach to determine their composition (CHN elemental analysis), morphology (by SEM), structure (by XRD), texture (by N_2 physisorption), thermal properties (TGA), chemical structure (by FT-IR and ss-NMR) and surface charge (by zeta potential analysis). A schematic chemical structure of QA-SOMS obtained from ss-NMR spectra is reported in Figure 1. The MO adsorption performance of the samples was tested. It was observed that increasing the amount of quaternary amino groups in the QA-SOMS materials resulted in an increase in the amount of MO adsorbed. For the QA-SOMS with the highest TMA:BTEB ratio (QA-SOMS 2:1), rapid MO adsorption in large amounts up to 720 mg/g was observed (Figure 2).

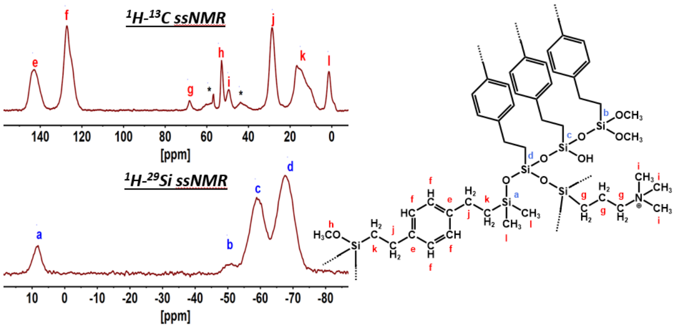

Figure 1. QA-SOMS schematic chemical structure obtained from ss-NMR.

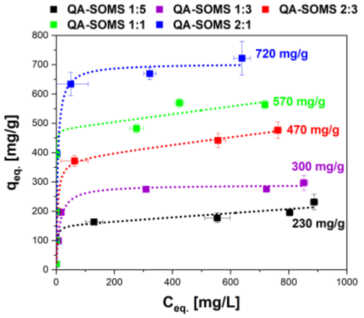

Figure 2. MO adsorption isotherms for QA-SOMS materials with varying TMA:BTEB ratios.

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OC114

INVESTIGATION OF THE MAGNETIC PROPERTIES OF IONIC LIQUID-BASED FERROFLUIDS

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Ionic liquids (ILs) have emerged as versatile solvents due to their tunable physicochemical properties, which make them ideal for applications in materials science and nanotechnology [1]. This study introduces a novel method for dispersing single-domain spinel ferrite magnetic nanoparticles (MNPs) directly into an ionic liquid, 3-ethyl-1-methylimidazolium acetate (EMIMAc), without water contamination. MNPs with different chemical compositions (γ-Fe_2O_3, $Co_{0.5}Zn_{0.5}Fe_2O_4$, and $CoFe_2O_4$) were synthesized via the polyol method, achieving uniform particle size (~5 nm) and tunable magnetic properties [2]. The particles were coated with dihydrocaffeic acid (DHCA) in tetrahydrofuran to ensure stability and compatibility with EMIMAc.

Direct (water-free) and indirect (water-involving) dispersion methods were compared, revealing that both approaches yield stable IL-based ferrofluids (IL-FFs) with minimal differences in aggregation or size distribution [3]. Magnetic characterization showed that dispersion in ILs modulates the interparticle interactions and magnetic anisotropy, with cobalt doping enhancing magnetic anisotropy due to strong Co^{2+} single-ion contributions. Additionally, the study highlights how the interplay between interparticle interactions and magnetic anisotropy impacts magnetization dynamics, offering insights into tailoring IL-FFs for advanced applications.

Acknowledgements: This study was funded by the European Commission PathFinder Open programme (grant No. 101046909, REMAP) and the European Union. The authors' views do not necessarily reflect those of the EU or EISMEA, which are not responsible for them. Additional support came from the "Network 4 Energy Sustainable Transition-NEST" project (code PE0000021) under MUR Decree No. 1561/2022.

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OC105 AN INNOVATIVE STRATEGY FOR RAPID SYNTHESIS OF ZnO@Au NANOSTRUCTURES AND THEIR APPLICATION IN PHOTOCATALYTIC PROCESSES

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Hybrid semiconductor/metal nanostructures have received significant attention due to their remarkable optical, electronic, and catalytic properties, which result from the combination of the unique features of both semiconductors and metals [1-3]. The integration of semiconductor photocatalysts with plasmonic metals is particularly effective in enhancing charge separation, thereby improving the overall catalytic efficiency [4]. However, challenges persist in their synthesis, stability, and scalability. In this work, we present an innovative and highly sustainable method for the rapid, one-step synthesis of piezoelectric zinc oxide (ZnO) nanostructures decorated with gold (Au) nanoparticles. Unlike conventional techniques that often require high energy inputs, prolonged reaction times, or complex processing steps, the proposed approach promotes the decoration of ZnO nanostructures with Au nanoparticles in just one minute. The process involves aqueous dispersions of piezoelectric ZnO nanostructures in the presence of Au^{3+} at three different concentrations, subjected to a standard ultrasonic bath for one minute. The successful formation of gold nanoparticles was confirmed by spectroscopic and morphological characterization (Fig.1) demonstrating that Au nanoparticle size and density can be precisely controlled by adjusting the concentration of Au ions and the ultrasound exposure time. The resulting hybrid materials were tested for H_2O_2 photocatalytic production in ultrapure water solution under solar simulator irradiation. The results revealed a specific trend in photocatalytic efficiency and mechanism selectivity, consistent with morphological and structural analyses, highlighting the potential of this novel approach for efficient photocatalytic applications.

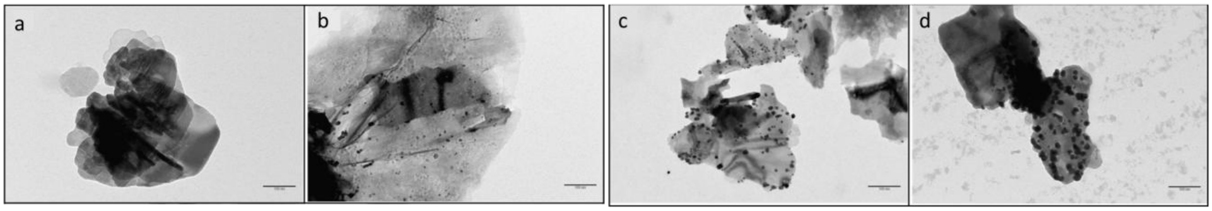

Figure 1. TEM images acquired for ZnO pristine (a) and ZnO with increasing concentration of Au nanoparticles (b-d)

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OC10

SYNTHESIS AND CHARACTERIZATION OF LIGNIN DERIVATE POROUS MATERIALS FROM BAMBOO CULMS (*Phyllostacys edulis*) FOR REMOVAL OF AROMATIC POLLUTANTS

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The use of plant biomasses for the production of new types of materials has been increasingly studied in recent decades. One of the most extensively studied plant biomasses is bamboo. The strong interest in this grass is mostly linked to its high growth rate, low water consumption during the growth phase and high absorption rate of CO_2 from the air and pollutants from the soil (heavy metals and organic pollutants). The chemical composition of bamboo makes it even more interesting from an engineering point of view. The composition of bamboo culms can be summarized as: cellulose and hemicellulose 65-70% and lignin 18-30%. Lignin is one of the most abundant biopolymers on earth. It is synthesized by plants from three different monomers: coniferyl alcohol, sinapyl alcohol and p-coumaryl alcohol. These three monomers react by a controlled radical reaction to form a three-dimensional network that is intended to give mechanical resistance to the plant. In addition, lignin, due to its random structure, helps plants to protect themselves from bacterial and fungal attacks by inhibiting tissue degradation. In this study, lignin was extracted from bamboo culms using hydrothermal extraction under basic conditions, and it was freeze-dried after extraction. The solid was then dispersed in a porogenic organic solvent and polymerized. The biopolymer was characterized by FTIR in order to study the superficial functionality and interaction between aromatic molecules probe as toluene. N_2 physisorption analysis at 77K was employed to better understand the surface properties. Moreover, the adsorption kinetics of organic pollutants (using Crystal Violet dye as a molecular probe) and UV-VIS spectroscopy were employed to assess the capacity of the material to act as an adsorbent for pollutants. In this instance, the adsorption capacity of Crystal Violet was determined to be over 98% within the initial four hours, as reported in Figure 1.

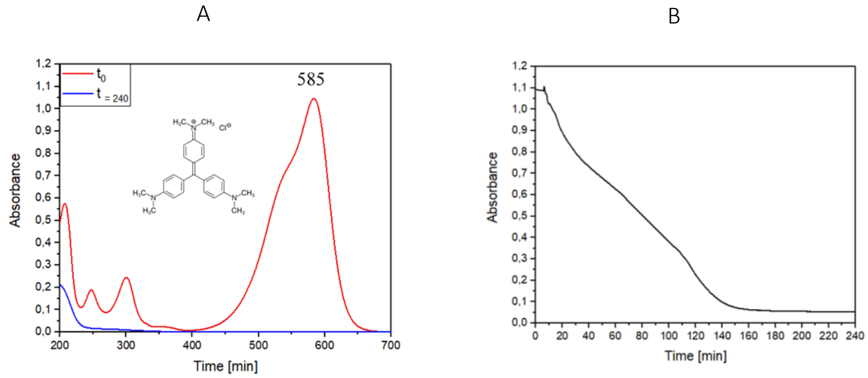

Figure 1: UV-Vis spectra of Crystal violet before and after adsorption process (panel A); Absorbance decreasing of Crystal violet solution during the adsorption process (panel B).

OC86

UNRAVELING MOLECULAR STRUCTURES AND DYNAMICS: THE ROLE OF ROTATIONAL SPECTROSCOPY AND QUANTUM SIMULATIONS

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Rotational spectroscopy is a powerful technique for determining molecular structures in the gas phase. It enables differentiation between conformers, isotopologues, excited states, and various degrees of solvation. However, this information is not directly available, and the support of quantum mechanical simulations is essential to guide the interpretation. The interplay between experimental and computational data is usually straightforward but can also be challenging. The difficulties arise from the internal dynamics and can be broadly categorized into three main areas: conformational complexity, large amplitude motions, and weak interactions. Recent studies involving small organic molecules such as nitroso compounds [1-4], substituted acetophenones (see Figure 1) [5-8], and di-tert-butylphenols [9-12] will be reviewed, highlighting the observed complex spectral features and the main issues in the interpretation of the data.

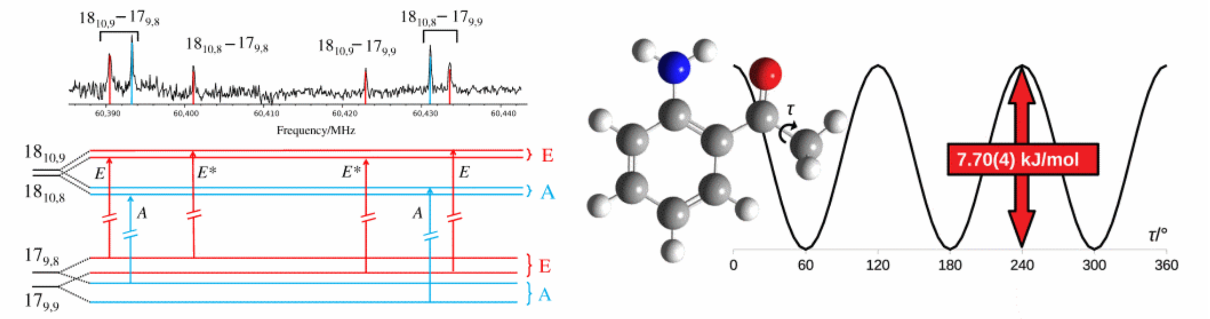

Figure 1. The structure of 2-hydroxyacetophenone is determined by a strong internal hydrogen bond between the substituents. The methyl internal rotation barrier is modeled based on the hyperfine structure observed in the spectrum.

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OC80

EXPLORING PEPTIDE-BASED STRATEGIES FOR TARGETING G-QUADRUPLEX DNA: A PHYSICOCHEMICAL STUDY

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Protein-DNA interactions are fundamental to essential cellular processes such as transcription and replication. Beyond binding to double-stranded DNA, proteins also recognize noncanonical DNA secondary structures like G-quadruplexes (G4s) [1]. G4s are polymorphic structures formed within guanine (G)-rich sequences and are characterized by at least two G-tetrads, i.e. cyclic planar arrays of four guanines [2].

In this context, we explored whether it is possible to exploit the DNA recognition motifs of G4-binding proteins to design peptides that selectively target these structures. Indeed, many G4-binding proteins contain an arginine- and glycine-rich motif known as the RGG or RG-rich motif, which plays a critical role in the recognition of such noncanonical structures [3]. However, the molecular details of these interactions remain poorly understood.

Aiming to develop peptide-based molecules capable of targeting G4s, we focused our attention on two peptides: one containing an RGG motif found in numerous human G4-binding proteins (NIQI) [4], and another derived from the DNA-binding domain of the yeast protein Rap1 (Myb$^{397\text{-}415}$) [5,6]. Their interactions with biologically relevant DNA G4 structures of different topologies (parallel, antiparallel, or hybrid) were investigated using a combination of physicochemical techniques, including circular dichroism spectroscopy, microscale thermophoresis, and isothermal titration calorimetry (ITC). Both peptides demonstrated selective binding and stabilization of specific G4s. ITC experiments provided thermodynamic insights into these interactions, while point mutagenesis helped identify key amino acids involved in G4s recognition. Our findings pave the way for developing a novel class of peptide-based G4 ligands, offering a promising alternative to small molecule G4 binders.

Acknowledgements: The research leading to these results has received funding from the Italian Association for Cancer Research (IG 24590 to B.P.).

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OC47

TWIN-CHAIN NETWORKS: GELATION KINETICS, MORPHOLOGY AND CLEANING ABILITIES

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Polyvinyl alcohol (PVA) cryogels are transversal materials, featuring key applications in many scientific and technological fields. We recently pioneered a new class of PVA-based cryogels, where the spontaneous micro-phase separation of PVA pairs in aqueous solution is harnessed to achieve a sponge-like, interconnected porosity at the micro- and nanoscale. The so-obtained “Twin-Chain” (TC) networks feature a boosted cleaning ability for the restoration of iconic artworks.[1]
The cryogelation kinetics relies on several key-parameters: while polymer concentration and temperature affect the size and number of PVA crystallites forming during freezing [2] (the gel physical “crosslinks”), the gelation mechanism changes when phase-separation phenomena are involved [3]. In this contribution the gelation kinetics of different TC pre-gel solutions, obtained by dissolving PVA pairs of different molecular weight and hydrolysis degree, will be unraveled, for the first time, through Small Angle Neutron Scattering (SANS). PVA solutions were subjected to low temperatures (0 and -10°C), and the scattering signal was acquired at regular time intervals until equilibrium. Figure 1 A shows the gelation kinetics of an illustrative sample. The effects of water-polymer phase-separation (i.e. the main process driving gelation) and PVA-PVA phase-separation on cryostructuration were explored, while polymer-solvent interactions were considered to explain the drastic changes in gels morphology (observed through Confocal Laser Scanning Microscopy, CLSM, imaging) as polymers-D_2O or polymers-H_2O systems are compared (Figure 1 B, C respectively).
The TC gels with modulated porosity were tested for their adhesive properties and cleaning ability on model surfaces (i.e. glass) and painting mockups. Their performances were interpreted in light of the gels surface roughness and pores interconnectivity/tortuosity.

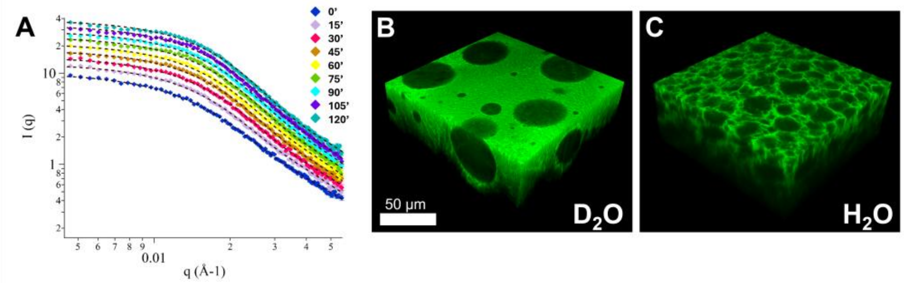

Figure 1. A) Gelation kinetics (SANS) of a D_2O solution containing two PVAs with different molecular weight and hydrolysis degree (curves were shifted along the y-axis for clarity); B) 3D CLSM image of the gel obtained from the same system in heavy water; C) 3D CLSM image of the gel obtained from the same system in water.

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OC72

MULTICOMPONENT LUMINESCENT/PLASMONIC MESOPOROUS SILICA NANOARCHITECTURES FOR TARGETED CHEMO-PHOTOTHERMAL TREATMENT OF COLORECTAL CANCER

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Multifunctional theranostic nanosystems represent a groundbreaking advancement in nanomedicine by combining both diagnostic and therapeutic capabilities in a single structure. Plasmonic $Cu_{2-x}S$ nanocrystals (NCs), with tunable localized surface plasmon resonance (LSPR) in the NIR region, are considered promising agents in cancer photothermal therapy (PTT). Hyperthermia-based therapies are often combined with chemotherapy, which becomes more effective when applied after hyperthermal treatments. Functionalizing plasmonic NPs with mesoporous structures enables synergistic drug delivery and PTT [1]. Mesoporous silica nanoparticles (MSNs) are attractive due to their high surface area, pore volume, biocompatibility, high loading capability, and ease of functionalization. Here, multifunctional core@shell nanostructures (MSN@MSN CR) were designed for colorectal cancer (CRC) targeted chemo-photothermal therapy. These structures feature a mesoporous silica core embedding $Cu_{2-x}S$ nanocrystals and a dahlia-like mesoporous silica shell loaded with paclitaxel. Additionally, a Ruthenium (Ru)-based luminescent complex was incorporated into the core for *in vitro* optical tracking. The luminescent/plasmonic $Cu_{2-x}S$_Ru@MSN@MSN CR were synthesized using a biphasic soft-templating approach and were surface modified with pH-sensitive polyacrylic acid and anti-PDGFRβ antibody for tumor targeting. A thorough morphological, optical, and photothermal analysis, along with drug loading and pH-dependent release assays, was conducted. $Cu_{2-x}S$_Ru@MSN@MSN CR exhibited an average size of 70 nm (σ% = 4%), high colloidal stability in aqueous media, large pores, 50% drug loading, and efficient pH-responsive behaviour. *In vitro* studies on normal colon epithelial (HCEC-1CT), non-metastatic (CACO-2), and metastatic (SW620) colorectal cancer (CRC) cells evaluated cell viability, CRC targeting, and the therapeutic efficacy of silica-based nanoformulations in the dark and under NIR irradiation. Additional tests performed on pancreatic ductal adenocarcinoma (MIAPACA, PANC1) and gastric cancer (KATO III, N87) cell lines further reinforced the targeting promise. pH-responsive, PDGFR-β antibody-functionalized $Cu_{2-x}S$_Ru@MSN@MSN CR demonstrated their strong potential for targeted, synergistic chemo/phototherapy, offering a promising avenue for CRC treatment.

Acknowledgements: Work supported by Bilateral Project CNR-RFBR Russia Joint research project (2021-2024), TITAN- PON ARS01_00906, NHYLODEA - European Union - Next Generation EU, Mission 4 C 1, CUP H53D23007980001, "Handling of mesenchymal-like circulating pancreatic cancer cells as an innovative approach to restrain disease progression" PNRR-MCNT2-2023-12377885- European Union - Next Generation EU, Mission 6 C 2, CUP F53C23001360008

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OC61

VALORISATION AND RECYCLING OF AGRI-FOOD WASTE: CIRCULAR ECONOMY IN AGRICULTURE

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The transition from a linear to a circular economy is a decisive step towards achieving the Sustainable Development Goals of the 2030 Agenda, adopted by the United Nations in 2015. To this end, it is necessary to act on the reduction of waste production and its optimal management, aiming at its reintegration into the production system. In this perspective, the management of waste produced within the agri-food chain plays a crucial role. Rethinking agri-food industry waste in terms of co-products can be a viable strategy to reduce environmental impact. For instance, agri-food waste can be exploited to extract bioactive compounds or used as adsorbent materials for the decontamination of wastewater.

In this work, waste from the initial phase of olive peeling used in modern olive mills, mainly consisting of olive tree (*Olea europaea* L.) leaves and small fragments of branches, was proposed and tested as an adsorbent material for the purification of water contaminated by Methylene Blue (MB), selected as model dye pollutant, even considering that olive production in the Apulia region (Italy) is one of the most important in the European Union and that the industry faces a pressing challenge on how to recycle and effectively manage the disposal of agricultural waste. This work is also in line with the need to find sustainable alternatives to the adsorbent materials classically used for wastewater decontamination, such as activated carbon or inorganic materials (zeolites, ion exchange resins). These materials, despite their effectiveness, pose a problem in terms of cost and sustainability due to their sourcing from non-renewable sources [2]. Here, the adsorption process of MB onto olive wastes was firstly studied from a physicochemical standpoint, in terms of kinetic and thermodynamic properties. Then, the environmental impact of the process was examined in terms of impact categories in the life cycle assessment (LCA). In fact, few studies have analyzed and quantified the environmental impact of new, non-commercial techniques for producing value-added products from waste materials. By filling this gap, our work contributes to a deeper understanding of the sustainability potential of these approaches. The main results showed that it is possible to carry out the process at neutral pH with removal efficiencies of over 90%, that this efficiency remains high even in simulated polluted matrices, and that it is possible to regenerate the adsorbent material by treatment with saline solutions. Finally, considering large-scale production, our material proved to be more environmentally friendly than activated carbon, which is regarded as the reference standard for adsorbent material.

Acknowledgements: This study was carried out within the project AGRITECH National Research Centre for Agricultural Technologies – Spoke 8 and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4 – D.D. 1032 17/06/2022, CN00000022). This abstract reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

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OC33

EFFECT OF TIN PRECURSOR LIGAND IN SnFe-N-C SINGLE-SITE CATALYSTS FOR OXYGEN REDUCTION REACTION

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Metal-doped nitrogen carbon materials have emerged as a suitable alternative to Pt-based catalysts. Of all, Fe, Cu, Co, Mn, and Ni are the most common ones, and Fe is recognized as the best choice to reach high activity and selectivity. Improvement of the activity is still needed. The addition of a second metal center has been more investigated in the last few years. First trials have been made using Mn, Co, Ni, and Cu showing to have an impact on site formation, final activity, or stability. Excluding d-block metal, the p-block (Sn, Sb, Bi) elements have been used for oxygen reduction in the last lustrum. More recently [1,2], Sn was used as a co-doping agent showing some improvement in activity, showing that Sn can regulate the charge distribution and control the intermediate adsorption energy [3]. Following our preliminary work, here several Sn precursors have been tested to prepare SnFe-N-C catalysts and to evaluate the influence on physical-chemical and electrochemical properties, in addition, ex-situ and in-situ XAS measurements have been performed. All materials show a good activity for ORR in acid media that well correlates with the nitrogen content and FeNx site density (Figure 1a). Different precursors fall into two categories, one forming only atomically dispersed Fe and Sn sites (STEM-EDX) of CL_2 in and the other forming a mixture of Fe and Sn single site together with Sn and $FeSn_2$ nanoparticles (STEM-EDX in Figure 1b). Interestingly, the presence of nanoparticles (addition of Sn precursor) does not hinder activity, therefore single site formation, as evidenced by XAS measurements. For the latter, a selection of spectra recorded (without Sn and $FeSn_2$ NPs) at Sn K-edge have been reported in Figures 1c,d.

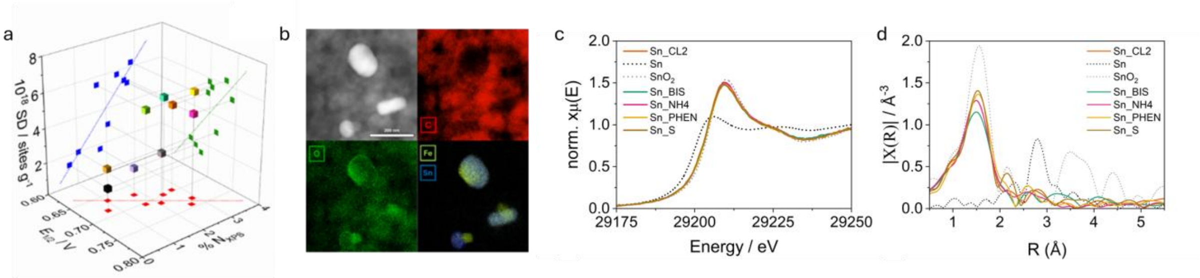

Figure 1. a) Correlation of activity, site density, and surface nitrogen content. b) STEM-EDX of two samples Cl_2 (no NPs) and TAR (Sn and $FeSn_2$ NPs) and c,d) selected XAS measurement on Sn K-edge for samples without NPs; c) XANES region and d) Fourier transform of EXAFS region.

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OC92

ADVANCING RO-VIBRATIONAL SPECTROSCOPY AND THERMOCHEMISTRY: NEW MODELS AND COMPUTATIONAL STRATEGIES

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The quest for a reliable yet practical modelling of large molecular systems has always played a central role in the field of theoretical and computational chemistry [1]. In this framework, despite the undisputed effectiveness of static structure-property correlations and the fundamental rigid rotor/harmonic-oscillator model, results that are directly comparable to experiment can only be achieved through a more advanced description either at the electronic or nuclear level. Among the various methods for the inclusion of anharmonic effects, vibrational second-order perturbation theory (VPT2) [2,3], allows for the effective study of medium-to-large sized molecular systems.

While VPT2 can be successfully applied in many cases, it is also characterized by some intrinsic drawbacks that prevent its use in some situations, in particular when large amplitude motions (LAMs) are present. Unfortunately, variational approaches such as the vibrational configuration interaction (VCI) [4] rapidly become prohibitive as the size of molecular systems increases. On the other hand, reduced-dimensionality methods tailored for describing one or a limited number of LAMs require an effective separation from the rest of the vibrations, usually referred to as small amplitude motions (SAMs). As shown in previous studies [5-8], defining a suitable set of internal coordinates capable to decoupling these two classes of vibration allows to treat each normal mode through the most appropriate method. Based on this premise, a general and effective VPT2 framework in terms of curvilinear coordinates was developed.

In this contribution, the versatility of internal coordinates and their application in the fields of rotational and vibrational spectroscopy will be described, starting with the calculation of transition energies [9], and proceeding to thermochemistry and vibro-rotational interaction parameters. The performance of the new engine will be illustrated through its application to systems of biological and technological interest.

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OC99 PLASMONIC NANOSTRUCTURES FOR NANOSCALE LASING: SPASERS AND RANDOM LASERS

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Metallic nanoparticles and nanostructures exhibit unique optical properties that enable a range of phenomena, including Surface-Enhanced Raman Scattering [1] (SERS) and Surface-Enhanced Fluorescence [2] (SEF). Recently, they have also found application in laser science, leading to novel plasmonic lasing architectures, primarily spasers and random lasers.

A spaser [3] (*Surface Plasmon Amplification by Stimulated Emission of Radiation,* Figure 1a) is based on a single metallic nanoparticle resonator embedded in an optically active medium, typically in the geometry of a metallic-dielectric coreshell nanoparticle. By replacing photons with surface plasmons and traditional resonant cavities with nanoscale plasmonic structures, spasers overcome the diffraction limit, enabling ultra-compact, nanoscale laser sources.

Conversely, random lasers [4] (Figure 1b) rely on scattering of light within an ensemble of randomly distributed metallic nanoparticles in an optically active medium. Plasmonic nanostructures enhance this process due to their significantly larger scattering cross sections compared to similar sized dieletric nanoparticles, improving feedback for lasing.

Despite their distinct mechanisms, spasing and random lasing can coexist, making it challenging to disentangle their respective contributions to the observed lasing signals.

Optimizing these systems requires careful selection of plasmonic nanostructures, precise tuning of plasmonic resonance bands, and controlled variation of the gain medium composition and concentration. A comprehensive investigation of both the structural and optical properties of these hybrid systems is therefore essential to advance their functionality and performance.

By careful adjustments of these parameters, this work explores the interplay between spasers and random lasers, providing insights into their functioning and optimization.

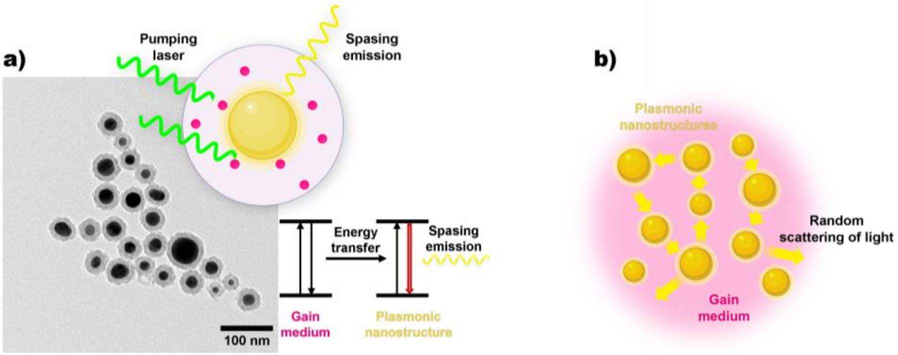

Figure 1. Spaser and plasmonic random laser schematic: (a) a spaser is based on an individual metallic nanoparticle with the optical feedback provided by the localized surface plasmon resonance; (b) a plasmonic random laser is based randomly dispersed plasmonic nanoparticles with the feedback provided by random scattering of light.

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OC118

PHOTOCATALYTIC-PHOTOTHERMAL EVAPORATORS: MECHANISMS BEHIND PROMOTED WATER PURIFICATION

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Solar-powered water evaporators are a low-cost, low-energy method to produce clean water by using solar energy to generate heat, enhance evaporation rates, and condense the vapor into purified water. Beyond emergency and remote applications, solar stills have shown economic potential for agricultural wastewater treatment. Interest in solar evaporators has grown since 2015 with the development of interfacial-heating solar-thermal desalinators [1]. These systems concentrate solar-thermal energy near the evaporation interface, keeping bulk water at lower temperatures to minimize heat loss and improve efficiency. These devices use photothermal absorbers with high solar energy absorption, mounted on porous hydrophilic supports that aid flotation and serve as thermal insulators [2]. These systems, however, suffer from biofouling and low rejection of volatile and semi-volatile contaminants [3], which compromise water quality. Recently, integrating photocatalysts has been proposed to address these challenges [4]. While studies show a reduction in volatile organic compounds in condensed water when photocatalysts are used, the underlying mechanisms remain unclear. This study investigates the competing mechanisms in photothermal evaporators coupled with photocatalysts. Using immobilized TiO_2 photocatalyst, we tested dyes and phenols as water contaminants, both separately and in mixtures. We conducted tests with photothermal evaporation alone and in combination with photocatalysis under different configurations (interfacial, submerged, and vapor-exposed photocatalysts), tracking reaction intermediates in both treated water and condensed phases. Our results reveal overlapping mechanisms, with their significance varying depending on the pollutant and operating conditions. For some organic pollutants, photothermal evaporation alone significantly reduces contamination in the collected condensed water, similarly to salt rejection. The inclusion of photocatalysts introduces additional pathways related to the partial photocatalytic breakdown of the target molecule. Our findings suggest that photocatalytic oxidation generates degradation intermediates that are less volatile, enhancing photothermal rejection. Finally, photocatalysis can also contribute to the decontamination of the VOC-rich vapours above the evaporator, a pathway that showed to be beneficial especially for mixtures of pollutants with different volatility. These findings can help improve the design of more efficient photothermal evaporators integrated with advanced oxidation processes.

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OC1

SOME MECHANISTIC INFERENCES RELEVANT TO CARBON MINERALIZATION, BY MECHANICAL TREATMENT, OVER STEEL SLAGS POWDERS

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Within the framework of CCUS, Carbon Capture Utilization and Storage strategies, wide attention is addressed to carbon mineralization processes, as a viable route to control and reduce the CO_2 emission in atmosphere. Recent literature reviewed the different classes of investigated materials, their reactivity, technological challenges, industrial application perspectives etc., highlighting the still needed deepening in basic science and applicative properties, to approach large-scale potential application [1-3]. To this regard, carbonation of industrial wastes deserves large interest, in view of a circular economy scenario and materials recovery and valorization [4,5].

Along this line, the present contribution focuses on the carbon mineralization properties by Electric Arc Furnace steel slags powders: the process, formally occurring at room temperature and atmospheric pressure, was induced by mechanical treatment in a suitably realized mechanochemical reactor, fed by a continuous flow of a mixture of N_2, O_2, CO_2 in a moist atmosphere [6].

The investigation of gaseous reagents conversion, and solid phases structural evolution, surmised a multi-step reaction mechanism: irrespective of different experimental conditions adopted, high CO_2 conversion values were monitored, governed by fast reaction kinetics, which followed activation steps dependent on specific conditions. The slags powders, a mixture of Ca-silicate, Fe-based oxides and SiO_2, evolved into Ca-carbonate formation, while a critical role seemed to be played by Fe oxidation state in allowing, or less, the occurrence of CO_2 reduction. In this framework, an investigation of magnetic properties and ^{57}Fe Mössbauer spectroscopy has been performed to gain new insight into the nature of iron compounds.

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OC7

PET-HYDROLYZING ENZYME COMPLEXES: MOLECULAR-LEVEL MECHANISTIC INSIGHTS

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The PETase enzyme can efficiently depolymerize plastics such as poly(ethylene terephthalate) (PET) at moderate temperatures, and has even shown promising activity toward poly(ethylene-2,5-furan dicarboxylate) (PEF), suggesting a potential route for sustainable plastic recycling. Building on these findings, we performed a systematic investigation combining classical molecular dynamics (MD) and hybrid QM/MM metadynamics enhanced sampling simulations to deepen the mechanistic understanding of PETase's activity and substrate interactions. First, we compared the wild-type enzyme with engineered variants (DuraPETase, ThermoPETase, FastPETase, and HotPETase) by analyzing their structural dynamics and binding to a tetrameric PET chain (PET4) under two temperature conditions (300 K and 350 K). Our classical MD results [1] confirm that stable enzyme–substrate complexes are formed at room temperature, primarily through aromatic interactions involving residues W185, Y87, and H237 (the "catalytic triad"), with the so-called "W185 wobbling" indicating a flexible binding pocket allowing substrate recognition. In contrast, increased temperatures reduce binding affinity, except in HotPETase, thus pinpointing the role of thermostability in catalytic performance.

Extending these insights, our QM/MM metadynamics simulations [2] investigated the catalytic cycle by mapping the free energy profiles of the acylation and deacylation steps for both PET and PEF hydrolysis. Consistent with earlier experimental observations, our results reveal that acylation is the rate-limiting step for both substrates. However, PET undergoes a concerted acylation process with a single energy barrier, whereas PEF follows a two-step mechanism involving a metastable intermediate smaller barriers—a finding that explains its enhanced reactivity, as shown in Figure 1. These mechanistic details, validated across multiple levels-of-theory, provide a thermodynamic and kinetic framework that not only consolidates existing knowledge but also helps the rational design of optimized biocatalysts for plastic recycling.

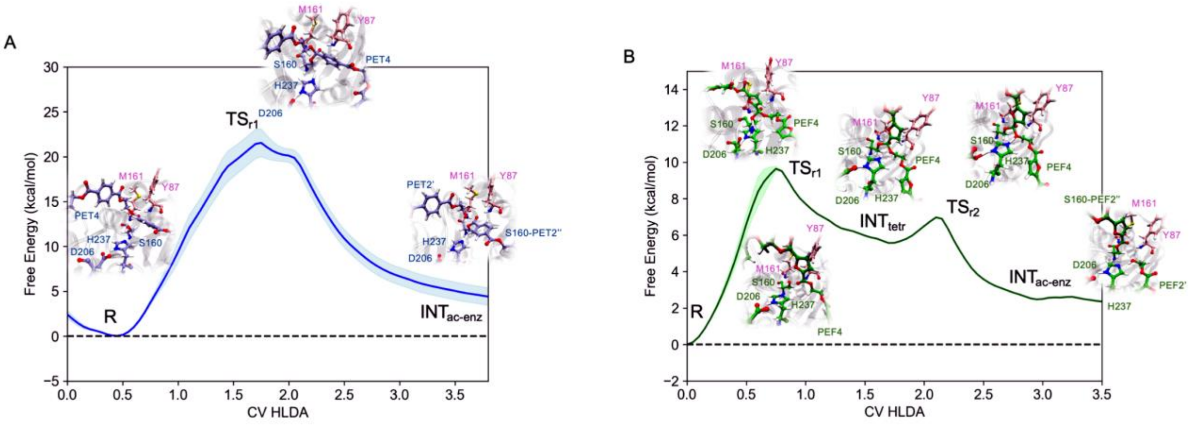

Figure 1. Free energy profiles of acylation calculated from well-tempered meta-dynamics simulations. The curves for (A) PET4 and (B) PEF4 acylation are calculated along the collective variable (CV) optimized via Harmonic Linear Discriminant Analysis (HLDA).

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OC64

FROM EXPRESS CATHODE SYNTHESES TO EFFICIENT RECYCLING: MICROWAVE-ASSISTED TREATMENTS FOR THE CLOSE LOOP SUPPLY CHAIN ON BATTERY INDUSTRY

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Microwave (MW) heating represents an innovative and energy-efficient technology that offers numerous advantages over conventional heating methods, thanks to its rapid heat transfer towards the sample. MW irradiation relies on the excitation of dipoles generating a rapid energy transfer, mainly from the core to the surface of materials.[1] To optimize heat transfer, materials called susceptors can be used, being capable of absorbing the electromagnetic energy from MW and efficiently converting it into heat. The use of susceptors further accelerates the heating process, reducing thermal loss from the surface of the sample, allowing for uniform heating. Key parameters to increase the efficiency of heat transfer are related to the nature of the material, such as its magnetic susceptibility, morphology, and particle size. Singling out the applications for electroactive materials, MW has been effectively employed to synthetize a broad number of materials, such as intermetallics, oxides, sulphides, etc.[2-4] The very short time needed for the syntheses not only are crucial for developing scalable protocols with reduced costs, but allows for the stabilization of kinetics products, not accessible with conventional heat treatment, thus widening the range of available electroactive materials.[4] On these bases, different transition metal oxides of Li, Na and K have been prepared via fast microwave irradiation and characterized by powder X-ray diffraction. Particular attention has been devoted to the comparison of the morphology and particle size distribution between materials prepared via conventional and MW routes, by means of high-resolution scanning electron microscopy. The electrochemical performance of the materials synthetized via MW irradiation has been assessed with various techniques, such as galvanostatic cycling, cyclic voltammetry and electrochemical impedance spectroscopy. Lastly, in a vision of circular economy for electrode raw materials, whose availability will be questioned in the next future,[6] MW irradiation has been also effectively employed to provide the thermal energy needed by thermolytic processes at the stage of metal separation, both on solid-state and in solution, for the treatment of spent cells. Preliminary results on the efficient treatment of spent $LiCoO_2$- and LiNMC-based electrodes will be showcased, demonstrating the versatility of the microwave-assisted treatments among the whole battery industry.

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OC14 PROBING HOST-GUEST INTERACTIONS IN POLYMERIC MEMBRANES BY SOLID-STATE NMR SPECTROSCOPY

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Solid State Nuclear Magnetic Resonance (SSNMR) spectroscopy has firmly established itself as a powerful technique for probing the structural and dynamic properties of polymeric and porous materials, as well as for revealing atomic-scale details of their interactions with guest molecules. These molecular features are closely linked to the functional properties of the materials, and gaining insight into them is crucial for optimizing the processes in which these materials are employed. A wide range of SSNMR experiments can be devised to probe various nuclear observables, such as isotropic chemical shifts, nuclear relaxation times and anisotropic line shapes, all of which are sensitive to the structure and dynamics of the host-guest systems under investigation [1,2,3].
In this contribution, SSNMR applications to polymeric membranes for CO_2 capture and storage and anion exchange membranes for water electrolysis will be presented, with a focus on host-guest interactions [4]. The results contribute to a deeper understanding of their functional properties and provide molecular-level insights that can support the rational design of next-generation materials with optimized performance.

Acknowledgments: PRIN PNRR 2022 "In MoTion-Influence of dynaMics on the adsorption and Transport properties in polymeric materials for membrane technologies" funded by the European Union - Next Generation EU is acknowledged for financial support.

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OC45

MULTISCALE QM/CLASSICAL APPROACHES FOR MOLECULAR SYSTEM IN SOLUTION: COUPLING THE GW APPROXIMATION WITH THE FLUCTUATING CHARGES FORCE FIELD

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Describing the interaction between a molecule and its surrounding environment is a fundamental challenge in quantum chemistry, as these interactions significantly influence electronic structure, energy levels, and response to external field. In this work, we develop a novel multiscale QM/classical approach that couples the GW approximation [1,2] with the Fluctuating Charges (FQ) and Fluctuating Charges and Dipoles (FQFμ) force fields [3]. This methodology allows for an accurate description of electron correlation effects, as captured by GW, while incorporating mutual polarization effects between the quantum system and its environment via FQ(Fμ). The new GW/FQ(Fμ) method is validated through the calculation of ionization potentials (IP) for solvated molecular systems, including nucleobases, and the Green Fluorescent Protein (GFP) chromophore. This work [4] provides a framework for extending GW-based multiscale methods to the calculation of excitonic states via the Bethe-Salpeter equation (BSE) within an atomistic embedding scheme.

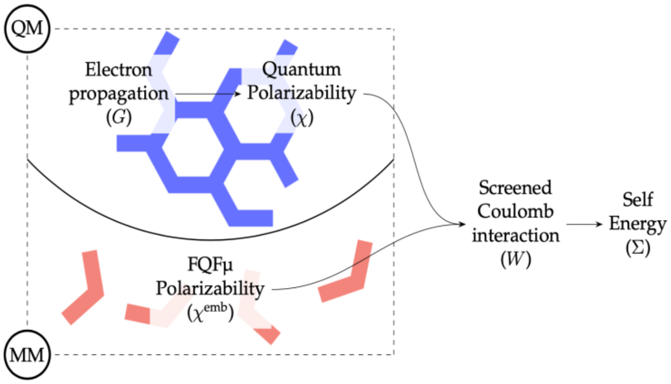

Figure 1. The system is composed of two moieties: the red moiety is treated classically (FQFμ force field), while the blue moiety is treated using the GW approximation. Each component provides a distinct contribution to the GW observables. The combination of all these quantities is necessary to evaluate the total self-energy.

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OC122

HARNESSING BIOACTIVE PEPTIDES TO MODULATE VIRAL BIOCONDENSATES

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Eukaryotic cells host functional membrane-bound organelles, but also some that are not delimited by a membrane. The latter are formed through a demixing of biomacromolecules, a process called liquid-liquid phase separation (LLPS) that leads to biocondensates (BCs) formation [1]. BCs are liquid-like structures used by the cell to control, in space and time, biochemical reactions fundamental to its life. Recently, it has been shown that BCs are also involved in the development and spread of diseases, defining the class of *condensatopathy*, like neurodegenerative diseases (Parkinson's), viral infections (SARS-CoV-2) and many types of cancer (Ewing sarcoma) [1,2]. Due to the emerging role of BCs in viral infection, they are attracting attention as targets for antiviral therapy. In this context, it has been shown that the SARS-CoV-2 nucleocapsid protein (N-P) undergoes liquid-liquid phase separation in the presence of RNA, resulting in BCs formation [3]. These structures are crucial for viral replication as they concentrate the viral RNA with the host cell 's protein machinery required for viral protein expression [3]. Thus, N-P BCs are promising targets to block or slow down viral RNA transcription and consequently virion assembly. Molecules that can act as N-P BCs modulators are antimicrobial peptides (AMPs), a class of bioactive pepiteds. AMPs are short peptides, usually cationic, active against several pathogens, including bacteria, viruses and even cancer cells [4]. They can act interacting directly with the membrane of pathogens and/or they can translocate across it reaching the intracellular space, interacting with intracellular components, like proteins and nucleic acids. In this work, we investigated the capability of three antimicrobial peptides to interfere with N-P/RNA condensates. Using microscopy techniques, supported by biophysical characterization, it was found that the AMP LL–III partitions into the droplets, leading to their clustering. Instead, the AMP *Cr*ACP1 partitions into the droplets without affecting their morphology but reducing their dynamics. Conversely, GKY20 leads to the formation of fibrillar structures after partitioning. It can be expected that such morphological transformation severely impairs the normal functionality of the N-P droplets and thus virion assembly [5]. These results could pave the way for the development of a new class of peptide-based antiviral agents targeting biocondensates, extending the applicability of this class of bioactive peptides to areas where they are not normally considered.

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OC113

SCHREIBERSITE CORROSION: A RESERVOIR OF PREBIOTIC LIVING PHOSPHORUS

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Phosphorus is an element of primary importance for all living creatures, being present in many biological activities in the form of phosphate (PO_4^{3-}). However, there are still open questions about the origin of this specific element and about the transformation which allowed it to be incorporated into biological systems. The most probable source of prebiotic phosphorus is the intense meteoritic bombardment during the Archean era, few million years after the solar system formation, which brought tons of iron-phosphide materials (schreibersite) on the early Earth crust [1]. It was recently demonstrated that by simple wetting/corrosion processes from this material various oxygenated phosphorus compounds are produced [2]. In the present work, the wetting process of schreibersite (Fe_2NiP) was studied by computer simulations using density functional theory, with the PBE functional supplemented with dispersive interactions through a posteriori empirical correction (D*0) [3,4]. Therefore, the two stable (110) and (001) Fe_2NiP surfaces were used simulating different water coverages, from which structures, water binding energies and vibrational spectra have been predicted. The computed (ana-)harmonic infrared spectra have been compared with the experimental ones, thus confirming the validity of the adopted methodology and models (see Figure 1) [5,6]. Moreover, water reactivity was inspected in several possible deprotonation reactions, also increasing the number of water molecules to lead to the formation of phosphonic and phosphoric acids and their corresponding deprotonated forms [7,8]. As a further step to the complexity of biological systems, the phosphorylation of organic matter was also considered, using methanol as a simple model system of the more complex sugars (such as ribose) [9].

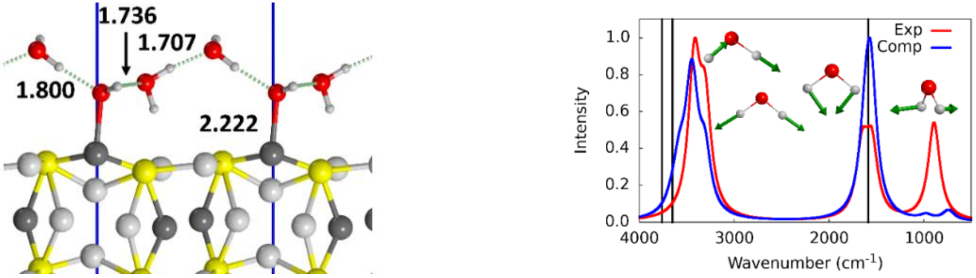

*Figure 1. PBE-D*0 optimized geometry of water monolayer on the (110) Fe_2NiP surface (left) and simulated vs experimental IR spectrum (at 125 K). Atom color legend: H in white, O in red, P in yellow, Fe in light grey, Ni in dark grey.*

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OC16

BIOHYBRID EGOTS: HARNESSING MICROALGAE FOR LIGHT-INDUCED CURRENT MODULATION

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Life on Earth is sustained by solar energy, harvested and converted into chemical energy through the photosynthetic activity of diverse organisms. Photo-bioelectrochemical devices harness these photosynthetic microorganisms to capture solar energy and generate electrical current by exploiting extracellular electron transfer (EET) mechanisms [1,2]. Devices capable of transducing and amplifying biological and chemical activity into electrical signals are highly desirable in fields such as sensing, neuromorphic computing, cellular computing, and self-powered electronics. In this context, electrolyte-gated organic transistors (EGOTs) have emerged as interesting candidates due to their ability to operate with aqueous electrolytes, biocompatibility, and low operating voltages [3].

This work explores the integration of photosynthetic microalgae with EGOTs to exploit their EET capabilities for light-driven modulation of the device. The EGOT features a biohybrid gate electrode, where indium tin oxide (ITO) is functionalized with living microalgae (Figure 1). Upon illumination, the photosynthetic activity of the microalgae induces faradaic reactions at the ITO interface via EET, transferring electrons from the biological system to the gate electrode. This electron flow at the gate electrode modulates the current in the EGOT channel, by altering the charge carrier density in the semiconductor, thereby regulating the source-drain current. The results demonstrate the potential of biohybrid interfaces in organic electronics and pave the way for the development of light-responsive bioelectronic devices.

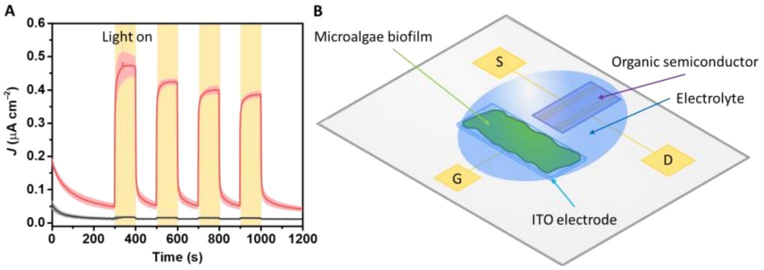

Figure 1. Current density measured at the ITO-biofilm hybrid electrode (red) in presence and absence of white light, compared to the bare ITO electrode (black) (A); scheme of the biohybrid EGOT device used in this study (B).

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OC81

PHYSICOCHEMICAL ANALYSES OF METAL-BASED DEEP EUTECTIC SOLVENTS

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Deep Eutectic Solvents (DESs) are mixtures of two or more compounds that exhibit a melting point lower than the one that they would have if the mixture behaved ideally (according to Raoult's law) in the liquid phase [1]. DESs show great potential in academic and industrial fields, and they have been proposed as an alternative to conventional solvents and/or ionic liquids for gas trapping, metal electroplating, organic and polymer synthesis, and material preparation. Among the others, an interesting application is their use for the extraction of high-added-value components from waste biomasses. [2]

This work aims to compare the physicochemical and thermogravimetric properties of type-II metal-based DESs (Figure 1), highlighting the influence of the metal on the system properties. A comparative study on the samples' thermal stability and the identification of thermal degradation products performed by thermogravimetry coupled with FTIR analysis of evolved gases will be presented. Moreover, the influence of water content and metal type on the system density, conductivity, and viscosity was evaluated. DESs' application for collagen extraction from tanned leather wastes will be described.

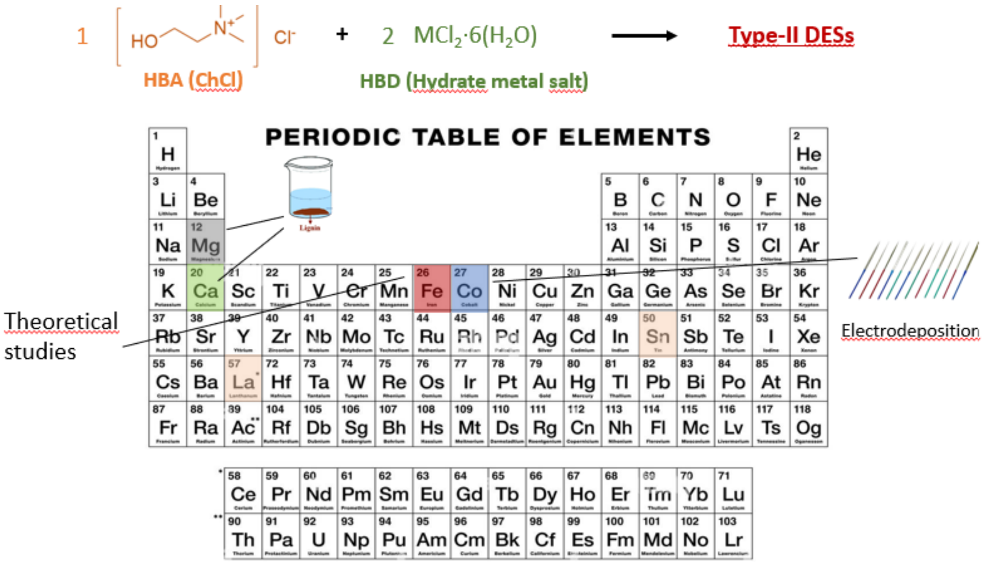

Figure 1. Type II DESs analyzed and compared.

Acknowledgements: This work is part of the MUR project PRIN 2022 PNRR ArtDECOW (project code P2022HWL7L). The project is financed by European Union-Next Generation EU, Mission 2, Component1(M2C1) CUPB53D23025330001.

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OC48

ETHANOL AND ETHYLAMINE ADSORPTION ON INTERSTELLAR ICE: A THEORETICAL AND EXPERIMENTAL APPROACH

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Experimental and computational chemistry are two essential tools in astrochemistry, providing crucial reference data for astronomical observations and modeling. These approaches not only complement each other but also help overcome their respective limitations. A key parameter in adsorption and desorption processes is the binding energy (BE), which quantifies the strength of interaction between a molecule and a surface. [1] BE also governs diffusion, as diffusion barriers are typically considered a fraction of this energy. [2-5]

Both a theoretical and an experimental approach were applied to characterize the BEs of ethanol (CH_3CH_2OH) and ethylamine ($CH_3CH_2NH_2$), two interstellar complex organic molecules (iCOMs), on both crystalline and amorphous water ices. The adsorption behavior was examined using density functional theory (DFT) calculations and temperature-programmed desorption (TPD) experiments. Experimentally, both molecules exhibit higher desorption temperatures on water ice than on a bare gold surface. The cohesive energies of pure ethanol and ethylamine bulk structures, computed through DFT, align well with the experimental BEs of these species deposited on gold, as inferred from TPD analyses.

For submonolayer coverages on water ice, direct BE extraction from TPD is not feasible due to co-desorption with water. However, DFT calculations reveal that their BEs exceed the cohesive energy of water. Interestingly, when multilayers of CH_3CH_2OH and $CH_3CH_2NH_2$ are deposited on amorphous ice, ethylamine exhibits weaker intermolecular interactions compared to ethanol and water, consistent with its computed cohesive energy. [6]

Finally, the computed BEs suggest that the snow lines of ethanol, ethylamine, and water in protoplanetary disks will be located at different distances from the central star. This indicates that a portion of ethanol and ethylamine is already frozen onto dust grains within the water snow line, facilitating their incorporation into water-rich planetesimals. [7]

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OC29

POSITIONAL MATTERS: WHEN BROMINE IN *PARA* IS ALL THYMOL NEEDS

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Natural terpenoids, such as carvacrol and thymol, as well as their synthetic derivatives, including 4-bromothymol[1] and thymyl acetate, are widely investigated for their activity as antibacterial and antimycotic agents. Recently, we demonstrated that 4-bromothymol antimycotic activity resulted up to 6 times higher than that of thymol on 8 yeast strains, even in the case of acclaimed resistant species. Hence, we have recently clarified 4-bromothymol mechanism of action on a eukaryotic-like membrane, namely the 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC), exploiting thorough computational studies, sweeping from Quantum Mechanics (QM) to Molecular Dynamics (DM) in comparison with that of thymol, carvacrol and thymyl acetate. QM afforded the characterization of compounds reactivity and affinity towards a hydrophobic environment, investigating the partition coefficients (LogP). MD, with the Minimum Bias Approach (MBA), reaped the “real” pose of terpenoids into the simulated double layer of POPC. Resulted showed that bromine deeply inserted into the bilayer, “anchoring” the 4-bromothymol at the lipid/water interface. Furthermore, thymol and carvacrol alter the dipole of the lipid heads only in one of the two possible positions (POSE_1 and POSE_2, Fig. 1), whilst 4-bromthymol induces a shrinkage of the lipid head, independently from its pose. These results clarify the importance of bromine as substituents, explaining 4-bromothymol higher efficacy than thymol and carvacrol. Taking advantage from these findings, other brominated thymol analogues, such as 2-bromothymol and 2,4-dibromothymol, was evaluated in the presence of charged and neutral lipids, such the anionic palmitoyloleoylphosphatidylglycerol (POPG) and the 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine (POPE), mimicking the bacterial membranes. MBA investigations were performed to foresee interactions of these new compounds with the bacterial membranes, comparing their placement with that of thymol and carvacrol. Among the brominated analogues, only 2-bromothymol induces a huge disbalance in number of lipids per Area, suggesting an even stronger biological efficacy with respect to 4-bromothymol. However, only 4-bromothymol formed hydrogen bond with the lipid head. Thus, 2-bromothymol and 4-bromothymol activity was evaluated *in-vivo*. Experiments performed on bacterial strains, confirmed the stunning efficacy of 4-bromthymol, highlighting its potential application in several fields.

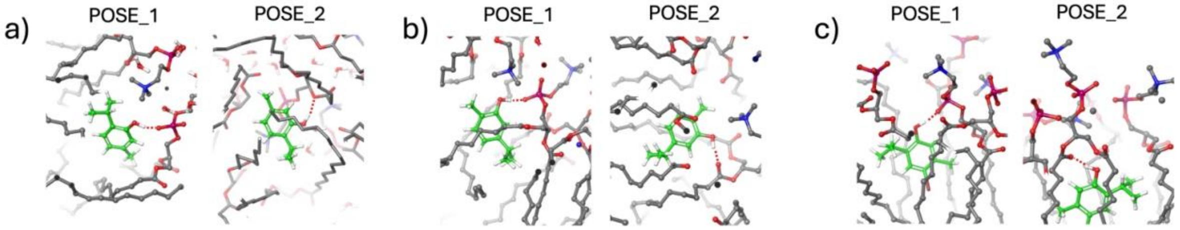

Figure 1. Thymol (a), carvacrol (b) and 4-bromothymol (c) poses into the double layer. POSE_1: H-bond between the -OH group of oxygens belonging to the phosphate group of POPC; POSE_2: H-bond between the phenolic -OH group and ester group of the palmitoyl chain. Dotted red line: hydrogen bond.

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OC91

ENHANCING THE THERMOELECTRIC PERFORMANCE OF Sb-BASED FILLED SKUTTERUDITES THROUGH FILLER MODIFICATIONS

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In recent years, the growing interest in thermoelectric materials, capable of directly converting heat into electricity and *vice versa*, has been driven by their potential applications in power generation, cooling technologies, and waste heat recovery [1]. Among these, Sb-based filled skutterudites have attracted significant attention due to their ability to host filler atoms within their crystal structure [2,3]. This feature enables in fact a substantial reduction in phonon thermal conductivity (κ_{ph}) through the rattling effect, which allows many skutterudites to achieve high values of the thermoelectric figure of merit ZT. This latter quantifies efficiency based on the electrical and thermal transport properties of the material: a higher ZT value indicates a better performance.

Filled skutterudites have the general formula $RE_yM_4X_{12}$ (where RE is a rare earth element, M is a transition metal, and X is a pnictogen) and crystallize in a body-centered cubic structure ($Im\bar{3}$ space group) with Sb_{12} icosahedral cages centred at the 2*a* (0,0,0) site. These oversized cavities are able to retain large ions, which effectively scatter phonons and enhance the thermoelectric performance by reducing κ_{ph}.

This study explores the relationship between crystal structure, filler content, and electronic properties in some filled skutterudite systems, with particular emphasis on the identification of the *p/n* crossover through X-ray diffraction. Additionally, the role of filler ions in modulating κ_{ph} is analyzed in terms of their concentration and chemical diversity, with the ultimate goal of optimizing the thermoelectric efficiency by fine-tuning the material composition.

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OC74

NANOSPECTROSCOPY AND CHEMICAL IMAGING OF APPLIED SELF-ASSEMBLED MONOLAYERS BY AFM-IR

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Chemically modified solid interfaces formed by self-assembled monolayers (SAMs) are applied in many fields ranging from medical diagnostics to catalysis and corrosion. These monolayers, especially when composed of mixed constituents, can form nanostructures spontaneously or can be induced to do so by targeted synthesis. We use nano-IR spectroscopy (AFM-IR) to study such nanostructured interfaces. With resolutions down to ~10 nm, this technique allows lateral topographical information to be combined with chemical information from IR absorption at the nanoscale. Recent examples of this research will be presented. One example is the fabrication of a recently developed aptasensor for the specific detection of the spike protein of SARS-CoV-2 [1, 2]. Phase separation into aptamer-rich and aptamer-deficient nanophases dominates this sensor surface and the chemical identity of the phases was assigned by AFM-IR (Figure 1). Furthermore, the analyte bound to the sensor was characterized at the single molecule level.

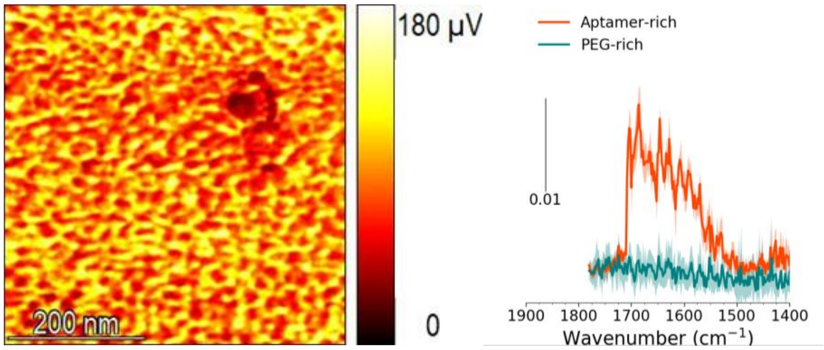

Figure 1. Left: IR imaging recorded at the v(C=O) of the DNA aptamer at 1680 cm^{-1} reveals nano-phase separation of aptasensor surface. Right: Nano-IR spectra of aptamer-rich and aptamer-deficient nano-phases.

Another example is the study of water adsorption on nanostructured polyethylene glycol (PEG) SAMs. Such monolayers are used as biofouling resistant surfaces, which has been hypothesised to be caused by the specific structure of water at this interface. It is shown that the properties of the adsorbed water depend on the conformational nanostructure of the nanodomains present in the studied system. Such studies shed light on the relationship between the lateral nanostructure and the functionality of nanostructured interfaces, providing important information for their improvement in applications.

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OC123

TOWARDS THE INCLUSION OF MOLECULAR DYNAMICS AND TRANSITION STATES SEARCH IN THE CRYSTAL CODE

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In the framework of Density Functional Theory (DFT), semilocal density functionals approximations can often be insufficient to achieve a good description of the electronic properties associated to the potential energy surface. This well-known problem can be partially mitigated by introducing hybrid density functionals, which incorporates a fraction of nonlocal exact exchange, but at the expense of a higher computational cost. Among the quantum-mechanical ab initio programs for the simulation of condensed matter systems, the CRYSTAL code has been heralded for its high efficiency in evaluating the exact exchange series, [1] thanks to the use of atom-centered basis functions within a linear combination of atomic orbitals to describe the crystalline wavefunction. The corresponding efficiency of the code has driven to the implementation of a rich variety of hybrid density functional approximations at a low computational cost, thus allowing to study electronic, magnetic, mechanical, spintronic and lattice-dynamical properties of materials using hybrid functionals.[1] In this work, the capabilities of the CRYSTAL code have been extended to include a computational package for the study of structural and electronic properties at a finite temperature, based on the Born-Oppenheimer ab initio molecular dynamics (AIMD) technique applied to the microcanonical and canonical ensembles, [2,3,4] as well as for the calculation and the characterization of transition states, using the Nudged Elastic Band (NEB) method. [5] Moreover, the possibility to perform structural optimizations based on AIMD concepts, using the Fast Inertial Relaxation Engine scheme,[6] has been introduced, [7] paving the way to the possibility of analyzing equilibrium crystalline structures at finite temperature. A brief description of the theoretical methodologies and of the algorithmic implementations, followed by a critical evaluation of the accuracy and parallel performance of this approach, will be given. Taking the periodic liquid water $(H_2O)_{32}$ and different phases of solid nitrogen as reference systems, the post-processing analysis of the AIMD trajectories leads to a detailed characterization of the structural and dynamical properties of these systems at different temperatures, which is capable of giving insights and shedding lights on their atomic-scale features, that have been debated for a long time in literature. [8,9]

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OC95 TIME-RESOLVED STUDY IN NITRO-DPP COMPOUNDS: THE ROLE OF ENVIRONMENTAL POLARITY AND STIFFNESS

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We investigated how structural rigidity and nitro group position influence the emission properties and excited-state dynamics of four diketopyrrolopyrrole (DPP)-based molecules: two rigid derivatives (K133 and K187) with a planar structure and two flexible ones (K132 and K186). The fluorescence properties of these molecules are controlled by shifting the nitro group on the DPP unit from the para to the ortho position. All molecules exhibit a quadrupolar charge distribution in both the ground and first excited state, showing poor solvatochromism. The excited-state dynamics of K132 and K186 are governed by an excited charge-transfer (CT) state. K132 is fluorescent in toluene but becomes non-emissive in polar solvents, where CT state stabilization promotes non-radiative decay. K186 is non-fluorescent in all solvents due to the rapid and efficient population of the CT state. The rigid molecules (K133 and K187) display a similar behavior, with fluorescence influenced by solvent polarity. However, no direct spectroscopic markers of the CT state were observed—only DFT calculations suggested its presence. A thermally activated CT state population was indicated by temperature-dependent fluorescence lifetime measurements in 2Me-THF. Conversely, the structural flexibility of K132 and K186 allowed the CT state to stabilize more effectively through interactions with the chemical environment. This enabled the direct observation of spectral markers: an excited-state absorption (ESA) that exhibits a progressive blue shift with increasing solvent polarity in the visible range, along with a growing excited-state absorption band in the mid-IR (observed with TRIR measurements). To assess solvent polarity and molecular rigidity effects, spectroscopic measurements were conducted in solvents of varying polarity and in solid-state matrices (PMMA and DPEPO). These experiments demonstrated that rigidity plays a minor role in excited-state relaxation: the CT state is populated in both matrices, with only a slight slowing of the ground-state recovery. Additionally, Br atoms attached to the DPP core in flexible molecules introduce a minor deactivation channel, leading to a long-lived triplet state. By combining experimental data with theoretical calculations, we developed a kinetic model describing the excited-state dynamics of these DPP derivatives. Global analysis of transient measurements provided kinetic constants and state lifetimes, offering a comprehensive understanding of their photophysical behavior. These findings illustrate how molecular rigidity and nitro group positioning influence excited-state relaxation pathways, providing valuable insights into the rational design of DPP-based materials with tailored optical properties for optoelectronic applications.

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OC73

α-CYCLODEXTRINS FOR THE FORMATION OF WATER-RESISTANT METAL ORGANIC FRAMEWORKS AS ADSORBENT TO REMOVE TEXTILE DYES FROM WATER

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Many substances could pollute water, and industrial, domestic, and agricultural effluents are reported to be the main contributors to this problem, discharging textile dyes, Contaminants of Emerging Concern, and heavy metals. [1] Among pollutants, textile azo dyes are worth mentioning. Indeed, these dyes are extensively employed in textiles, food production, and cosmetics, contaminating water to different extents, increasing the environmental risk regarding toxicological, mutagenic, and carcinogenic aspects. [2] Consequently, strategies for obtaining clean water have been developed over the years, and for this purpose, stable crosslinked Metal Organic Frameworks α-Cyclodextrin-based are presented during this work for environmental applications as high performant adsorbent. The chemical and physical features of the adsorbent were thus searched through the synergistic use of complementary techniques and unveiled after its use. If α-Cyclodextrin, and the corresponding Metal Organic Frameworks α-Cyclodextrin-based, assembled via K^+ ion coordination, occurred highly water soluble, on the other hand, the crosslinked structures occurred stable, with a Z-potential of -15 mV, and with a reduced crystalline order and thermal stability. The adsorbent used exhibited high performances in removing Direct Blue-78, selected as a model textile dye, alone, and even when in mixture with Direct Red 83:1 and Direct Yellow 86. The role of different parameters affecting the adsorption process, such as pH, ionic strength, and temperature was assessed, demonstrating the key role of electrostatic attraction between the pollutant and adsorbent. Specifically, the mechanism of adsorption was multiple, also involving hydrophobic interaction.

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OC4 A STUDY OF THE TRANSPORT PROPERTIES OF MMMS BASED ON TRIPTYCENE PIMS

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Membrane technology represents a growing field for gas separation applications [1]. Embedding fillers to the polymeric matrix is one of the most promising possibilities for developing membranes that overcome the well-known Robeson upper bound [2].

Dense mixed-matrix membranes based on glassy polymers such as 6FDA-DAM, PIM-1, and BTFMA-DPE were prepared by solution casting and solvent evaporation, including 20 wt% of highly microporous hyper crosslinked functionalized triptycene PIMs, namely Trip-Hydrocarbon, Trip-NO_2, Trip-NH_2 and Trip-SO_3H fillers, referred to the total solid content in the polymer solution.

Single-gas transport properties of the MMMs were studied in terms of permeability, diffusion, and solubility coefficients at 35°C and 1 bar by the so-called time-lag method. The effect of different fillers in the MMMs is evaluated regarding gas separation performance for the CO_2/N_2 and CO_2/CH_4 separations. The selected polymeric matrices combined with the highly porous fillers enhanced the gas selectivity for CO_2/CH_4, whereas a lower permeability was found for CO_2 in some cases, depending on the filler type. Adding the fillers in the lower free-volume polymeric matrix enhanced the permselective properties.

The correlation of the transport properties and the polymers with different amount of free volume is explained in terms of the change in slope of the plot of the diffusion coefficient as a function of the gas diameter, where a stronger size-selective trend for the larger gas molecules is observed than for the smaller He and H_2. Ageing studies confirmed that diffusivity is differentially influenced by larger gas molecules, thus further enhancing their size-selectivity.

Acknowledgements: This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101115488. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Innovation Council and SMEs Executive Agency (EISMEA). Neither the European Union nor the granting authority can be held responsible for them.

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OC111 SYSTEMS AND THEIR CONTROL – FROM PHOTOCHEMICALLY CONTROLLING IMINE EXCHANGE TO OFETS

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Systems of chemicals are as interesting as they are complicated. As more chemicals and processes are added to a system, justifying what happens to it over time gets more and more involved. In order to get around this, scientists often build up systems slowly, adding element by element. Here I will present work on one such system, a mixture of three imines which interconvert by imine reactions. This builds on literature work on systems of two imines.[1] We show and ability to control the composition photochemically and justify it. I will present evidence that energy transfer occurs in these systems leading to relatively wavelength independent perturbations. The system control is shown in Figure 1.

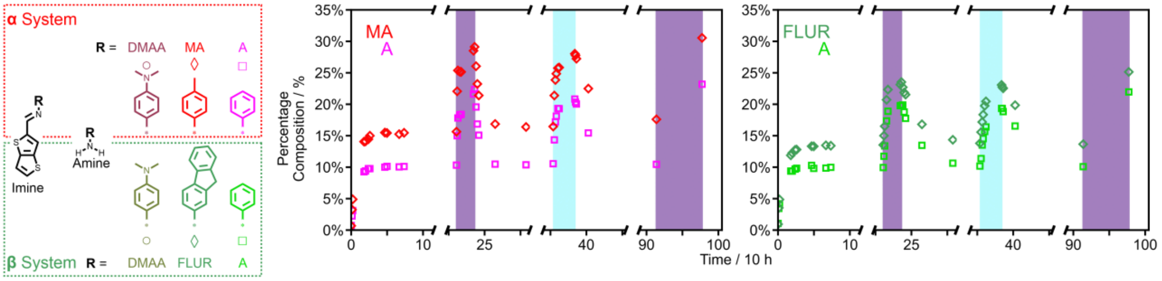

Figure 1: The compositional control of a system of imines, under 400 (purple) and 500 nm (blue) irradiation.

In addition, I will show our latest research towards applying system chemistry to organic field effect transistors (OFETs). OFETs are formed by forming films on top of a surface with electrodes either on it or electrodes applied after on top of the film. When films are formed they are often assumed to form amorphously. Some ordering has been reported dependent on deposition method and interaction strength at the solid-solid interface.[2,3] However, a semi-disordered mix of molecules can be thought of as being a frozen system of semi-randomly rotating molecules. We intend to explore previously published work on controlling these systems,[4] and apply the thought process of systems chemistry to them (figure 2). I will show our latest work towards this goal.

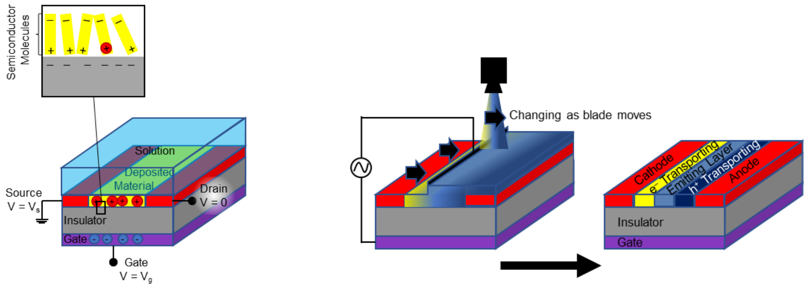

Figure 2: The proposed OFET systems to be studied.

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OC53

SYNTHESIS AND APPLICATION OF GIANT UNILAMELLAR VESICLES FOR CELLULAR MODELING AND ADVANCED MATERIALS

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We report the synthesis and versatile applications of Giant Unilamellar Vesicles (GUVs) in both cellular modeling and the engineering of advanced functional materials. GUVs, which closely mimic natural cell membranes, create compartmentalized microenvironments ideal for studying biological processes and enabling material synthesis. In cellular modeling, GUVs serve as simplified yet dynamic systems to investigate complex behaviors such as enzymatic reaction networks, signal transduction, and self-division, providing insights into the mechanisms of cellular communication and function. Importantly, the integration of photoswitchable amphiphilic molecules into GUV membranes permits reversible modulation of membrane properties in response to external stimuli such as light, advancing the development of stimulus-responsive biomimetic systems with applications in smart drug delivery and adaptive biointerfaces.

A key advancement in this platform is the encapsulation of magnetic nanoparticles (NPs) within GUVs, enabling precise spatial control and protection of functional nanomaterials within biologically relevant environments. This capability facilitates studies on nanoparticle–membrane interactions, targeted delivery strategies, and localized catalytic processes. Additionally, GUVs act as confined microreactors for the in situ synthesis of nanostructured materials, such as Metal-Organic Frameworks (MOFs) like Zeolitic Imidazolate Frameworks 8 (ZIF-8). Collectively, the multifaceted use of GUVs as biomimetic platforms highlights their potential in bridging synthetic biology with nanotechnology and materials science.

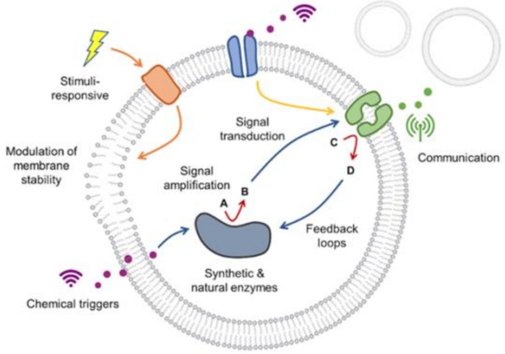

Figure 1. GUVs as tunable and smart synthetic environment.

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TIME-RESOLVED PHYSICO-CHEMICAL INVESTIGATION OF OUT-OF-EQUILIBRIUM INTERFACIAL ADSORPTION AT THE AIR/WATER INTERFACE

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The formation of colloidal nanoparticle monolayers at liquid interfaces has attracted significant research interest due to their potential for designing novel functional responsive materials. [1] The interface acts as a scaffold for nanoparticle self-assembly, where dimensional confinement and asymmetric environments enable the creation of nanostructured interfaces.[2] Moreover, as the adsorption is irreversible, interfacial NPs represent an easy and versatile model case of out-of-equilibrium system. While previous studies have demonstrated how surfactant-decorated NP monolayers can be tuned by controlling the NP/surfactant ratio in bulk [3,4], fundamental physicochemical insights still need to be elucidated. In particular, the role of surfactants and electrolytes in both adsorption kinetics and interfacial surface excess remains unclear. In this perspective, we developed a methodology to follow the NP adsorption at the air/water interface. This approach is based on Time-Resolved Grazing Incidence Small-Angle X-ray Scattering (TR-GISAXS), enabling real-time, high spatiotemporal resolution analysis of NP adsorption upon the addition of micromolar amounts of a cationic surfactant. Two distinct adsorption regimes were identified: an initial diffusion-controlled process followed by a kinetically limited phase. Additionally, fitting of the time-dependent NP surface excess curves enabled us to quantify, for the first time, the non-equilibrium surface excess and its dependence on the dispersion composition. These findings highlight the critical yet distinct roles of the cationic surfactant and ionic strength. Indeed, while the surfactant is essential to promote the adsorption of oppositely charged NPs, the salt concentration enables the modulation of long-range electrostatic interactions, which strongly influence both the adsorption kinetics and surface excess. Our experimental setup allowed us to investigate with unprecedented spatiotemporal resolution nanoscale interfacial phenomena, paving the way to a more quantitative description of out-of-equilibrium interfacial processes.

Acknowledgements: We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian MUR, funded by the European Union – NextGenerationEU – Project Title: Reconfigurable Low-Dimensional Nano-Structures at Liquid Interfaces - ReLoDS – CUP E53D23008600006 – Code 2022ZP453S- Grant Assignment Decree No. 958 adopted on 3.6.2023 by the Italian MUR.

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OC25

NOVEL LUMINESCENT MULTI-COMPONENT COMPOSITES INSPIRED BY ANCIENT PIGMENTS: A MODERN INNOVATION IN ANTI-COUNTERFEITING SYSTEMS

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Multimodal luminescent systems have the ability to emit distinct signals depending on the excitation used to illuminate them. The study here reported aimed to obtain luminescent multi-component composites that could emit in red and near-infrared range depending on the excitation used to illuminate them, possessing at least three levels of safety [1]. Various luminescent materials, having different natures and properties, mixed together, may work in synergy. Egyptian Blue (EB, $CaCuSi_4O_{10}$) and Han Blue (HB, $BaCuSi_4O_{10}$) have been chosen as blue pigments, able to convert efficiently red radiation into infrared one.

HB [2], also known as Chinese Blue, is an ancient material with a history that dates back to ancient China. Like its counterpart, Egyptian Blue (EB) [3], Han Blue has intriguing features and has been employed as a pigment in antiquity. The main constituent of Han Blue is a two-layered barium and copper silicate, $BaCuSi_4O_{10}$, which shares a structural similarity with $CaCuSi_4O_{10}$ found in EB, differing only in the presence of Ba^{2+} instead of Ca^{2+}. Han Blue shares with EB intriguing photoluminescent properties, particularly in the Near Infrared region (NIR) between 900 and 1000 nm.

Red phosphors such as $YPO4:Eu^{3+}$, $YAG:Eu^{3+}$ and $Y2O2S:Eu^{3+},Mg^{2+},Ti^{4+}$ have been added to the blue pigments and dispersed in an aqueous solution, by using two different polyvinyl alcohol (PVA) or arabic gum (AG) as medium, or into a silica matrix.

The composite preparation included systematic studies to prepare a stable colloidal system and to investigate the role of parameters such as concentration, pH and the presence of any additives affecting its stability, the transparency and the optical properties. All counted parameters are important for following using of investigated composites as the security markers. The kind of interactions responsible for the stability of composite was also investigated. Based on the tests, the specific luminescent characteristics of the composites tested were selected to allow their application in the field of security and anti-counterfeiting.

Acknowledgements: Join Chairs Project "Materiali Nanostrutturati Innovativi con proprietà di Luminescenza per i Beni Culturali (NanoLuBC)"- Doc. n. 184 del 14/05/2024 del CdA del CNR.

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OC106 TRIARYLPHOSPHONIUM BODIPY-BASED [2] ROTAXANES NANOPARTICLES FOR LIGHT-DRIVEN ANTIBACTERIAL APPLICATIONS

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Self-assembled molecular aggregates often have peculiar spectroscopic properties, which make them optimal candidates for photodynamic therapy and photopharmacology applications. [1]
We synthesized new BODIPY chromophores, functionalized with triarylphosphonium rotaxanes as potential antimicrobial photosensitizers for photodynamic therapy. Three compounds additionally linked Br atoms to increase their triplet formation yields. We studied the photophysical properties of these compounds with different techniques, including transient absorption spectroscopy. [2]
While in acetonitrile the brominated compounds showed a fast intersystem crossing with good triplet yields (ΦΔ 17-59%), the addition of water led to aggregates formation, as shown in Figure 1.

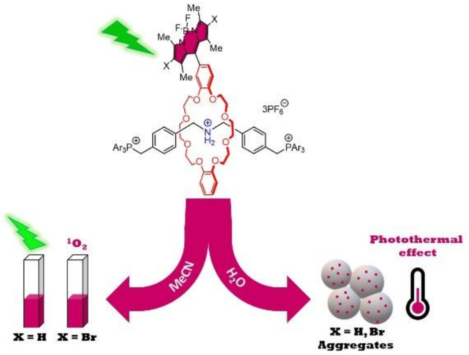

Figure 1: Schematic illustration of BODIPY-based rotaxanes (X = H, Br). In acetonitrile, brominated compounds show singlet oxygen generation, while water induces aggregation, leading to enhanced photothermal effects.

The aggregates presented an extremely fast excited-state non-radiative deactivation, with completely suppressed triplet formation.
Analysis of the photothermal properties of the nanoparticles revealed photothermal efficiencies ranging from 70 to 98% for all the investigated samples, suggesting that the presence of the heavy atoms is not a key factor for their photothermal conversion ability.
The antibacterial efficacy of the BODIPY-based nanoparticles was evaluated against Gram-positive and Gram-negative bacterial strains. The brominated compounds showed good antimicrobial activity. Interestingly, one halogen-free BODIPY also showed light-induced antibacterial effects. These findings highlight the potential of self-assembled BODIPY nanoparticles as biocompatible, metal-free antimicrobial agents for photomedicine applications.

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OC67

NQR SPECTROSCOPY FOR THE STUDY OF MAPb(Br_xI_{1-x})$_3$ PEROVSKITES AND THEIR PHOTOINDUCED HALIDE SEGREGATION

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Over the past decade, metal halide perovskites have emerged as one of the most promising classes of materials in photovoltaics due to their remarkable optoelectronic properties. A key factor in their success is the ability to tune their properties by varying their composition, which simultaneously makes the structural characterization of these materials particularly challenging due to the high degree of structural and dynamic disorder [1].
Recently, Nuclear Quadrupole Resonance (NQR) spectroscopy has gained increasing interest for its ability to provide in-depth local investigations of halide environments [2-4], which are notoriously difficult to study directly by observing halide nuclei by means of Solid-State Nuclear Magnetic Resonance (SSNMR).
In this study, we investigated the halogens chemical environment of various compositions of mixed-halide perovskites MAPb(Br_xI_{1-x})$_3$, where MA is Methylammonium, using ^{127}I and $^{79/81}$Br NQR. Additionally, through *in situ* illumination experiments, we observed for the first time the reversible effect of photoinduced halide segregation in mixed-halide perovskites [5] by means of NQR spectroscopy. This kind of study opens up the possibility of obtaining local structural information associated with this phenomenon, thus increasing the experimental data available to understand its origins.

Acknowledgements: We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title NUTSHELL: NMR Under illuminaTion SHEd Light on materiaLs– CUP I53D23003870006- Grant Assignment Decree No. 958 adopted on 06/30/2023 by the Italian Ministry of Ministry of University and Research (MUR).

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OC58

PANI-CuHCF HYBRID FILMS FOR ADVANCED ENVIRONMENTAL SENSING

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Conductive polymer (CP) are innovative and promising materials which combine the mechanical proprieties and metal-like conductivity. Among them, one of the most attractive is the polyaniline (PAni) because its conductive proprieties can be easily tuned through doping with acids, which allows it to transition between its insulating, semi-conducting, and highly conducting forms [1]. Also, the emeraldine salt form of PANI exhibits high conductivity, making it particularly valuable in sensors, batteries, and capacitors [2].

Polyaniline (PANI) is a cost-effective and easy-to-synthesize conductive polymer that exhibits exceptional electrochemical and electrical properties, making it suitable as sensor, energy storage devices, and electronic or electrochromic devices [3]. In this context, it has been studied both in layered systems and in hybrid systems containing metal hexacyanoferrates or Prussian Blue analogues (MHCF or PBA), an important class of mixed-valence compounds of great interest due to their remarkable electrocatalytic capabilities, ion-exchange properties (ESIX materials), and ion-sensing capabilities, with significant relevance as reversible redox species [4,5].

In particular, the in situ electrosynthesis of copper hexacyanoferrate (CuHCF) has been employed to design hybrid sensors capable of detecting ROS species, such as H_2O_2, through Fenton-like reactions [6,7].

Testing new electro- and redox-active nanocomposites for their potential environmental applications, such as water-pollutants sensing, is a challenge in order to limit the Reactive Oxygen Species (ROS) impact on cells. Thus, this work aims to develop PAni/CuHCF LbL systems and their physico-chemical investigation including stability, electrical conductivity, electrochemical response, and their ability to interact with specific chemical species. Preliminary tests conducted with hydrogen peroxide (H_2O_2) have demonstrated the responsiveness and sensitivity of these films, highlighting their significant potential for advanced applications in environmental sensing.

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OC119

DYNAMIC LIPID VESICLE RESPONSE TO OSMOTIC PRESSURE: MODELING AND EXPERIMENTAL INSIGHTS INTO BILAYER PERMEABILITY

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Understanding passive transport across lipid bilayers is crucial for both elucidating fundamental cellular processes and advancing drug delivery strategies [1]. In this study, we developed a robust procedure by combining liposome swelling/shrinkage assays under osmotic stress [2] and a detailed mathematical model [3]. The curve-fitting of the experimental results allows the quantitation of the permeability coefficient of both water and the permeant species. The model takes into explicit consideration both the partition to and the diffusion through the lipids, such that their relative weight on the overall permeation process can be discerned. By comparing a non-permeant, a slightly permeant and a permeant species, our results revealed that lipid bilayer permeability is markedly influenced by the solution composition. The presence of specific solutes can alter lipid packing and/or diffusivity, thus modifying even the bilayer permeability to water.

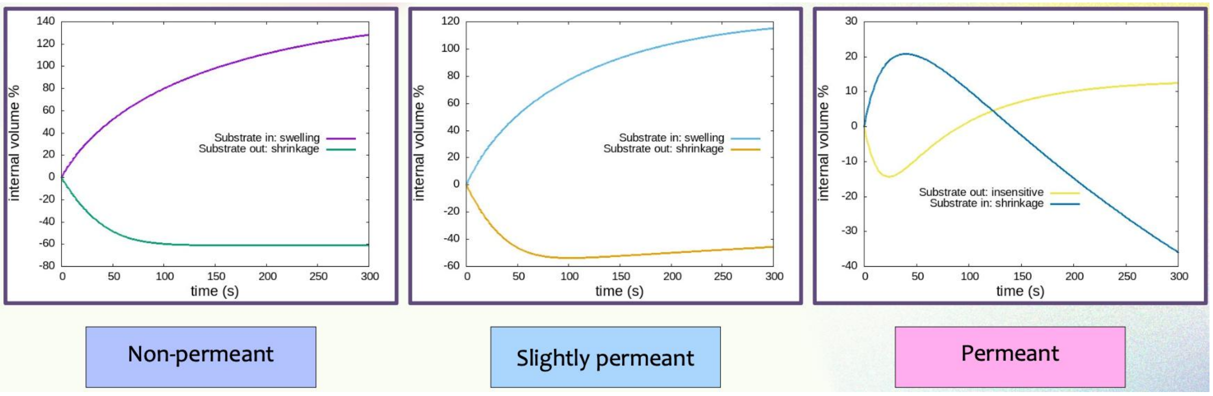

Figure 1. Example of simulated curves with our algorithm, for different species and different system setup.

A key finding during our investigation was the intrinsic asymmetry of the experimental response. Additional experiments demonstrated that system dynamics is not equivalent in swelling and shrinkage modes, with the former being considerably more hindered. This necessitated the incorporation of distinct damping factors into the mathematical model, ensuring adequate treatment of both regimes. The refined model led to a remarkable improvement in curve-fitting accuracy, bolstering its validity. Although restricted to non-electrogenic processes, at the moment, our integrated experimental and modeling strategy offers a reliable method to probe mechanistic aspects of passive membrane transport and could have broad application in the fields of pharmacology, biotechnology, and biophysical chemistry. The model represents an analytical tool, on the one hand, but also a predictive tool, on the other, allowing the fast simulation and comparison of different scenarios before moving to the bench.

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OC60

HIGHLY ACTIVE CATALYSTS FOR CO_2 METHANATION BY DISPERSION OF A Ni-BASED ACTIVE PHASE ON MESOPOROUS CeO_2

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Due to the increasing attention toward global warming, current research is focusing on green fuels obtained by the reduction of captured CO_2 (e-fuels) with hydrogen obtained from renewable energy sources (green hydrogen). A prominent example of these e-fuels is methane, that is obtained from CO_2 through a reduction reaction called the “Sabatier reaction”. Ni-based catalysts are currently among the most investigated systems for CO_2 methanation, due to their high activity and selectivity at relatively low temperatures and due to their low cost compared to catalysts based on noble metals. Ni is often paired with a support/promoter, like CeO_2 [1,2]. In this work, composite catalysts consisting of a NiO active phase dispersed on mesoporous CeO_2 are presented. The use of a mesoporous support allows to obtain a high dispersion of NiO in form of small nanoparticles, leading to a high catalytic activity with a reduced amount of active phase. For comparison, a chemically inert mesostructured siliceous material (SBA-15) has also been used as a support to determine the effect of CeO_2 as a promoter on the catalytic performance of the catalysts.

To disperse the NiO phase over the CeO_2 support an impregnation approach compared with a self-combustion reaction was used; three composite catalysts with a Ni wt% loading of 5, 10, and 15% were obtained. For comparison, a 5%Ni catalyst was obtained, with the same approach, using SBA-15 as support in place of mesoporous CeO_2.

XRD characterization suggests that NiO is dispersed over the mesoporous support in form of very small nanoparticles. Particularly, the pattern of the 5%Ni composite does not show any diffraction signal attributed to Ni-based crystal phases, while the 10%Ni and, particularly, 15%Ni show weak and broad peaks. Furthermore, the chemical mapping obtained both with EDX and EELS highlights how decreasing the load of active phase from 15 to 5% the dispersion of NiO over CeO_2 becomes more homogeneous. These results are also supported by H_2-pulse chemisorption on reduced samples, which points out a higher Ni dispersion decreasing the Ni load from 5% (16.7%) to 15% (5.3%).

To determine their catalytic activity the catalysts were tested for CO_2 methanation at different values of temperature and gas hourly space velocity (GHSV). The tests point out a high catalytic activity for all the catalysts supported on mesoporous CeO_2, with a CO_2 conversion ranging from 80 mol% (5%Ni@CeO_2) to 85 mol% (15%Ni@CeO_2), comparable or, in the case of 5%Ni@CeO_2, higher than most of the similar catalysts reported in the literature. On the other hand, the catalyst obtained on the siliceous support (5%Ni@SBA-15) shows a much lower CO_2 conversion (about 10 mol%), indicating the fundamental role of CeO_2 not only as a support but also as a strong promoter. Another important result is that the value of CO_2 conversion is not strongly influenced by the amount of the active phase, indicating that a low amount of Ni (5 wt%) can reach a high activity, due to its superior dispersion in form of ultra-small nanoparticles. This point is particularly important since it allows to minimize the amount of Ni (both a carcinogenic element and a critical raw material) in the catalyst, maintaining a high performance.

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OC42

A GENERAL PROTOCOL FOR QUANTUM MECHANICALLY DERIVED FORCE FIELDS IN ACCURATE POLYMER MODELING

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Polymers are essential in applications ranging from advanced electronics [1] to packaging materials [2]. Enhancing key properties such as biodegradability, mechanical strength, thermal stability, and electronic performance requires an atomic-level understanding of polymer behavior. However, the structural complexity and diverse chemical interactions within polymer systems pose significant challenges. Traditional force fields, originally designed for small molecules or biomacromolecules, often fail to accurately capture crucial electronic effects, including short-range steric interactions, large conformational flexibility in conjugated segments, and π-π interactions [3]. To overcome these shortcomings, various methods have been proposed to refine classical force fields, primarily by recalculating partial charges and reparameterizing dihedral angles to better approximate polymer-specific behavior [4,5]. However, this may introduce inconsistencies in the potential energy model, leading to errors in predicting properties that are sensitive to subtle conformational changes and overall polymer structure [6].

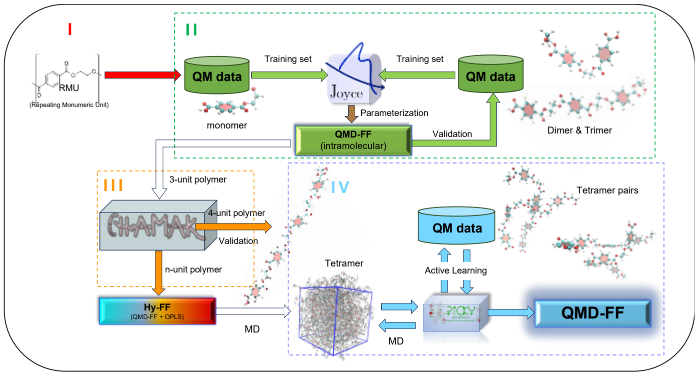

Figure 1. Workflow of the devised computational protocol.

In this work, we introduce a novel parameterization protocol for developing polymer-specific force fields relying solely on the knowledge of the polymer's chemical structure. Our approach leverages Quantum Mechanically Derived Force Fields (QMD-FFs), implemented using the Joyce method and code [7], to offer enhanced tunability and a more accurate representation of polymer properties. We validate this methodology on two polymer chains, known for their wide applications in industry, and complicated Potential Energy Surface,—Polyethylene Terephthalate (PET) and Polyethylene Furanoate (PEF)—demonstrating that QMD-FFs outperform traditional force fields and yield predictions that closely align with experimental data.

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OC17

MÖSSBAUER SPECTROSCOPY: OPPORTUNITIES AND PERSPECTIVE FOR (NANO)MATERIALS PHYSICAL CHEMISTRY

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Mössbauer Spectroscopy (MS) has now established itself as a very powerful technique, being able to provide chemical, structural and magnetic information on a wide variety of materials. In this context this technique is used in a broad range of research areas (e.g. chemistry, Physics, Biology, Geology), for both fundamental and industrial applications. The present communication, by shortly discussing several examples, will show how MS on condensed matter open interesting opportunities and perspective in the research area of Materials Physical Chemistry, with particular attention to the nanoscale.

MS probes the effects of hyperfine interactions between the nucleus and the surrounding environment; even if the energy contribution due to hyperfine effects is very low, this method allows to detect that thanks to its very high energy resolution (e.g. $\Delta E \sim$ 10-8 eV for the ^{57}Fe I= 1/2 → 3/2 14.4 keV transition). In this regard MS allow a quick and quantitative evaluation of Fe^{3+} and Iron Fe^{2+} that represent often a tricky problem in several systems. Taking as a case study nanostructured spinel iron oxide, the longstanding distinction among magnetite (Fe_3O_4) and maghemite (γ-Fe_2O_3) will be discussed [1], showing how MS can give a resolutive contribution in this scientific debate. The extraordinary sensitivity in investigating hyperfine interactions also allow the study of interface between different materials, as demonstrated in the $SrFe_{12}O_{19}/CoFe_2O_4$ system, where we can identify the crystallographic site at which the interface iron atoms are located [2]. MS has very low experimental time windows ($t_w = 5\times10^{-9}$ s) allowing a careful investigation of the magnetization dynamics of nanostructured materials and revealing interesting futures such as superspinglass regime. [3]. Mossbauer spectroscopy under intense magnetic field (MSHF) allow to investigate magnetic structure of the materials. Using nanostructured spinel ferrite as a model system the interplay among inversion degree and surface magnetic disorder (i.e. spin canting) on the magnetic properties will be discussed. Finally, the perspectives related to the use of ^{57}Fe-enriched precursors for the synthesis of nano-heterostructures will be discussed.

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OC71

FULLY ATOMISTIC QM/CLASSICAL APPROACHES TO SURFACE-ENHANCED RAMAN SPECTROSCOPY: FROM THEORY TO APPLICATIONS

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Raman spectroscopy provides detailed molecular fingerprint information but suffers from inherently low sensitivity due to weak scattering cross-sections. Surface-enhanced Raman scattering (SERS) overcomes this limitation by leveraging localized surface plasmon resonances in metallic nanostructures, dramatically amplifying Raman signals. This enhancement enables detection down to the single-molecule level, making SERS a powerful tool for (bio)chemical sensing and analysis. [1-2]

Multiscale approaches can effectively model the enhanced spectroscopic response of molecules embedded in plasmonic environments under irradiation.[3,4] Recently, our group proposed a Quantum Mechanics (QM)/Molecular Mechanics (MM) approach for calculating SERS spectra.[5,6] In this framework, the molecule is described at the TDDFT level, while the plasmonic substrate is treated classically, preserving its atomistic nature. The frequency-dependent Fluctuating Charges and Fluctuating Dipoles (ωFQFμ) electromagnetic model [7] is employed to account for the plasmonic behavior of metal nanostructures with complex morphologies (such as edges, tips, defects, and junctions) and compositions, including homogeneous, core-shell, or alloyed colloidal noble metal systems.[8-9]

Our fully atomistic multiscale strategy enables *in-silico* tuning of key experimental parameters, such as molecular orientation, substrate morphology, composition, plasmonic response, and solvent effects.[6] Using the QM/ωFQFμ methods, we compute SERS spectra for selected (bio)molecular systems, such as DNA nucleobases and amino acids, and validate our predictions against experimental data.

Acknowledgements: This work has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 818064).

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OC100

AC-MODULATED AND LOCALIZED-XPS FOR CAPTURING METAL/IONIC LIQUID INTERFACES

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Electrochemical devices are based on the fundamental process of ion migration and accumulation on surfaces. Complex molecular properties of ions and device dimensions control the entire process and define the overall dynamics of the system. For ionic liquid-based electrolytes it is often not clear which property and to what extent contributes to the overall performance of the device. Herein we use X-ray photoelectron spectroscopy (XPS), while the device is under electrical bias. Such a procedure reveals localized electrical potential developments, through binding energy shifts of the atomic core levels, in a chemically specific fashion. Combining it with Square-Wave AC Modulation, the information can also be extended to time domain, and investigate devices configured as a coplanar capacitor, having an ionic liquid as the electrolyte, in macro-dimensions (see Figure 1). Our analysis reveals that nonlinear voltage profile across the device emerges from spatially nonuniform electrical double layer formation on electrode surfaces. Interestingly, the coplanar capacitor has extremely slow responses, which is particularly controlled by IL film thickness. XPS measurements can capture the ion dynamics in tens of seconds to microseconds range and reveal that ionic motion is all over the device, including those on metallic electrode regions. This behavior can only be attributed to motion in more than one dimension. The ion dynamics can also be faithfully simulated by using a modified PNP equation, considering steric effects, and device dimensions. XPS measurements on two devices with different dimensions corroborated with and validated the simulation results. The present results propose a new experimental approach and provide new insights into the dynamics of ions across electrochemical devices. [1-3]

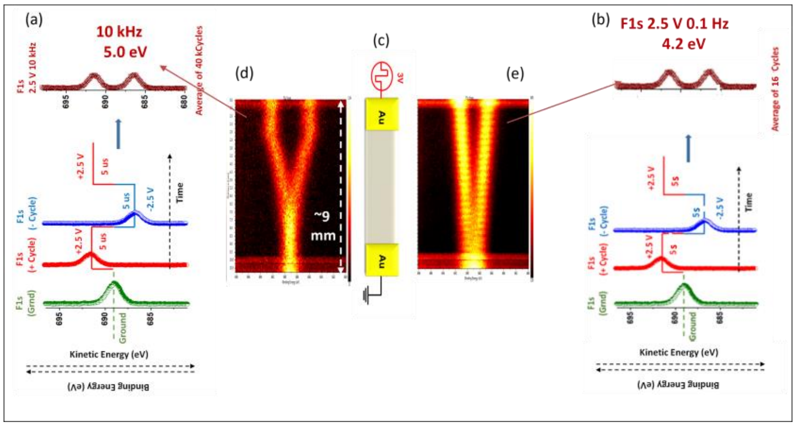

Figure 1. F1s XP Spectra recorded as Line-Scans at 2 different Frequencies.

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OC120

DIRECT AMIDE-BOND FORMATION REACTION ON ANATASE TiO_2 FROM FIRST PRINCIPLES MODELING

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Amide bonds - widespread in chemical products of key relevance for many applications - can be formally synthesized from condensation reactions between amines and carboxylic acids, producing water as a byproduct. However, conventional amidation approaches make use of drastic reaction conditions and large amounts of chemicals. Hetereogeneous catalysts may help overcome these limitations, yet key microscopic-level insight on the reaction mechanisms is missing.

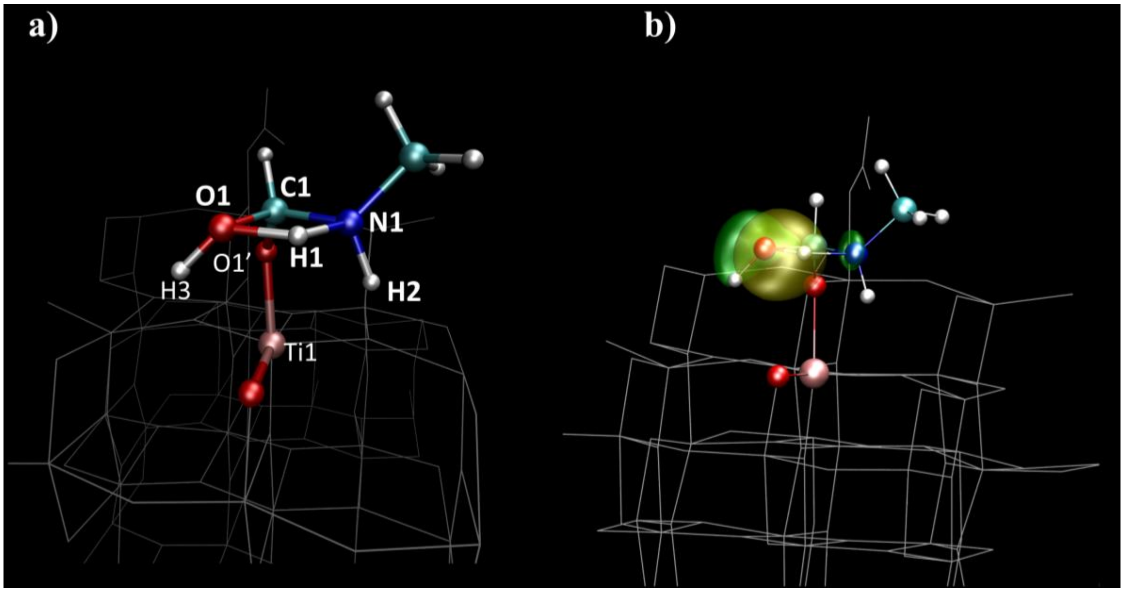

Figure 1. a) Transition state structure for the direct amide-bond formation reaction $HCOOH+CH_3NH_2 \rightarrow CH_3NHCHO+H_2O$ on anatase $TiO_2(101)$ surface. b) Wannier molecular orbital associated to the formation of the water molecule via proton transfer from the $–NH_2$ group of methylamine. Atom color codes: blue=N, red=O, cyan=C, pink=Ti, white=H. The reaction center is shown as ball-and-sticks, while the rest of the system including the TiO_2 slab is shown as grey sticks.

By using density functional theory, ab initio molecular dynamics, and abinitio metadynamics, we show that gas-phase methylamine directly attacks the carbonyl group of formic acid adsorbed on anatase $TiO_2(101)$ surface in an Eley–Rideal-type mechanism, yielding adsorbed methylformamide and a water molecule equivalent. [1] Such a direct amidation process does not rely on the presence of surface defects (e.g., –OH groups or oxygen vacancies). After the formation of an adduct, involving a strong interaction between methylamine N1 atom and the C1 atom of adsorbed formic acid, the actual condensation occurs. The transition state (see Figure 1) exhibits a 4-center ring moiety involving the N1, H1, O1, and C1 atoms, which assists the transfer of the H1 proton from the amine N1 atom to the carboxylate O1 atom. [1] The computed energy barrier -60 kJ mol^{-1} (14.3 kcal mol^{-1}) [1]- is compatible with the mild reaction conditions experimentally adopted in direct solvent-free amidation processes on TiO_2 nanoparticles. [2]

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OC23

SELF-AGGREGATION OF RHAMNOLIPIDS STABILIZES ENDOGENOUS RADICALS IN CONCENTRATED AQUEOUS SOLUTION

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The self-assembly of amphiphilic molecules is key to designing functional formulations, yet the aggregation behavior of biosurfactants at high concentrations is not well understood. Rhamnolipids (Rha), biosurfactants from Pseudomonas aeruginosa, form complex aggregates influenced by their composition and environment [1,2]. While their micellization in dilute solutions is well-studied, the molecular organization, phase transitions, and polarity of concentrated Rha systems need further investigation [3]. To address this, we employed Electron Paramagnetic Resonance (EPR) spectroscopy, a powerful tool for probing local molecular dynamics and organization, to analyze aqueous Rha mixtures from 20% to 90% w/w. Two spin-labeled probes, 5-doxyl stearic acid (5-DSA) and 16-doxyl stearic acid (16-DSA), were used to selectively monitor different regions of the surfactant assembly [4,5]. Computational analysis of the EPR spectra revealed a transition from micellar to lyotropic liquid phases above 80% w/w, characterized by a decrease in spin mobility and an increase in molecular ordering. The emergence of a slow-motion component in the 16-DSA spectra at high Rha concentrations highlights the formation of highly packed, anisotropic aggregates.

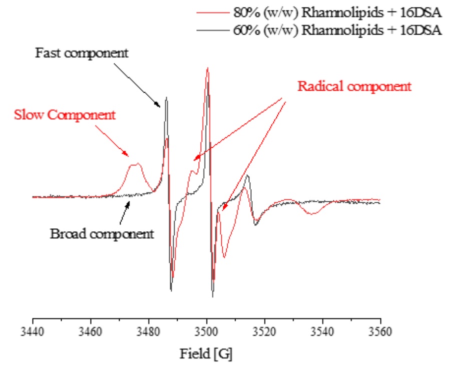

Figure 1 Spectra of 16-DSAin water Rha mixturesat two different rhamnolipids percentages (60 and 80 % w/w)

The detection of an endogenous radical component, even without spin probes, indicates that high Rha concentrations stabilize radicals, potentially giving them antioxidant properties [6]. This phenomenon, likely due to lipid peroxidation or radical trapping within the aggregates, highlights the interfacial redox properties of biosurfactants. These findings reinforce the value of EPR spectroscopy in studying the molecular organization and dynamics of concentrated amphiphilic systems, aiding the design of bio-based formulations for industrial and environmental use.

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OC6

UNRAVELLING THE METHANE TO METHANOL CONVERSION OVER A NOVEL Fe-BASED METAL ORGANIC FRAMEWORK CATALYST: AN X-RAY MULTITECHNIQUE CHARACTERIZATION

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Achieving the direct oxidation of methane to methanol (MTM) under mild conditions is considered the holy grail of modern catalysis, as the current large-scale methanol production technologies rely on expensive and non-environmentally friendly processes operated at elevated temperatures and pressures (T>400 °C, P>30 bar) [1]. Natural enzymes efficiently perform the MTM reaction [2-3], and have therefore inspired the development of upscalable artificial catalysts able to reproduce this exceptional reactivity. Metal-organic frameworks (MOFs) are hybrid porous materials composed of metal nodes and organic linkers that are regarded as promising candidates to realize the MTM oxidation because of their intrinsically high chemical tunability. MIL-100(Fe) is a MOF containing trimeric Fe(III) units and the benzene-1,3,5-tricarboxylate (BTC) linker, which is known to form open Fe(II) sites upon thermal treatment above 200 °C [4]. These open metal sites can perform the N_2O-based MTM oxidation through a highly reactive Fe(IV)=O intermediate [4], but an in-depth spectroscopic characterization of their formation process is lacking. Additionally, the low availability of N_2O limits the applicability of this gas for the MTM process only of academic interest, therefore it is quite interesting to explore a more economically convenient process based on molecular oxygen.

Here, we present a detailed spectroscopic characterization of the direct MTM conversion at ambient pressure and moderate (200 and 100 °C) temperatures over MIL-100(Fe) (see Figure 1), using O_2 as the oxidant [5]. We first characterize the thermally induced self-reduction underwent by a portion of the Fe(III) with operando high energy-resolution fluorescence detected X-ray absorption spectroscopy (HERFD-XAS), determining the intermediate species involved in this process as well as the final Fe(II) abundance. Subsequently, we characterize the MOF under catalytic conditions, highlighting the fate of the Fe(II) sites during the MTM reaction and the propensity of the material towards active site regeneration. We also identify the species formed upon catalyst deactivation with the help of valence-to-core X-ray emission spectroscopy (VtC-XES). To monitor the catalyst stability, we employ operando powder X-ray diffraction (PXRD) throughout the entire process. Finally, we complement this experimental characterization with density functional theory (DFT) calculations steered by experimental evidence, validating both proposed mechanisms for the activation and MTM conversion processes.

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OC32 A COMBINED PHYSICO-CHEMICAL APPROACH DEFINES THE STRUCTURAL EFFECTS OF ANTI-THROMBIN APTAMERS ON HUMAN PROTHROMBIN ACTIVATION

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Blood coagulation disorders remain a major cause of mortality and disability worldwide, driving the search for novel therapeutic agents capable of finely modulating the coagulation cascade [1,2]. Among them, oligonucleotide aptamers targeting specific coagulation factors represent promising candidates, sometimes evaluated in preclinical and clinical studies [3]. In this context, anti-thrombin aptamers attracted significant interest due to their dual mechanism of action. They not only inhibit thrombin activity but also limit thrombin production by binding its precursor prothrombin [4-7]. Understanding the structural basis of this dual targeting is crucial for optimizing their anticoagulant potential and designing next-generation therapeutic agents with improved safety profiles and reduced side effects.

To elucidate the interaction between anti-thrombin aptamers and prothrombin, we employed calorimetric and spectroscopic analyses, revealing that these aptamers recognize exosite I of thrombin and proexosite I of prothrombin with comparable affinity. Small-angle X-ray scattering (SAXS) experiments on the prothrombin complex with NU172, the only anti-thrombin aptamer in advanced clinical trials [8], provided structural insights into their recognition mechanism. Notably, aptamer binding to proexosite I shifts the prothrombin open-closed equilibrium [9] toward the open conformation. These results have allowed to propose a reasonable mechanism to explain the high inhibition ability of the examined aptamers against the conversion of prothrombin into thrombin [10]. Further spectroscopic studies are ongoing to confirm and characterize this conformational equilibrium shift in greater detail.

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OC85

INKJET PRINTING OF FLEXIBLE KESTERITE SOLAR CELLS

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Among the emerging inorganic thin-film photovoltaic technologies, kesterite $Cu_2ZnSn(S,Se)_4$ (CZTSSe) is one of the most promising material thanks to its tunable bandgap of 1.0-1.5 eV according to the [S]/([S]+[Se]) ratio, which allows for an efficient harvest of an abundant portion of the solar spectrum. This material can be easily grown through different processes, both on rigid and flexible substrates, but solution-based methods, relying on the deposition of multiple layers to reach the desired thickness of the film, are currently considered as the best choice [1]. The most common are spin-coating, blade-coating, spray pyrolysis, and dip-coating. Specifically, spin-coating led to the current record efficiency of η = 15.1% [2], even though the small-area limitations of this technology together with the waste of a non-negligible amount of precursor solution, still hinder the scalability of the process. Drop-on-demand inkjet printing is a promising solution-based technique that is appealing from an industrial point of view [3]. In this work, for the first time the inkjet printing method has been applied to flexible substrates for CZTSSe thin-film solar cells. A novel 2-methoxyethanol (MOE) -based precursor solution has been properly optimized, together with the surface engineering of the flexible substrate, to allow for inkjet printing of the CZTSSe thin-film absorber. The obtained results show the first example of a working inkjet-printed flexible kesterite CZTSSe solar cell, overcoming the performance of its corresponding spin-coated counterpart by 20%, relying on a more homogenous and compact material. With inkjet printing technology, a significant reduction of preparation cost and better raw materials utilization has been possible, proving it as the most reliable path for a sustainable industrial scale-up of flexible CZTSSe solar cells.

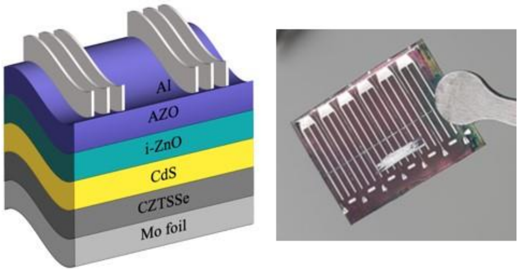

Figure 1. Architecture (left) and appearance (right) of a flexible CZTSSe solar cell.

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OC66

SUPERPARAMAGNETIC NANOPARTICLES AS MOLECULAR MESSENGERS FOR SECURE INTRA-BODY COMMUNICATION AMONG IMPLANTED MEDICAL DEVICES

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Synthetic Molecular Communication (SMC) is an emerging paradigm inspired by natural biological communication, in which molecules are used to encode, transmit, and decode information [1]. This approach is particularly promising for implanted medical devices (IMDs),[2] where traditional wireless communication methods face severe limitations due to signal attenuation, tissue interference, and power constraints. By leveraging molecular messengers instead of electromagnetic waves, SMC offers a bio-compatible and energy-efficient solution for intra-body information transfer. However, one of the major challenges in implementing SMC for IMDs lies in the development of reliable and detectable molecular carriers, capable of controlled propagation through biological fluids while ensuring efficient signal retrieval by a receiver. Among the various candidates for molecular messengers, superparamagnetic iron oxide nanoparticles (SPIONs) stand out due to their unique magnetic properties [3]. Their high biocompatibility and precise controllability via external magnetic fields, reducing the aggregations, make them particularly suited for communication in biological environments. Unlike traditional chemical messengers, which rely purely on diffusion, SPIONs can be actively guided within the body, potentially enhancing the precision and speed of signal delivery. Moreover, their magnetic properties allow remote detection, enabling non-invasive information retrieval via inductive sensing through the skin, which eliminates the need for direct contact with the communication medium. These advantages position SPIONs-based communication as a groundbreaking solution for intra-body IMD connectivity, offering a hybrid approach that bridges molecular and electromagnetic communication strategies. We present our experimental testbed demonstrating the feasibility of SPION-based synthetic molecular communication. By developing a controlled release system and an inductive receiver, we validate the capability of this communication framework to encode and transmit information reliably within a vascular-like environment. Our preliminary results highlight the potential of SPIONs as efficient molecular messengers, opening new perspectives for secure, biocompatible, and long-range intra-body communication. These findings pave the way for future developments in next-generation smart implants and advanced biomedical communication networks.

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OC76

UNRAVELING THE OXIDATION MECHANISM OF THIOPHENE IN BIOMASS GASIFICATION: A CROSSED MOLECULAR BEAM STUDY

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The gasification of solid feedstocks has recently emerged as a promising pathway toward an environmentally sustainable and decarbonized energy sector. This process can convert municipal solid waste, plastics, or biomass-derived materials into syngas, a key intermediate for chemical production and hydrogen generation. However, the widespread implementation of gasification is still hindered by operational challenges and a limited understanding of its fundamental reaction mechanisms. In particular, sulfur-containing species present in biomass feedstocks can significantly influence the composition and reactivity of the resulting syngas, affecting both process efficiency and environmental impact.

In this study, we investigate the gas-phase reaction of atomic oxygen ($O(^3P)$) with thiophene as a model system for sulfur-containing compounds in biomass-derived pyrolysis and gasification processes. We have employed the crossed-molecular-beam (CMB) technique with universal, soft ionization, mass-spectrometric detection, and time-of-flight analysis to identify the reaction mechanism and the branching fractions (BFs) of all possible reaction products [1]. Preliminary results indicate that atomic oxygen efficiently degrades thiophene, breaking its aromatic ring to form thioacrolein and CO, suggesting a selective oxidative cleavage of the thiophene ring. Similar spin-forbidden CO-forming pathways were observed in benzene and pyridine oxidation, where intersystem crossing played a crucial role [2,3].

These findings contribute to a deeper understanding of the elementary reaction mechanisms governing the oxidation of sulfur-containing species in biomass conversion. By providing experimental insights into the molecular-scale kinetics of these transformations, this study supports the development of more accurate models for gasifier design and optimization, ultimately aiding in the broader effort to improve the efficiency and viability of gasification technologies.

Acknowledgments: We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 02.02.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title 20227W5CLJ Biomass gasification for hydrogen production (Bio4H2) – CUP J53D23001970006 - Grant Assignment Decree No. 961 adopted on 30.06.2023 by the Italian Ministry of Ministry of University and Research (MUR). We also acknowledge support from the European Union – NewxtGenerationEU under the Italian Ministry of University and Research (MUR) National Innovation Ecosystem grant ECS0000041 – VITALITY. CUP: B43C22000470005.

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OC36

SILVER NANOPARTICLES DECORATION OF POLYOXO-TITANIUM CLUSTERS FOR ADVANCED OXIDATION

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Metal-oxo clusters (MOCs) are structures composed of multiple metal centers linked to each other by bridging oxygen atoms. A specific subclass of MOCs is represented by poly oxo-titanium clusters (PTCs), whose structure is based on a $[Ti_xO_y(OR)_z]$ (OR = alkoxyl) core coordinated with organic ligands. By the selection of proper organic ligands, it is possible to modulate the properties of these compounds by combining the excellent photoactivity of TiO_2 with the unique characteristics of the chosen ligands [1]. In this work the synthesis of the robust cluster $[Ti_6O_4(OiPr)_{10}(O_3P\text{-}Phen)_2]^{2+}$ (OiPr = isopropyl group, O_3P-Phen = phenylphosphonic acid), functionalized with isonicotinic acid was carried out. This structure (Figure 1) is already known in the literature as "PTC-3" [2]. Our aim was to exploit nitrogen atoms given by pyridinic ligands to coordinate silver species (i.e. silver nanoparticles "AgNPs"), in accordance with the Pearson's soft and hard acid-base theory, so that AgNPs could be incorporated within the structure. According to the well-known properties of AgNPs, such as excellent electrical conductivity, chemical stability, catalytic, and antimicrobial properties, the application's fields of the composite material (PTC-3@AgNPs) could be broadened. PTC-3@AgNPs was synthesized through the solvothermal method by means of a one-pot reaction. Proper amounts of isopropanol, isonicotinic acid, phenylposphonic acid, silver acetate, and titanium isopropoxide were mixed in a glass reactor and subjected to the synthesis process, performed for three days at 80° C. Synthesized samples were comprehensively characterized by means of: X-Ray Diffraction (XRD), Thermo-Gravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC), Transmission Electron Microscopy (TEM), UV-Vis diffuse reflectance spectroscopy (DRS), Fourier-Transformed Infrared (FTIR), and micro-Raman Spectroscopy. Both PTC-3 and PTC-3@AgNPs showed promising properties towards the degradation of methylene blue in combination with hydrogen peroxide, despite the role of silver still need to be clarified. In a successive step we tried to replicate these syntheses by replacing isonicotinic acid with polycarboxylate ligands (2-amminoterephthalic acid, 2, 5-pyridinedicarboxylic acid and 1, 3, 5-benzenetrycarboxylic acid) to increase the dimensionality of the structure and obtain an extended framework.

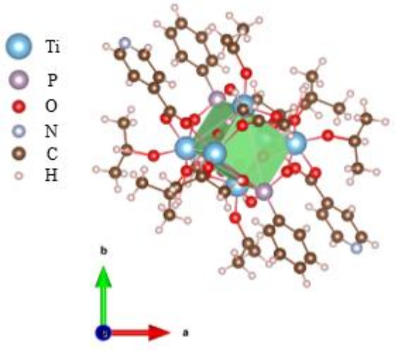

Figure 1. Structure of PTC-3 cluster.

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OC21

IMPUTATION AND MACHINE LEARNING TECHNIQUES FOR POLYMER GAS PERMEABILITY ANALYSIS

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The development of polymer membranes for gas separation processes faces significant challenges due to limited availability of comprehensive permeability data in scientific literature[1]. This computational framework addresses this limitation by maximizing the utility of sparse experimental datasets through advanced data integration and predictive modeling techniques. The approach emphasizes data collection, curation, and intelligent imputation strategies to overcome the fragmented nature of available permeability measurements across diverse polymer structures and gas types. In this work, we established a unified and comprehensive database by consolidating scattered polymer permeability data from multiple literature sources. The integration process involved standardizing polymer representations using Simplified Molecular Input Line Entry System (SMILES) notation, which enabled consistent structural encoding across diverse polymer families. This standardization was crucial for subsequent molecular descriptor generation and structure-property relationship analysis.

To address the challenge of missing permeability values, we implemented several advanced imputation techniques specifically tailored for gas permeability data[2]. These methods considered both the molecular structure of polymers and the physicochemical properties of the penetrant gases to estimate missing values with high accuracy. The imputation approach particularly focused on membrane permeability toward industrially relevant gases, enabling the creation of complete permeability profiles for polymers with previously partial characterization.

Machine learning algorithms, including Random Forest and XGBoost, were employed to develop predictive models that capture the complex relationships between polymer structures and their gas transport properties.

This research highlights the value of systematic data collection efforts in the field and provides tools to bridge existing data gaps. By facilitating more holistic analysis of polymer performance across multiple gas pairs, the approach contributes to accelerating the discovery and development of advanced membrane materials for sustainable separation processes, while emphasizing the continued need for expanded experimental data generation and sharing within the research community.

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OC98 STUDY OF THE PHOTO-BEHAVIOUR OF AZO MOLECULES IN SOLUTIONS, THIN FILMS AND GRAPHENE-LIKE MATRICES

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Azobenzene (AB) is a notorious organic dye, and its photophysical properties in solution are very well known, in particular AB presents a high photo-isomerization yield and a very low fluorescence [1,2,3]. Also, the Azo group, when properly functionalized, is able to undergo a controlled photo-switching capability [4], and over the years these systems have been included in a variety of photo-responsive devices, for application like visible-light-controlled molecular systems [5], till photocatalysis [6] and solar thermal fuels [7,8]. However, when AB is adsorbed onto solid surfaces, the isomerization is inhibited, and the fluorescence efficiency is enhanced (Figure 1) together with the decay time of the singlet excited state, which is increased by ten times than in solution [9].

In this study, AB and an alkyl derivative AB (FAAzo) compound were optically characterized, thorough UV-VIS absorbance, luminescence, time-correlated single photon counting and evaluating the kinetics of photoisomerization. Both compounds were studied in solutions, organic and water, in thin films and in graphenic matrix. The obtained results are discussed in terms of nature of the interactions between Azo units in the different experimental conditions, and adsorbed on graphene-like matrices.

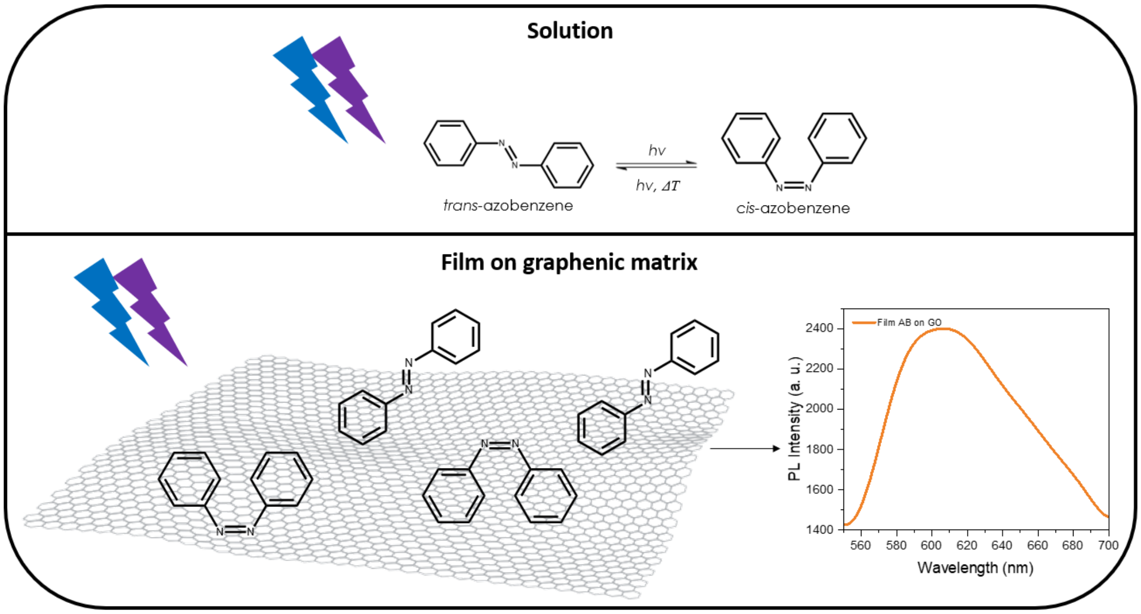

Figure 1. Scheme of different behavior of AB molecules in solution and thin film, when shined with UV light.

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OC116 3D-ENGINEERED IN VITRO MODELS FOR BIOMEDICAL APPLICATIONS BASED ON PVA-SHELLED DECAFLUOROPENTANE DROPLETS

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Three-dimensional (3D) *in vitro* cell culturing is gaining increasing attention due to its advantages over traditional two-dimensional (2D) models. Although 2D cultures are easier to establish and manipulate, they have significant limitations, such as the inability to replicate the *in vivo* microenvironment and the lack of critical cell-cell and cell-matrix interactions [1]. By contrast, 3D models preserve cellular polarity and support complex structures like spheroids, organoids, and multicellular aggregates, which more closely resemble the *in vivo* state. Currently, a broad range of techniques for developing advanced 3D cell culture models are in use, including hydrogels, microfluidic devices, and scaffold-based systems.

In this context, we developed a 3D-scaffold system based on meso-droplets (DPs) consisting of a polyvinyl alcohol (PVA) shell and a perfluorocarbon (DFP, decafluoropentane) core for biomedical applications [2]. Indeed, PVA is known for its well-established biocompatibility and its ability to form a stable, flexible matrix for cell culture. The system's biocompatibility was first assessed through MTT and Trypan Blue assays. Subsequent experiments involved culturing normal and tumor-derived human cell lines on DPs and comparing their behavior with cells grown in traditional 2D cultures. As expected, 3D cultured cells displayed enhanced cellular aggregation and more robust growth patterns, compared to their 2D counterparts. Cells in these structures were labelled with various fluoroprobes to assess their viability and distribution. Confocal laser scanning microscopy (CLSM) was used for imaging 3D structures due to its ability to visualize cells in three dimensions, offering insights into cell morphology and spatial organization within the scaffold. Taking advantage of the chemical versatility of the PVA shell, the DPs were functionalized with type I collagen derived from rat tails, a well-established extracellular matrix protein known to promote cellular bio-adhesion and facilitate tissue engineering.

Finally, we explored the potential biomedical application of the DPs-cell system in the functionalization of Nitinol Flow Diverter (FD) stents with Human Fibroblast (HFFF2) cells. Nitinol stents are commonly used in vascular interventions, but they face challenges related to post-operative complications such as restenosis and thrombosis [3]. By functionalizing the stent surface with human fibroblasts, the reendothelialization process can be accelerated, improving the biocompatibility of the device and reducing the risk of restenosis.

Acknowledgments: the research was funded by INAIL under the grant agreement BRiC2022 ID53.

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OC65

GESTALT PERCEPTION OF COMPLEX FTIR SPECTRA

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Fourier Transform Infrared (FTIR) spectroscopy captures rich molecular information, but conventional analysis struggles with complex mixtures due to noise, baseline drift, and lack of standardisation. Inspired by biological olfaction [1], we treat FTIR spectra as holistic signatures of latent chemical archetypes, bypassing preprocessing entirely. We generated a large synthetic dataset of 100 archetypal mixtures, each measured 120 times under varied noise and artifact conditions—resulting in 12,000 complex spectra—to train and validate our machine learning models. Crucially, our framework accounts for non-Gaussian variance in component distributions, better reflecting real-world chemical diversity. Using modern machine learning and neuromorphic [2] architecture, we achieve high classification accuracy even in the presence of measurement artifacts. We validate these findings using real FTIR spectra from essential oils, fuel oil types, and natural vinegars, showing that our approach enables reliable, calibration-free classification of complex natural products. This supports the use of FTIR as a universal, standardised platform for machine olfaction.

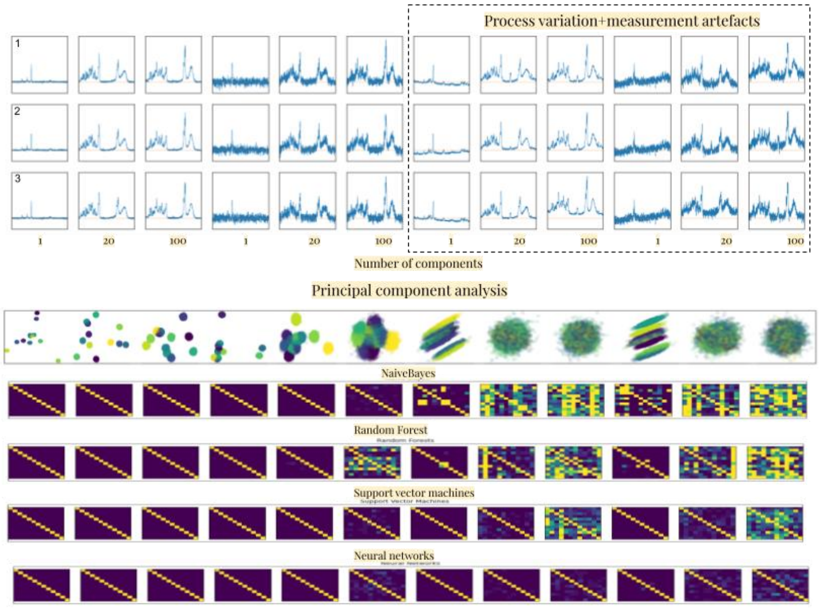

Figure 1. Classification of Complex Mixture Spectra. Top: FTIR spectra from simulated mixture archetypes with increasing numbers of components (3, 20, 100), showing process variability and realistic measurement artifacts (e.g. baseline shift, water/CO_2 interference). Middle: PCA projections illustrate class separability deteriorating with increased mixture complexity. Bottom: Confusion matrices for four classifiers—Naive Bayes, Random Forest, Support Vector Machines, and Neural Networks—demonstrate that despite high spectral variance and lack of preprocessing, neural networks retain superior classification performance across all datasets.

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OC87

PoLA (POROSITY LOCAL ANALYSIS): A NOVEL DESCRIPTOR OF MICROPOROUS VOLUME TO PREDICT GAS ADSORPTION IN AMORPHOUS MATERIALS

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A procedure is presented to describe the porosity of microporous solids (e.g. activated carbons): unlike many methods commonly used at present, PoLA (Porosity Local Analysis) is not based on pores of pre-defined regular shape (like spheres or cylinders) but rather on a local analysis of the cavities geometry.

PoLA is particularly suited to describe amorphous porous materials, like activated carbons, accurately: the procedure can be applied to any atomistic model and it is much faster than other methods in wide use (as for instance the popular PoreBlazer tool [1]). More importantly, the porous volume distribution provided by PoLA is strongly correlated to gas adsorption isotherms and it can be used to accurately and efficiently predict gas adsorption.

As proof of concept, we tested the new descriptor by preparing a dataset of porous carbon models which were analyzed by PoLA, and for which N2 adsorption isotherms at 77 K were simulated with Grand Canonical Monte Carlo. A machine learning model (Random Forest) approach was trained on isotherms and porosity distribution and performed excellently in predicting absorption isotherms (Figure 1) for carbon models not included in the training set (Figure 1), outperforming other porosity measures (e.g. PSD[1], Figure 2).

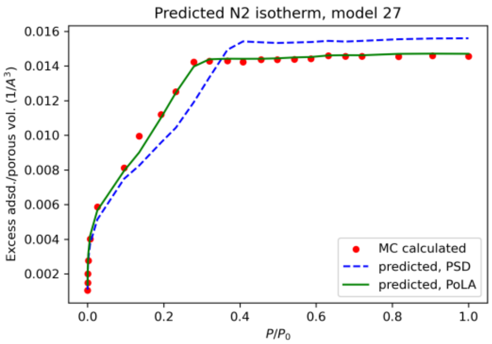

Figure 1: N_2 at 77 K adsorption isotherm in a large carbon model, computed by high level GCMC and predicted on the basis of PoLA and PSD porous volume distributions.

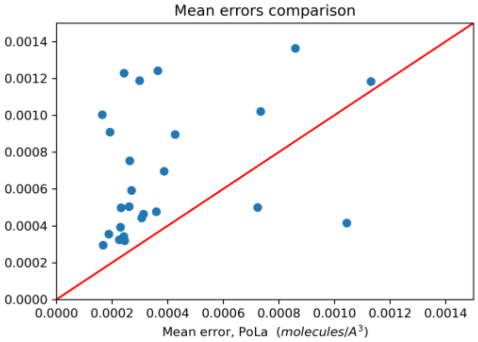

Figure 2: Mean unsigned errors of PoLA and PSD predicted isotherms with respect to Grand Canonical Monte Carlo calculations

PoLA can also be used to deduce the porous volume distribution from experimental nitrogen or argon adsorption isotherms and predict the performance towards other gases of interest, like hydrogen, methane or carbon dioxide.

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FC16

CHIRALITY INDUCED SPIN SELECTIVITY: THE ROLE OF TWO-ELECTRON SPIN-ORBIT COUPLING

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Chirality-Induced Spin Selectivity (CISS) is a phenomenon where electrons in chiral systems exhibit spin-dependent behaviour.[1] While CISS holds great promise for spintronics, chiral sensing, and quantum technologies, its fundamental mechanisms remain elusive.[2] Theoretical models suggest that spin-orbit coupling (SOC) plays a crucial role; however, in systems without heavy atoms, SOC is typically weak, leading to discrepancies of several orders of magnitude between theoretical predictions and experimental data.[3]

In this work, we explicitly incorporate two-electron SOC terms into the theoretical description of CISS. Going beyond conventional Hartree-Fock (mean-field) approximation, we derive SOC operators in second quantization, enabling an accurate evaluation of matrix elements in real-space and valence-bond basis. Our findings reveal that a purely one-electron description fails to capture key features of SOC. We demonstrate that the imaginary part of the SOC coupling—responsible for encoding chirality information—undergoes a sign inversion upon enantiomeric inversion. The two-electron treatment fundamentally reshapes the interaction landscape, cancelling certain couplings, introducing new ones, and significantly remodulating existing interactions, ultimately leading to a sign inversion in spin polarization. It underscores the need to include two-electron contributions for a physically consistent description (Figure 1).

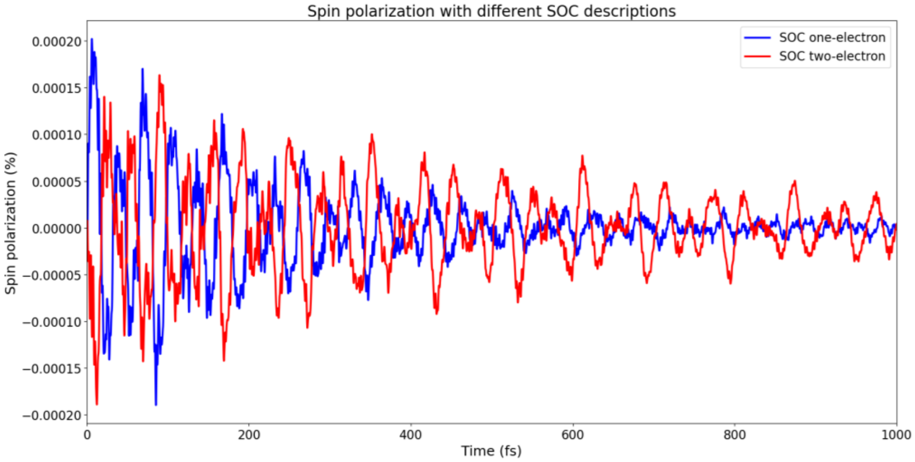

Figure 1: Evolution of spin polarization with one-electron and two-electron SOC terms, calculated using Redfield theory.

This work establishes a new theoretical framework for modelling SOC in chiral systems, laying the foundation for future studies aimed at developing a fully quantitative description of the CISS effect.

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FC17

DECODING SINGLET-TRIPLET INVERSION: A PPP-BASED FRAMEWORK FOR HIGH-THROUGHPUT SCREENING

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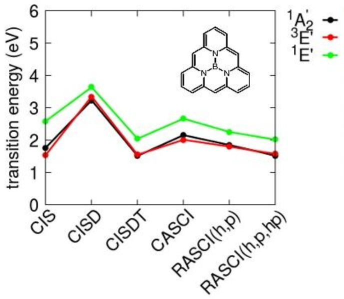
Recent experiments [1,2] and theoretical predictions [3-5] have unveiled a fascinating phenomenon known as the inversion of the lowest singlet and triplet excited states (ST inversion) in certain triangle-shaped organic molecules. These molecules, rich in conjugated carbon and various heteroatoms like nitrogen and boron, defy Hund's rule and hold immense promises for revolutionizing organic light-emitting diodes (OLEDs) by enabling efficient triplet harvesting. However, dealing with the complexities of ST inversion poses a formidable computational challenge, particularly when exploring larger molecular systems using current ab initio methods.

In this contribution, we introduce a novel approach to ST inversion based on the Pariser-Parr-Pople (PPP) model, the simplest model for correlated electrons in π-conjugated systems [4,5]. Using a combination of PPP-CISDT and restricted active space configuration interaction calculations, we show that ST inversion does not strictly require non-overlapping HOMO and LUMO orbitals. Rather, it emerges from a delicate interplay between a narrow gap and a small exchange integral between the frontier orbitals. Moreover, we show the critical role of triply excited configurations in accurately modeling ST inversion (see Figure 1). By combining precision with computational efficiency, the PPP model paves the way for systematic screening of the growing molecular landscape exhibiting ST inversion.



Method	CPU time (minutes)
CIS	1.51
CISD	99.98
CISDT	40,770.62
CASCI	0.91
RASCI(h,p)	31.23
RASCI(h,p,hp)	266.76

Figure 1: Comparison of the first few excitation energies for the sketched triangular boron carbon nitride across different theoretical models, along with corresponding computational time analysis.

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FC1

INVESTIGATING CO_2 CAPTURE AT DIFFERENT TEMPERATURES USING 3D PRINTED ZEOLITE, MOF AND LDH MONOLITHS

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Carbon capture from post-combustion processes using solid adsorbents has attracted increasing attention in recent years as a promising approach to counter CO_2 emissions.[1] Two possible adsorbents for the CO_2 capture at medium-low temperature are zeolites and MOFs due to their textural, structural, and chemical properties.[2,3] On the other side, layered double hydroxides (LDHs) or layered double oxides (LDOs), obtained through the thermal activation of LDHs, were shown to readily adsorb CO_2 at elevated temperatures. [4] However, to increase their industrial applicability, all these powder adsorbents should meet important requirements such as low cost and availability into already shaped form.

In this work, different 3D printed materials were produced by Direct Ink Writing and evaluated as possible CO_2 adsorbents: a binderless Lynde type A (LTA) zeolite monoliths and a bentonite-MOF (F4_MIL-140A(Ce)) composite for capture at medium-low temperature (25-100°C) and a geopolymer-LDH ($Mg_3Al_1CO_3$) composite scaffolds for adsorption at elevated temperature (300°C).

After a basic characterization, capture tests were carried out measuring pure CO_2 adsorption/desorption isotherms at different temperatures. Dynamic breakthrough measurements were also performed using different geometries (Figure 1a) to evaluate the effect on the dynamic CO_2 adsorption. Interestingly, all the monoliths exhibited a CO_2 adsorption capacity comparable to the powder materials (see Figure 1b for 3D LTA monoliths). For the geopolymer-LDH composite regeneration strategies were also evaluated to obtain a stable performance through several adsorption cycles.

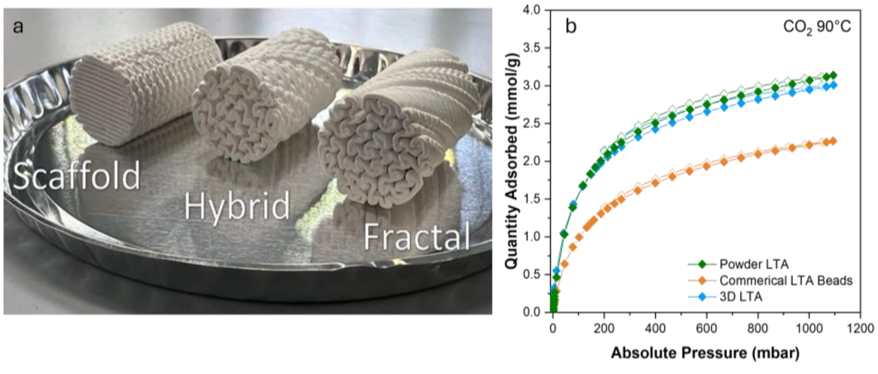

Figure 1. Binderless 3D printed monoliths of LTA zeolite in different geometries (a) and CO_2 adsorption/desorption isotherms at 90°C of Binderless 3D LTA printed monoliths in comparison with powder and beads commercial LTA samples (b).

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FC2

COFFEE SILVER SKIN AS ADSORBENT TO REMOVE NORFLOXACIN FROM WATER

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Coffee Silver Skin (CSS), the coffee roasting factories' by-product,[1-3] has been recycled as adsorbent material for water treatment to remove Norfloxacin, a fluoroquinolone antibiotic classified as a Contaminant of Emerging Concern (CECs).[4,5] The adsorbent was obtained by washing the CSS with water, and its main features were investigated before and after the pollutant removal, by adopting synergically ATR-FTIR, SEM, and TG techniques. UV-Vis spectroscopy was employed to monitor the antibiotic concentrations in water during adsorption. The role of various experimental parameters, like adsorbent/pollutant amounts, pH, and ionic strength, in the adsorption process was examined to elucidate the adsorption process and the nature of adsorbent-adsorbate interactions. Adsorption isotherms, kinetics, and thermodynamics were also studied to clarify the process and the adsorbent's characteristics. Moreover, to increase the adsorbent operability, the application of desorption and Advanced Oxidation Processes (AOPs) was proposed to remove the pollutant from the CSS surface. Particularly, in line with the sustainability principles, the desorption approach was performed by adopting water at 50 °C or diluted salts solutions. On the other hand, different AOPs based on UV, TiO_2, and H_2O_2 were studied to degrade adsorbed antibiotic onto CSS. Hence, the best experimental conditions were set for both approaches and conducted to reuse CSS for several cycles, retaining the adsorption performance of the proposed substrate.

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FC18 STRUCTURAL AND THERMODYNAMIC STUDY OF A NEW HYDRATE EUTECTIC SALT

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The search for new liquid media capable of meeting the requirements of efficiency, cost-effectiveness, eco-friendliness, and low toxicity is a critical area of current chemistry research.

In this context, over the past few decades, ionic liquids [1], molten salts used as PCMs (Phase Change Materials) [2], and DES (Deep Eutectic Solvents) [3] have emerged as promising classes of solvents with applications among others as electrolytes and extractive liquids. From this perspective, it is evident that a deeper understanding of the microscopic behavior of these complex systems will aid in elucidating macroscopic fluid phenomena, guiding research toward optimizing their applications [1].

In this study, eutectic and molten salt chemistry are combined to obtain a novel room temperature liquid mixture of two inorganic hydrate salts: $CoCl_2 \cdot 6H_2O$ and $Zn(NO_3)_2 \cdot 6H_2O$.

By employing spectroscopic and thermal analyses, it was possible to fully characterize the structure and the thermodynamic properties of the solvent. As widely known from literature, the physicochemical properties of the system can be tailored by using cosolvents, often offering good advantages in terms of cost and efficiency. For this reason, the effects of adding water at different concentrations were also investigated.

The metal speciation has been probed with X-ray Absorption Fine Structure (XAFS) experiments performed with synchrotron light, providing insights into Zn^{2+}, an ion not easily detectable by conventional techniques [4]. Calculation of theoretical signals and fitting of the experimental data were performed with the GNXAS software package, while Principal Component Analysis (PCA) was used to extrapolate the number and concentration of the Zn^{2+} complexes in the $CoCl_2 \cdot 6H_2O$:$Zn(NO_3)_2 \cdot 6H_2O$:water mixtures with different 1:1:water ratios.

The XAFS results were then combined with conventional UV-Vis and NIR measurements, confirming the previous findings. The medium and long-range structure was instead probed with X-ray diffraction, again obtained with synchrotron light. Moreover, thermal behavior (particularly important for the application of these kinds of systems) was assessed using thermogravimetric and calorimetric analysis.

The multi-perspective approach used in this research provides a detailed and comprehensive understanding of the system, offering valuable insights into the potential technological employment of the solvent.

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FC19

THE ELUSIVE NATURE OF Si (111)-7X7 SURFACE

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Two stable allotropes of silicon are known to occur on Si111 surfaces that produce the2×1 and 7×7 structures. The 2×1 was determined to arise from π-bonded chains of Si atoms on the surface. However, the nature of the 7×7 proved to be more elusive. A structure for the 7×7 surface was proposed and referred to as the dimer adatom stacking fault structure or DAS. Recently the nature and our understanding of the Si (111)7x7 surface has been questioned [1-3] due to the failures of all DFT calculations to describe various properties of this system [4]. The most obvious is the ground state of the widely accepted DAS structure that shows a metallic electronic structure whereas numerous experiments show a gapped electronic structure near E_f. In addition, several structural measures including X-ray measurements show that the height of the adatoms predicted is at least 0.2 Å smaller than those measured, an error well beyond the accepted accuracy of DFT calculations. Here we present DFT calculations that more accurately describe the exchange-correlation, k-pt sampling and the surface point group symmetry of the 7x7 than considered previously. Calculations of the DAS structure using VASP are shown to relax to a new lower energy structure with distinctly different properties. Several other more subtle paradoxes such as the incorrect symmetry of both the Patterson map as well as the systematic lateral distortions in the adlayer are also corrected predicted.

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FC9

MECHANICISTIC INSIGHTS INTO BETA-3 ADRENERGIC RECEPTOR MODULATION VIA MOLECULAR DYNAMICS SIMULATIONS

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G-protein coupled receptors (GPCRs) are key signaling proteins whose activation by agonists initiates numerous physiological processes [1]. The human β_3-adrenergic receptor (β_3AR) is a class A GPCR of therapeutic interest for vasodilation and metabolic disorders. Although mirabegron is recognized as a β_3AR agonist [2], the activity of SR-59230A remains under debate, with evidence suggesting both antagonist and partial agonist behavior [3] (Figure 1).

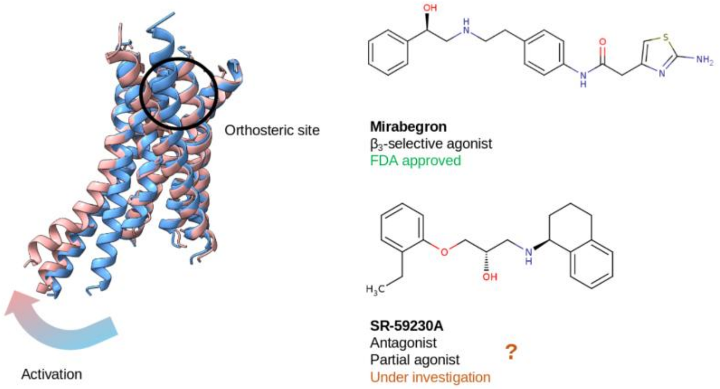

Figure 1. On the left the aligned active (red) and inactive (blue) states of the β_3AR, on the right the ligands under study.

In this study, we elucidate the molecular mechanisms by which these ligands affect the configurational landscape of β_3AR. Recently, the active structure of the human β_3AR was determined by Cryo-EM [4]; however, its inactive conformation remains unresolved. To address this, we generated an inactive-state model via homology modeling using the available turkey β_1AR structure [5].

Our molecular dynamics simulations of the apo receptor revealed an intermediate state characterized by a partial deactivation, evidenced by an inward movement of TM6. Incorporating the G-protein to maintain a fully active conformation, we performed ensemble docking to capture dynamic receptor fluctuations and obtain initial binding poses for both receptor states.

Notably, µs-long MD simulations demonstrate that SR-59230A-bound β_3AR (in the absence of G-protein) persists in an active-like conformation, supporting its classification as a partial agonist.

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FC3

DEVELOPING SOLID-STATE NMR METHODS TO PROBE SURFACES IN LEAD HALIDE PEROVSKITES

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Lead Halide Perovskites (LHPs) with general formula $APbX_3$ (where A^+ = methylammonium (MA^+), formamidinium (FA^+) or Cs^+ and X^- = Br^-, Cl^- and I^-) are attracting significant interest for many optoelectronic applications, particularly in solar cells and light emitting diodes (LEDs), thanks to their remarkable properties such as high absorption coefficients, long charge carrier lifetimes and diffusion lengths, combined with the low cost of materials and ease of processability [1]. However, a major issue to be addressed is the instability over moisture, temperature and/or oxygen exposure of 3D perovskites [2,3]. A promising strategy to enhance their environmental stability consists in reducing the dimensionality from 3 to 2 dimensions [3]. Recently, the combination of 2D/3D perovskites has established itself as one of the most attractive approaches, as they combine the stability of 2D systems, with the high performances of the 3D counterparts [2]. Most perovskite-based devices rely on polycrystalline thin films, which, while easy to fabricate, suffer from high instability in humid environments and are prone to grain boundary defects and structural disorder. These factors promote non-radiative recombination, thereby limiting device efficiency. One way to overcome these limitations is employing perovskite single crystals (SCs).

The knowledge of atomic level structure and dynamics is fundamental to achieve a deep comprehension of the properties of perovskites materials. In this view, solid-state NMR (SSNMR) spectroscopy has established itself as a powerful technique to investigate perovskite materials at the atomic level, providing information on dopant incorporation, phase segregation, halide mixing, local dynamics [5]. Preliminary studies also proved the potential of SSNMR to investigate surfaces and interfaces [6].

The main goal of this work is to develop tools for the characterization of the surface/interface properties in 2D/3D structures, by combining crystal engineering for isotopic enrichment of surfaces and SSNMR methods.

To this aim, a surface modification with isotopically enriched cations (^2H-enriched MA^+ on the methyl group, $CD_3NH_3^+$) in $MAPbI_3$ and $MAPbBr_3$ powder and single crystal perovskites was performed using two different synthetic approaches. The successful substitution of $CH_3NH_3^+$ by $CD_3NH_3^+$ was probed by the direct observation of ^2H NMR static spectra on both SCs and powders. Furthermore, surface properties were investigated through ^2H spin-lattice relaxation time measurements, providing deeper insights into the structural and dynamic behavior of the modified perovskite surfaces.

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FC4

INVESTIGATING THE PERSISTENT LUMINESCENCE IN $Cs_2(Ag_xNa_{1-x})InCl_6:Mn^{2+}$ DOUBLE PEROVSKITES

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Persistent Luminescence (PeL) is a phenomenon in which a material continues to emit light for extended period after removing the excitation source (X-rays, electrons, or ultraviolet/visible light). This effect arises from metastable localized electronic levels in the bandgap that temporarily store the excitation energy. While the majority of PeL materials (>75%) are oxides, recent studies have demonstrated the occurrence of PeL in bulk halide double perovskites (HDPs) as well. Notably, $Cs_2(Ag_xNa_{1-x})InCl_6:Mn^{2+}$ single crystals (SCs) exhibit a persistent red emission (~620 nm) for over an hour after UV excitation. However, moving from bulk to nanostructured samples the PeL disappears (scheme in Figure 1a) [1-4].

In this work, we investigate the impact of stoichiometry, size and shape on the PeL behavior of HDPs. We synthesized various compositions of $Cs_2(Ag_xNa_{1-x})InCl_6:Mn^{2+}$ SCs and extended our study to their micrometric and nanometric counterparts, including nanocubes (NCs) and nanoplates (NPs). To understand the underlying mechanisms, we performed optical analyses, including photoluminescence excitation, photoluminescence, PeL, and thermally stimulated luminescence measurements across a broad temperature range (10 K–450 K). Since PeL is related to the presence of trapping sites, which may originate from local structural defects, we further investigated these defects using X-ray Powder Diffraction, Pair Distribution Function analysis (across 15 K and 373 K), and X-ray Absorption Near Edge Structure (XANES) spectroscopy at the K-edge of Mn (the emissive center) at three different temperatures: 15 K, 290 K and 430 K.

Our results indicate a strong size-dependent behavior. We hypothesize that the PeL disappearance from bulk to nanocrystals is ascribed to differences in the position of the traps in the bandgap between bulk and nanostructured samples. In addition, from the XANES analysis, the pre-edge peak is broader for the bulk sample (Figure 1b), so we hypothesize that in the bulk sample, Mn coexists in the 2+ and 3+ oxidation states, with the 3+ responsible for the PeL.

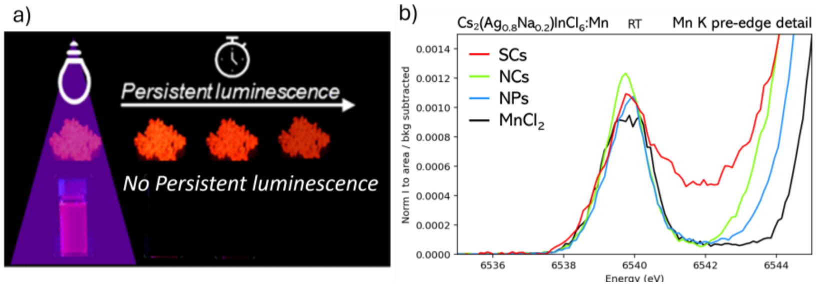

Figure 1. a) PeL disappears at RT moving from bulk to nanostructured samples in $Cs_2(Ag_xNa_{1-x})InCl_6:Mn^{2+}$ compounds; b) XANES at Mn K-edge at RT for $Cs_2(Ag0.8Na0.2)InCl_6$:Mn SCs, NCs, NPs samples and MnCl2: Mn K pre-edge detail.

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FC5

POTENTIAL HYDROGEN PRODUCTION METHODS FROM INDUSTRIAL WASTEWATER

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Hydrogen (H_2) is regarded as the most promising and significant fuel for the future because of its incredible capacity to reduce pollution and improve the environment. Hydrogen has gained considerable attention in recent years as a promising sustainable clean energy source. As a result, there is a growing global interest in reducing the greenhouse effect and other environmental pollutant gases. Significant research and investment in hydrogen production technologies are necessary to achieve a fully developed hydrogen economy and make hydrogen a vital component of the energy market. The objective is to make hydrogen production systems more efficient, economical, dependable, safe, and adaptable to a variety of end-user requirements, including small/large scale, portable/stationary, and so on. This study is mainly focused on both hydrogen production and its potential from synthetic wastewater or real industrial wastewater treatment. These include different industrial wastewaters from food processing such as sugary wastewater, beverage wastewater, rice winery wastewater, brewery wastewater, dairy wastewater, cattle wastewater, probiotic wastewater, tannery wastewater, olive mill wastewaters, coffee drink manufacturing wastewater, and the filtered leachate of municipal solid wastes. It can be suggested that they are excellent potential for the production of H_2 from wastewater-containing carbohydrates. Therefore, the present study summarizes more attention to solar driven hydrogen production from wastewater, by highlighting the potential of several technologies for simultaneous water treatment and green hydrogen production from wastewater.

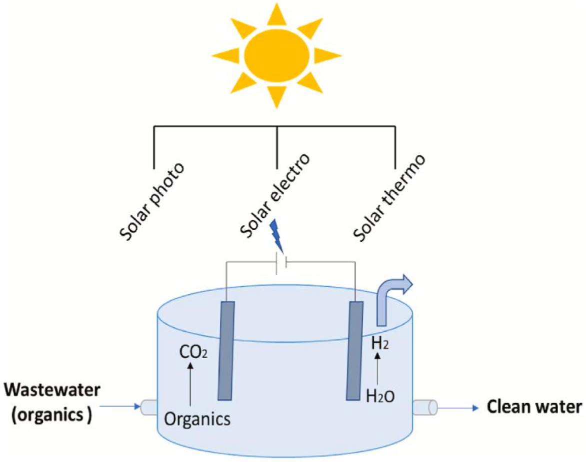

Figure 1. Solar-driven hydrogen production.

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FC10

UNVEIL OXYGEN TRANSPORT FEATURES OF HEMOCYANIN: A QM/MM-NEVPT2 PERSPECTIVE

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Modeling oxygen transport in hemocyanin (Hc) remains challenging due to the multireference nature of the Cu_2O_2 core and its structural flexibility, which allows for multiple isomeric forms, such as peroxo and bis-µ-oxo configurations [1-6], significantly influencing Hc response to oxidative stress and reactive oxygen species (ROS). Therefore, in this study, we employ advanced quantum mechanics/molecular mechanics (QM/MM) approach at the multireference NEVPT2 level of theory (QM[NEVPT2]/MM) [8,9] to explore the oxygen-binding mechanism and the peroxo-to-bis-µ-oxo isomerization in Hc (Figure 1) [10]. While Density Functional Theory (DFT) is effective in predicting oxygen binding, it struggles to accurately describe highly correlated electronic states, such as superoxide species and mixed Cu_2 oxidation states. In contrast, NEVPT2 provides a more reliable description by accounting for both static and dynamic correlation effects [8]. Integrating NEVPT2 within a QM/MM framework enables us to capture both electronic complexity and the influence of the protein environment at a feasible computational cost. Our results align with the previously proposed Hc oxygen binding mechanism [1,6], involving two nearly simultaneous electron-transfer (ET) steps and a triplet-singlet intersystem crossing (ISC). However, we find that the first ET step occurs prior to ISC, resulting in the formation of a stable singlet superoxide intermediate through a low-energy barrier. The second ET leads to the formation of a singlet oxy-hemocyanin species featuring the characteristic peroxo-Cu_2 O_2 "butterfly" core. Furthermore, QM[NEVPT2]/MM simulations reveal a lower-energy barrier for the peroxo-to-bis-µ-oxo isomerization compared to QM[DFT]/MM calculations. However, the peroxo form remains energetically favored within the protein environment. Overall, our findings offer new insights into the behavior of the hemocyanin active site, highlighting the importance of considering both electronic correlation and the protein environment in accurately modeling copper-oxygen interactions in biological systems.

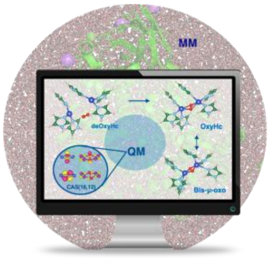

Figure 1. Scheme of QM[NEVPT2]/MM approach to unveil oxygen binding and peroxo-to-bis-µ-oxo isomerization in Hc.

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FC11

CONTROLLING THE SIZE AND STABILITY OF AMORPHOUS CALCIUM PHOSPHATE-BASED PARTICLES: INNOVATIVE STRATEGIES AND APPLICATIONS

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The ability to control the size of nanoparticles is crucial for their application in nanomedicine (such as in drug delivery, targeting, imaging) as it plays a key role in regulating the *in vivo* transport behavior due to the existence of multiple physiological size thresholds within the body and size-dependent nano-bio interactions [1]. In this scenario, amorphous calcium phosphate (ACP)-based nanoparticles represent a promising class owing to their biocompatibility, biodegradability, bio-relevance, low cost, pH-responsiveness and porous nature that allows for the loading of active molecules. Despite such premises, their use in the biomedical field is hindered by the tendency to aggregate in aqueous media, typically forming micron-sized structures that are also susceptible to crystallization. The challenge of obtaining stable ACP-based particles, both in terms of size and phase, is thus open. In this scenario, this contribution will showcase some strategies developed by our group for the preparation of ACP-based particles with tunable size and stability, focusing on the physico-chemical understanding of the formation mechanism and interactions with stabilizing agents (Figure 1). We will show that the glycoprotein Fetuin-A, either alone or in combination with albumin, is able to reduce ACP particle size from several microns to a few hundreds of nm, and to delay the amorphous to crystalline transition in a concentration-dependent fashion [2,3]. Besides proteins, we will show that bisphosphonates (alendronate and etidronate) can modulate the size of ACP-based nanoparticles, due to their interaction with Ca^{2+} ions in solution during particles' formation. The role of polyacrylic acid in achieving ACP-based particles with excellent re-dispersibility will also be outlined [4]. All these systems were studied taking advantage of a multi-technique approach which included, among others, the analysis of the size in solution by means of dynamic light scattering, the morphology with electron microscopy techniques, the crystallinity by combining X-rays diffraction and IR spectroscopy and the thermal properties. Overall, our results provide valuable insights into the preparation of ACP-based nanoparticles with tunable size and crystallinity, paving the way for the application of these promising platforms in nanomedicine.

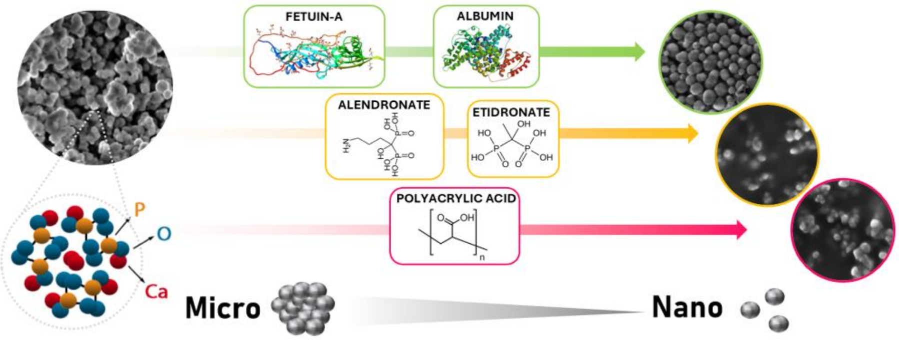

Figure 1. Graphical abstract of the contribution.

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FC12

SOLID-STATE NMR STUDY OF STRUCTURAL AND DYNAMIC PROPERTIES OF THE TWO POLYMORPHS OF LEFLUNOMIDE

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Active pharmaceutical ingredients (APIs) in solid formulations are influenced by their chemical and physical properties in the solid-state, impacting crucial characteristics like solubility and stability [1]. Polymorphism, the ability of a compound to exist in multiple solid forms, significantly affects these properties [2]. Leflunomide, a Disease Modifying Antirheumatic Drug (DMARD) primarily used for rheumatoid arthritis[3], exhibits two known polymorphs, Form α and Form β. While their structures are known [4,5], dynamic insights remain unexplored. Here, we utilize solid-state Nuclear Magnetic Resonance spectroscopy (ssNMR) to characterize the structural and dynamic aspects of leflunomide polymorphs. High-resolution spectra of various nuclei (^{1}H, ^{19}F, ^{13}C and ^{15}N) (Figure 1) allowed the differentiation of the two forms, confirming their structural properties, and provided further insights into their intermolecular environment. The measurement and analysis of spin-lattice relaxation times enabled the quantitative characterization of internal motions in terms of activation energies and correlation times. This comprehensive study enhances our understanding of leflunomide polymorphs and underscores the utility of ssNMR in pharmaceutical research.

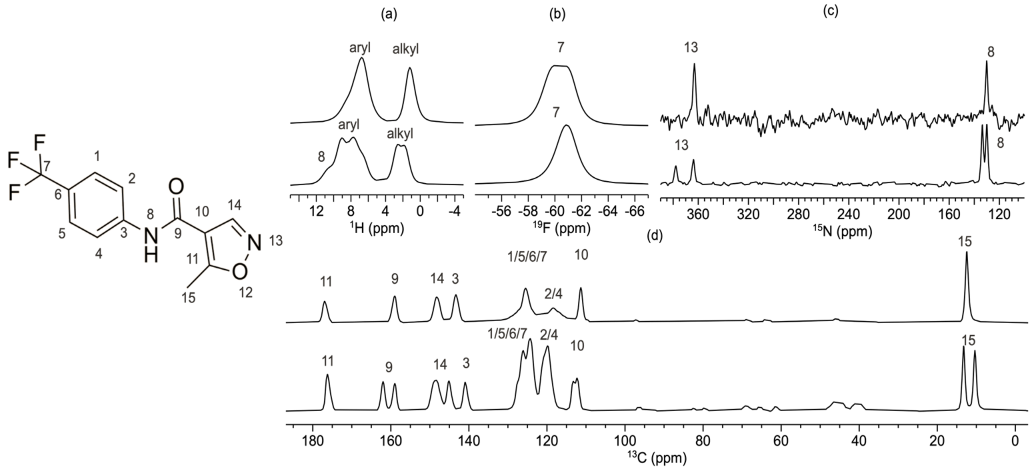

Figure 1. ^{1}H (a), ^{19}F (b), ^{15}N (c) and ^{13}C (d) MAS spectra of the two different polymorphs of the active ingredient Leflunomide, α and β with signal assignment.

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FC6

SYNTHESIS AND SOLID STATE NMR CHARACTERISATION OF POLYKETONE-BASED ANION EXCHANGE MEMBRANES

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The need for a green transition requires new ways to produce and store energy. Among different possibilities, green hydrogen is emerging as a promising strategy to decarbonize various sectors of human activity. Green hydrogen can be produced with different setups, and, among them, anion exchange membrane water electrolysis (AEM-WE) is considered the most appealing to achieve high productivity at low cost. However, AEMs are not yet ready for large-scale applications and still suffer from several limitations that affect the lifecycle and efficiency [1].

Because of this issue, different polymeric backbones and charged groups can be tested to tune properties to a satisfying level [2].

In this abstract, we present our research concerning AEMs for water electrolyzers based on a functionalized low molecular weight polyketone (PK). We report the functionalization of PK via a Paal-Knorr reaction using 1-(3-aminopropyl)piperidine. The obtained polymer can then be used in a casting/quaternization procedure in the presence of alkyl iodides to obtain an AEM [3].

We employed different diiodides, ranging from diiododecane to diiodobutane, together with iodobutane in different ratios to explore thermal and mechanical properties of the resulting membranes.

We characterized the membranes with common techniques coupled with Solid State NMR (SSNMR). Specifically, multinuclear SSNMR was used to seek evidence regarding the cross-linking process. Low field proton spin-lattice relaxation times have also been measured as a function of temperature to understand the polymer behavior near the glass transition.

Acknowledgments: PRIN PNRR 2022 "In MoTion-Influence of dynaMics on the adsorption and Transport properties in polymeric materials for membrane technologies" funded by the European Union - Next Generation EU is acknowledged for financial support.

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FC20

EXPERIMENTAL RECONSTRUCTION OF HISTORICAL DAGUERREOTYPES AND PHOTOMECHANICAL REPRODUCTION PROCESSES

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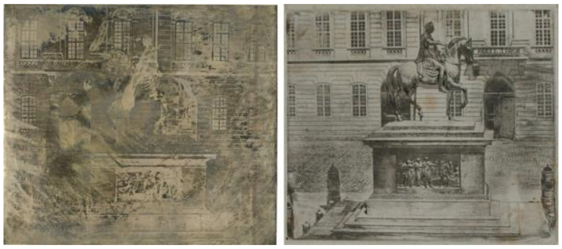
Two crucial techniques were developed in the late 1830s that significantly influenced the graphic arts and the quantity of print runs. Electrotyping [1] was successfully used for the production and reproduction of printing plates shortly after its invention by the German physicist Moritz Hermann von Jacobi in 1838. Photography [2] is the second pioneering innovation within this context, developed and published by Louis Jacques Mandé Daguerre just one year later in 1839. Initially, the process could only be used to depict landscapes due to the lack of technical equipment and long exposure times. However, a number of technical advances, which were developed in Vienna in the early years in particular, led to serious improvements in the quality but also to a shortening of the exposure time enabling first portraits to be taken. This pioneering development was based on the photosensitivity of the halides Br, Cl, and not only I, on a silver-plated copper support plate [3]. Moreover, reproduction of large numbers of prints from daguerreotypes through the direct application of a new etching technique on daguerreotypes and their galvanic reproduction became possible for the first time (Figure: Etched Daguerreotype and print).



The surface morphology and elemental composition of historical daguerreotypes from museum collections have been analysed [3,4]. In addition to ageing and corrosion features studied by optical microscopes and SEM/EDX, µXRF scanning was used to see how image information is stored in the nanoparticles. Moreover, daguerreotype series were produced according to controlled parameters in order to enable a better interpretation of the aged and light-damaged daguerreotypes, but also to identify the sensitisation, exposure and development processes used. The etched plates produced in this way were used for printing. The durability and the mechanical properties of these etched plates together with the quality of the prints were investigated. This study compared the chemistry and morphology of historical and new daguerreotypes in order to assess the historical manufacturing processes.

Acknowledgments: Partial funding is acknowledged by the Project PHELETYPIA, “The impact of early photography and electrotyping media on the creation of images and contemporary art", Heritage 2020-060 PHELETYPIA, Heritage Science Austria grant program of the Austrian Academy of Sciences.

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FC13

A NEW ROUTE FOR SYNTHESIZING LOW-POLYDISPERSITY HYDROXYPROPYL CELLULOSE NANOGELS

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Hydroxypropyl cellulose (HPC) nanogels were synthesized using a novel methodology. In our approach the optimal synthesis conditions for different HPC molecular weights were determined by correlating surfactant concentration and reaction temperature through dynamic light scattering (DLS) analysis of the solution dispersity. The results indicate that the polymer chains remain in a monodisperse phase at elevated temperatures (78°C) and at surfactant concentrations above the critical micellar concentration (cmc) of dodecyltrimethylammonium bromide (DTAB). By means of this new route it is possible to synthesize nanogels with low polydispersity. The polymeric network was crosslinked using divinyl sulfone. The dependence of the nanogel size on the crosslinker concentration was characterized under synthesis conditions equal to 78°C and 2 cmc of DTAB. DLS measurements revealed that the nanogel size decreases with increasing crosslinker molarity. Furthermore, the internal structure of the nanogels was characterized as a function of temperature using small-angle neutron scattering (SANS).

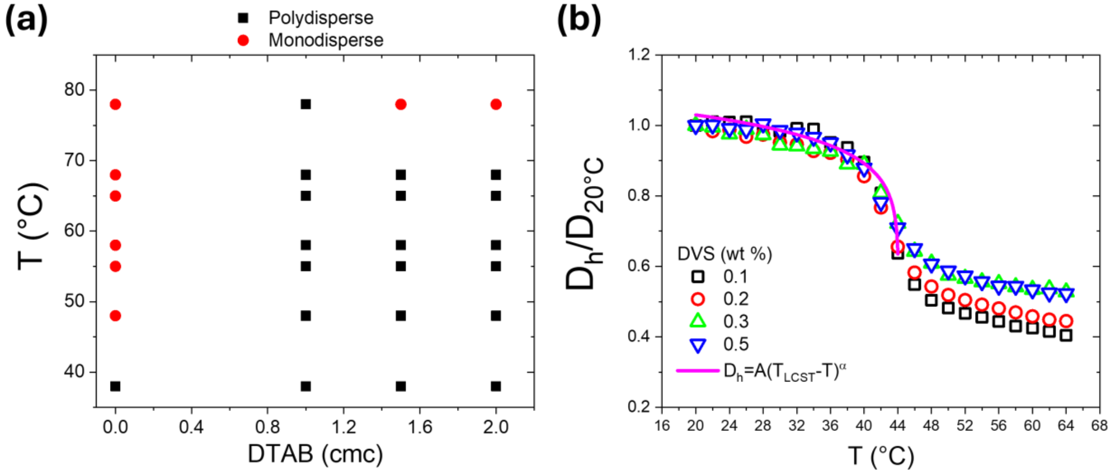

Figure 1. (a) Phase diagram of polymer Hydroxypropyl cellulose (HPC) as a function of the surfactant concentration. (b) Temperature dependence of the hydrodynamic diameter (D_h) normalized by D_h=20°C as a function of the temperature.

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FC14

PVA-SHELLED PERFLUOROCARBON DROPLETS AS A VERSATILE PHASE-CHANGE PLATFORM FOR OCCUPATIONAL DOSIMETRY OF IONIZING RADIATION

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Within the broad domain of imaging and theranostics, phase-change perfluorocarbon microdroplets (MDs) are of crucial importance thanks to their ability of efficiently converting into echogenic and optically detectable microbubbles, when exposed to ultrasound (US), laser and ionizing radiation (IR) beams [1]. Recently, the use of such systems has demonstrated to be an invaluable and new radiosensitive tool for external and internal IR dosimetry [2]. Regarding this, a key concern is the significant increase in professional use of IR during the last 20 years [3]. People involved in the production, testing and use of IR source machines exhibit a higher risk of tumor growth [3]. Hence, it is of fundamental urgency the development of a system able to evaluate the exposure to IR and process the signal rapidly and in real-time. Substantial progress in this respect can be pursued optimizing MDs stability, sensitivity, chemical versatility and synthesis efficiency.

Here we introduce a new dosimetry system based on meso-droplets (DPs) with a polymer shell of polyvinyl alcohol (PVA) and a perfluorocarbon core (alternatively DFP, decafluoropentane, and/or PFP, perfluoro-n-pentane). The latter can undergo liquid-vapor phase transition upon interaction with US, hadrons and X rays, leading to the formation of echogenic bubbles. Thanks to the possibility of detecting vaporization events by echography and optical imaging rapidly, this platform offers the chance of intervening immediately in case of accidental high-dose exposure. Furthermore, given the last technological advances in terms of artificial intelligence (AI), these techniques could also be coupled to informatics tools for a faster image analysis.

We developed and optimized different synthesis methods according to the system chemical composition and the employed homogenization technique. The final products were characterized in terms of morphology, mean diameter and number density by optical and confocal laser scanning microscopy (CLSM); exploiting the chance to introduce different fluorescent dyes inside the DPs core (Nile-Red) or linked to the shell surface (FITC). In order to obtain a wearable dosimeter for occupational use, we encapsulated these DPs inside "ergonomic" hydrogels before exposing them to US, hadronic irradiation and X rays in different dose ranges. Our results show that the platform morphology is modified after exposure both in water and in gel matrices and that the signal is clearly detectable in rapid time scales by a vast spectrum of imaging techniques. According to these promising outcomes, we aim to present this platform in the near future as an innovative and versatile professional dosimeter.

Acknowledgments: the research was funded by INAIL under the grant agreement BRiC2022 ID53.

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FC15

DEVELOPMENT OF INNOVATIVE BARIUM PECTINATE GELS BY IONOTROPIC CROSS-LINKING OF HIGH AND LOW METHOXYL PECTIN USEFUL FOR BIOMEDICAL APPLICATIONS

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Pectin has garnered significant attention for its potential as a sustainable alternative to fossil fuel-derived materials. Its versatile properties make it applicable across a wide range of fields, including food products, biomedical applications, and tissue engineering [1-4]. Pectin is a complex polysaccharide primarily composed of D-galacturonic acid (GalA) and rhamnogalacturonan. It is found in the cell walls of plants, where it plays a crucial role in maintaining the structural integrity of plant tissues [5].

In the study reported in this contribution, pectin, extracted from the residual citrus peels remaining after the extraction of essential oils, was ionotropically cross-linked using barium and calcium ions.

In particular, the ionotropic cross-linking has been studied in the high concentration domain, in which pectin behaved as non-Newtonian fluid. The rheological analysis showed that cross-linking is effective for both low and high methoxylated pectins. Moreover, the strength of the pectin gel depends on the molecular weight and the degree of methylation of pectin, and the pH as well. Indeed, by comparing the gels obtained with $BaCl_2$ and $Ba(OH)_2$, the latter showed significantly higher storage modulus values, indicating a stronger gel. Finally, the results highlight a higher affinity of barium ions for pectin compared to calcium ions. Overall, these findings are promising for the use of these gels in 3D printing, as the improved viscoelastic properties could allow the use of these gels without the need for covalent cross-linking by cross-linking agents, which are not always environmentally friendly and biocompatible. Furthermore, the presence of barium ions could pave the way for the use of these gels in the biomedical field as contrast agents with limited side effects.

Figure 1. Different samples of pectin from different citrus fruits on the left, 3d printing test in the middle, 3D extrusion printer on the right.

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FC21

THE PROCESS OF PHYSICAL CHEMISTRY BECOMING A SCIENCE

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There are some approaches about the development of physical chemistry as an independent discipline in the world. For example, one of them is evaluating the contents of it, and it can go to the beginning of the modern chemistry. Another approach is to accept the terminology of physical chemistry in scientific literature. In the middle of 18. century (1752-54), Russian scientist Lomonosov had used this term firstly. Lomonosov had written a book named ''An Introduction into True Physical Chemistry'', also ''A Plan to a Course in Physical Chemistry'' and ''Experiment in Physical Chemistry''. Then, Wallerius written ''Chemica Physica'' and also Spielman written ''Chemie Physique'' in 18. century respectively. Also, Scheele, Davy, Thenard, Berzelius, Volta, Lavoisier, etc. had studied on physical chemistry in 18.-19. centuries. In 1887, the Oswald, Nerst and Van't Hoff had published the first journal named as ''Zeitschrift für physikalische Chemie'' at Leibzig University, so that ''physical chemistry'' had become an independent discipline by this way. In ''Chemistry In Britain Journal'', Oswald has named as ''the father of physical chemistry'' in 2003. At 23 November 1923, the first physical chemistry lesson added into the curriculum in Turkey. From 18.c. to now, there are many developments is this scientific branch in all over the world.

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THE ROLE OF WATER IN CO_2 PHYSISORPTION INSIDE MESOSTRUCTURED SILICA: INSIGHTS FROM MOLECULAR SIMULATIONS OF FUNCTIONALIZED MCM-41

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Mesoporous silica-based materials are widely utilized in adsorption and catalysis due to their high surface area and tunable textural features. The surface chemistry can be tailored through the addition of a variety of functional moieties, by exploiting the native surface silanol groups [1]. Among them, MCM-41 is an ideal model, characterized by a highly ordered 2D hexagonal pore symmetry. Most of the previous studies have focused on amine-functionalized materials for CO_2 capture through chemisorption. Physisorption, although crucial in dictating gas uptake and molecular orientation before chemisorption occurs, remains underrated and less explored. Similarly, despite many investigations have provided evidence of the role of humidity in the adsorption performance of these materials, conclusions are inconsistent [2-4].

This work extends our previous studies [5-7] by adding water molecules into the computational models of both bare and aminopropyl-functionalized MCM-41. By using Grand Canonical Monte Carlo and Molecular Dynamics simulations, water adsorption was first analyzed at different relative humidity. Bare MCM-41 exhibited greater water uptake than its functionalized counterpart, due to the preferential interaction of water molecules with the silanol groups. In the functionalized MCM-41, water preferentially adsorbs in silanol-rich regions but, at higher humidity, progressively infiltrates the spaces between aminopropyl chains forming a network of H-bonds with both silanol and amine groups. Then, physisorption of CO_2 and CH_4 was investigated at different humidity and pressures. CO_2 was found to preferentially interact with both the silanol groups and the adsorbed water molecules, while the probability of contacts with the amine groups was remarkably low. This was not due to the competition between CO_2 and water for the surface sites, since the same observations were previously reported in dry conditions [7]. Overall, the adsorption capacity, selectivity and gas diffusivity were not significantly altered by the presence of water, up to the maximum humidity tested (15% RH). In agreement with the literature [3,4], this result would imply no need for strict control of humidity prior to material's application as sorbent. We moved further with a series of statistical analyses of the simulation trajectories in order to characterize molecule relative orientation and position in the mixed adsorbed layers in detail. The goal was to clarify whether the presence of water molecules might favor the correct orientation of CO_2 and the amine groups, thus promoting their reaction during the stage of chemisorption.

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FC8

TAPPING INTO CHARGE STORAGE WITH OPERANDO-XPS USING MULTI-LAYER-GRAPHENE ELECTRODES IN CONTACT WITH A MIXED IONIC LIQUID MEDIUM

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X-Ray Photoelectron Spectroscopy (XPS) under bias is used to track both changes in surface population of various entities as well their electrical potentials on two multilayered graphene electrodes, configured as a coplanar-capacitor, having an ionic liquid mixture consisting (TFSI-) anions but different cations (DEME+ and Rb+), as the electrolyte. As the capacitor is electrified by increasing bias in steps of 0.5 until 3.5 V, intensity enhancement of peaks representing ions is accompanied by depletion of C1s peak of graphene electrodes, under both positive and negative bias. Peak positions shift to higher/lower binding energies under positive/negative bias, since kinetic energy of photoelectrons decreases/increases, such that they are as the most direct reporters of the local electrical potential(s). Under bias, although intensity ratio of anionic to cationic N1s peaks exhibit an increase, this change is compensated by an increase of the other cation Rb+, to preserve electro-neutrality. The schematic representation of the co-planar capacitor device with one electrified and one grounded multilayer graphene electrode is shown in Figure 1(a). The chemical structure of DEME cation, TFSI anion and Rb cation making up the electrolyte is shown in Figure 1(b). XPS Survey and other spectral regions are shown in Figure 1(c). C1s region grounded and under +2.5 V bias is shown in Figure 1(d). This information provides valuable insights for the development of new energy storage systems.

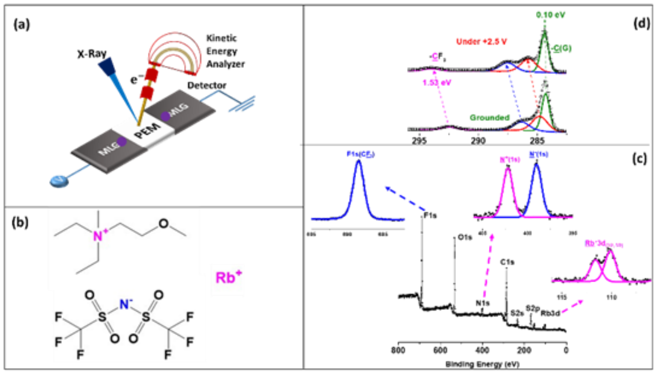

Figure 1. (a) Schematic representation of the co-planar capacitor device with one electrified and one grounded multilayer graphene electrodes. (b) Chemical structure of DEME cation, TFSI anion and Rb cation making up the electrolyte. (c) XPS Survey and other spectral regions. (d) C1s regıon grounded and under +2.5 V bias.

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FROM GELATIN TO ANIMAL GLUE: IS ADHESIVENESS REALLY RELATED TO COLLAGEN-LIKE 3D STRUCTURE?

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Gelatin-based adhesives, also known as animal glues, are reversible adhesives obtained through the partial hydrolysis of collagen, derived from processed livestock by-products. These adhesives have been used for centuries in various applications. With the advent of synthetic glues, their use has significantly declined [1]. However, there is renewed interest in understanding their properties and exploring their potential applications, particularly in restoration and wood decoration. In this study we characterized commercial animal-based glues derived from animal bone and hide tissues commonly used in restoration in Europe and three Japanese glues traditionally employed in Urushi lacquer artworks and restoration (Figure 1). In particular, we used rheology to confirm their adhesive suitability, in terms glue strength, viscosity and viscoelastic properties, XRD and FTIR to evaluate the secondary structure of gelatin before and after the application on a surface. FTIR showed a high β-structure content in all samples. The β-structure, lost in solution, was restored after drying, suggesting its key role in structure-dependent mechanical properties. Moreover, DSC evidences the presence of glues’ physical aging, essential for long-term adhesive properties [2].

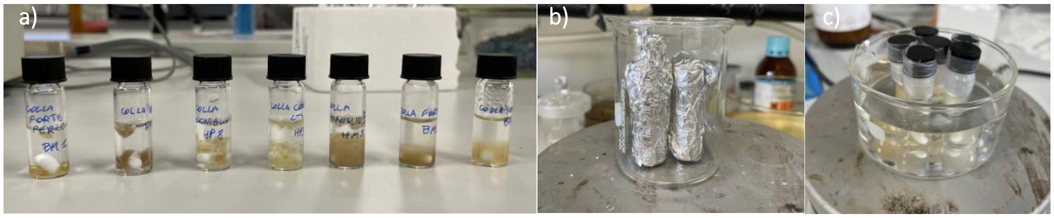

Figure 1. Production of glues’ gels: a) dissolution in water, b) twenty-four hours stirring in the dark, c) heating at 60°C for 30 minutes.

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INTERACTION OF FLUORESCENT CHROMOPHORES AND NANOSTRUCTURES WITH GRAPHENE SHEETS

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The adsorption of various molecules and nanostructures onto graphene is widely studied for applications in flexible optoelectronic devices, energy storage systems, light-harvesting technologies, and biosensing [1-4]. However, many studies do not thoroughly investigate the nature of the interaction between the adsorbed species and graphene. In this work, we offer a contribution to this topic by examining how different fluorophores interact when adsorbed onto graphene, focusing on their physicochemical properties. To this end, we selected highly emissive molecules and nanostructures as fluorophores, specifically two fluorescein derivatives and different types of carbon dots (CDs). CDs are intrinsically fluorescent, core–shell-like nanoparticles with dimensions below 10 nm, consisting of an inner carbonaceous core and an outer shell of functional groups [5]. Our study wants to provide insights into the interaction mechanisms between these species and graphene, which can occur either through the fluorophores' functional groups or their aromatic moieties. The interaction with molecular species was primarily explored by analyzing the absorption, emission, and Raman spectra of chromophore-graphene compounds in different environments. The results suggest that the selected fluorophores interact with graphene mainly through their aromatic moieties, leaving the functional groups exposed. This observation may indicate a similar interaction mechanism for CDs.

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PC1

INVESTIGATION ON THE PIEZO-PHOTOCATALYTIC ACTIVITY OF BFO-BASED NANOSCALED SYSTEMS

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Bismuth ferrite, $BiFeO_3$ "BFO", exhibits a rhombohedral structure at room temperature and the ABO_3 formula typical of perovskites; this material shows multiferroic properties, that can be mainly attributed to the ferro-electric behavior, due to the location of Bi in the A-sites, and to the magnetic order induced by the 3d orbital of Fe cation in the B ones. The ferroelectric polarization of BFO aligns along the [111] direction of the perovskite unit cell, making it a potential piezo-photocatalytic material [1] (Fig. 1).

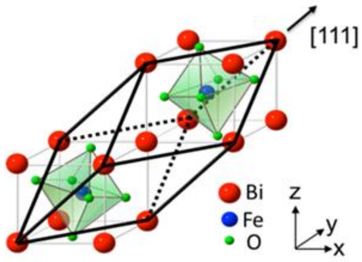

Figure 1. $BiFeO_3$ crystal structure with detail of the ferroelectric polarization alignment along [111] direction.

Single phase $BiFeO_3$ and $BiFeO_3$-based systems were prepared by a simple, one-pot, sol-gel synthesis method using amino acid glycine as chelating agent, followed by different annealing steps (first, at 300 °C for 30 min, then at 500 °C for 60min) [2]. Synthesized nanoparticles present agglomeration, with an average size of ~30 nm, as obtained by the analysis of crystallites with XRPD. The piezo-photocatalytic activity was investigated by testing the degradation of a model pollutant, i.e., Methylene Blue, in different conditions. A Xenon solar lamp (300 W) was used as the irradiation source while the sono-mechanical vibration was provided by an ultrasonic bath (35 kHz, 120 W). Various experimental conditions were considered, such as different pollutant as well as different piezo-photocatalyst's concentration, different time and temperature values. Moreover, a new ring-magnetic separator system has been developed to provide increasing magnetic field gradient to maximize the magnetic separation at a higher speed compared to traditional single magnet, which shows a significant separation of the materials and demonstrates to be a promising system to tackle the separation problem of suspended powders.

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PC2

PHYSICO-CHEMICAL CHANGES IN EARLY 1900S GELATIN-BASED PHOTOGRAPHIC FILMS: A MULTISCALE APPROACH

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This study addresses the degradation of gelatin-based photographic films from the early 1900s, highlighting the critical role of molecular-level understanding in the development of effective conservation strategies. A major challenge in previous research has been the gap between methodologies: high-resolution techniques focus on intricate details of artefacts, while low-resolution approaches assess the artefact as a whole. This methodological gap often results in an incomplete understanding of degradation processes, as detailed chemical insights are not linked to the broader spatial context.

To overcome this, the study proposes a multi-scale approach that integrates hyperspectral ultraviolet induced visible fluorescence mapping (HUVFM) and time-of-flight secondary ion mass spectrometry (ToF-SIMS). This combined methodology provides a link between microscale chemical changes and mediated macroscale chemical information. HUVFM detects fluorescence quenching in degraded areas, indicating protein and collagen degradation in the gelatin matrix. Multivariate analysis methods confirm these findings by identifying distinct spectral patterns in degraded regions. ToF-SIMS further reveals molecular and elemental changes, including loss of the protective paraffin coating and exposure of the underlying gelatin, while depth profiling maps the spatial distribution of degradation products.

The study also addresses opaque regions associated with silver reflection and proposes the oxidation-migration-reaggregation model as a plausible explanation. These findings provide insight into the interrelated chemical and structural degradation mechanisms of gelatin-based photographic films, providing valuable knowledge for their preservation.

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PC3

LAYER-BY-LAYER GROWN COPPER-BASED SURFACE-SUPPORTED METAL-ORGANIC FRAMEWORKS: A SURFACE STUDY

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Metal-organic frameworks (MOFs) are porous coordination polymers consisting of organic linkers connected to metal or metal cluster nodes. Known for their stability, porosity, and tuneable properties, MOFs have been applied in areas like gas storage, separation, catalysis, and sensing. They are also explored as precursors for high surface area materials, though their role as co-catalysts in operational photoelectrochemical cells is still under investigation.

To enhance their usability for advanced applications, MOFs—typically synthesized as powders—must be deposited onto solid substrates. Surface-supported metal-organic frameworks (SurMOFs) created using a layer-by-layer (LbL) growth method are gaining traction for integrating novel functionalities into photoelectrodes. Despite their potential, LbL-grown SurMOFs remain challenging to characterize, especially in understanding their formation mechanisms.

In this preliminary study, we investigated the growth of a copper-based SurMOF (HKUST-1) on a flat thermal SiO_2 substrate pre-treated with a zirconium phosphate layer. In order to characterise the SurMOF at different stages of its formation, we used a combination of surface techniques. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) provided detailed insights into the surface composition at the molecular level, X-ray photoelectron spectroscopy (XPS) provided semi-quantitative data on the elemental composition, while atomic force microscopy (AFM) was used to probe the surface topography, revealing morphological features of the layered structure such as roughness, uniformity and potential defects. The combination of these techniques provided a comprehensive characterisation of the SurMOF system, facilitating a deeper understanding of its growth mechanism and structural properties.

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PC4

SURFACE FUNCTIONALISATION OF ELECTRODES FOR SIMULTANEOUS POLLUTANT REMOVAL AND HYDROGEN PRODUCTION BY PHOTOELECTROCATALYSIS

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The presence of emerging pollutants in water, such as pesticides, pharmaceuticals, microplastics, organic dyes, etc. is a critical priority in today's world because of their potential negative effects on the environment and human health. At the same time, the need for a green economy with reduced use of fossil fuels has increased the need for new sustainable energy sources. A possible strategy to address both these environmental concerns, is to use water pollutants as sacrificial agents for photoelectrocatalityc hydrogen (H_2) production, converting solar energy into an energy carrier, such as H_2, while reducing water contaminations.

In this contest, titanium dioxide (TiO_2) is one of the most widely utilized material due to its promising properties. Nevertheless, it has several disadvantages including the wide bandgap that limits light absorption to the UV-A region of the solar spectrum, a low quantum efficiency and a relatively fast charge-carrier recombination.

In this study, nanostructured TiO_2-based films underwent surface modifications aimed at enhancing their photoelectrocatalytic efficiency. The goal was to achieve dual functionality: the removal of a water contaminant (Rhodamine B dye) and the generation of hydrogen within a custom designed dual-chamber reactor. To this end, the TiO_2 nanostructures, intended for use as photoanodes photoelectrocatalytic experiments, were functionalized by introducing a zirconium phosphate (ZP) monolayer to their surfaces.

The ZP-modified photoanodes showed improved performance in the simultaneous removal of dye pollutants and generation of hydrogen. These results suggest that such modified photoanodes are viable candidates for advancing an integrated approach to environmental remediation and green energy production, offering a suitable strategy for a sustainable and circular solution that contributes to both environmental protection and renewable energy production.

Acknowledgements: This work has been partially funded by European Union (NextGeneration EU), through the MUR-PNRR project SAMOTHRACE (ECS00000022)

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PC5

COPPER – BASED SILICATES: SYNTHESIS AND OPTOELECTRONIC PROPERTIES

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Alkaline earth copper silicates with the general formula $ACuSi_4O_{10}$ (where A = Ca^{2+} and Ba^{2+}) represent a family of materials known since antiquity.[1] In particular, $CaCuSi_4O_{10}$ and $BaCuSi_4O_{10}$ traced back in 2500 BC and 1200 BC, and are known as Egyptian blue and Han blue, respectively; they are characterized by an intense blue color and high stability over time.[2] Besides historical interest, the peculiar layered crystalline structure (Figure 1a and b) and their emission in the near infrared region (NIR, figure 1c) makes them interesting new materials for optoelectronic applications.[3] The chromophore group is characterized by a $[CuO_4]$ in a square planar geometry surrounding by $[SiO_4]$ tetrahedra.[4]

Recent studies have demonstrated the possibility of obtaining them in nanometric dimensions through exfoliation. This opportunity opens a new class of two-dimensional nanomaterials with potential applications in the field of biomedical imaging, solar light-to-electricity conversion devices, and IR light-emitting devices, and telecommunications.[5]

Herein, we show our recent results on the preparation of 2D nanosheets based on the aforementioned compounds and the $SrCuSi_4O_{10}$. Playing with the exfoliation conditions (e.g. temperature, solvents, surfactants) it is possible to govern the exfoliation processes. Moreover, we tried the first attempt synthesis of alkaline earth copper nano-silicates through a bottom-up strategy, following hydrothermal or colloidal synthesis.

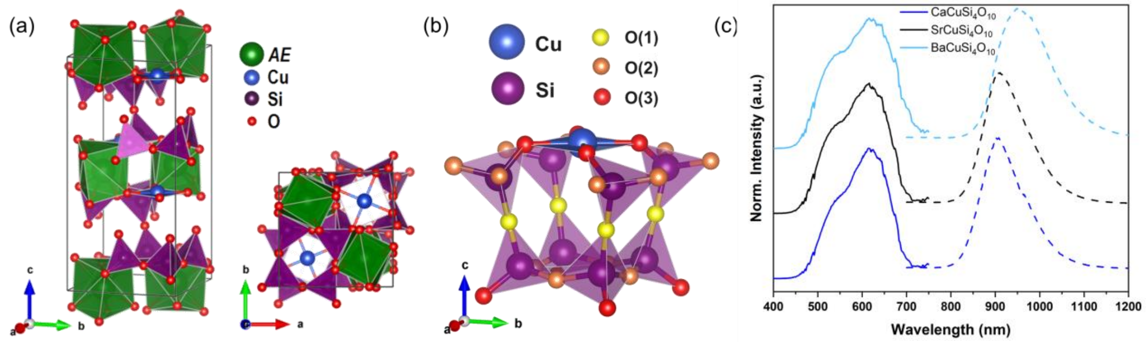

Figure 1. (a) Crystal structure of $AECuSi_4O_{10}$ (b) highlighting the chromophore group; (c) photoexcitation and photoemission of the $AECuSi_4O_{10}$ materials [3].

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PC6

HISTORICAL SYNTHESIS AND POTENTIAL DEGRADATION OF YELLOW AND RED CADMIUM PIGMENTS

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Cd-based pigments were introduced in the 19th century and revolutionized the colour palette of artists. The primary component is the orange CdS, with ternary compounds fabricated later to achieve adjustable hues [1,2]. Adding Zn, the colour tunes to yellow increasing the Zn amount, whereas red pigments can be obtained by substituting sulfur with selenium (Figure 1). Extensive research has demonstrated how Cd-based pigments are characterized by a high level of heterogeneity in terms of colour, presence of impurities, coexisting of different phases, and particle size. This heterogeneity is induced by the variability of the synthetic methods employed by the different companies, with direct influence of the long-term stability of these materials. Indeed, the lack of precise information of the composition of the pigments obtained following the historical syntheses limits the prediction of the possible deterioration in real paintings [3].
In this study, we synthesized a series of $Cd_xZn_{1-x}S$ and $CdS_{1-x}Se_x$ pigments following established historical formulations. The synthesized pigments exhibit similar hues but vary in crystalline structure, particle morphology, and size. Additionally, different secondary phases are identified. The materials underwent artificial aging under simulated solar illumination to assess potential degradation. Subsequently, photocatalytic tests were conducted to correlate the observed alterations with their intrinsic semiconductor properties.
The results revealed important information about the deterioration behavior of historical pigments, identifying key indicators of pigment reactivity in real artworks and demonstrating the inherent instability of historically synthesized pigments based on fabrication methods.

Figure 1. Chromatic variations of cadmium-based pigments: yellow (ZnxCd1-xS), orange (CdS), and red (CdS1-xSex)

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PC7

ELECTRON PARAMAGNETIC RESONANCE TO EVALUTE AGRIFOOD QUALITY, TRACEABILITY AND SAFETY

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EPR (Electron Paramagnetic Resonance) spectroscopy is a powerful and non-destructive technique for the identification of organic free radicals and most transition metal ions in soils, as well as to study oxidative processes due to the formation of radical species in food systems [1,2]. The spectroscopy is recognized for the traceability of different types of food [3] and for its quality control [4]. EPR approach on food analysis is aimed for the quantification of radical species, the characterization of chemical reactions in foods that involve radical species formation [1,2], the assessment of antioxidant capacity of food, its quality, stability and shelf life [5,6].
The research has been developed inside the PNRR project to apply EPR technique for the analysis of the whole chain of wine and olive oil, starting from traceability purposes and then the final product for quality control, stability and shelf-life analysis.
In this work the oxidative stability and quality of oils have been investigated. Thirteen extra-virgin olive oils from the Tuscany region were analysed, through EPR spin-trapping technique using PBN to address oil stability. EPR radical scavenging assays towards galvinoxyl radical (GOR) and DPPH radical were used for endogenous antioxidant capacity determination. The fitting of EPR-PBN adduct curve, based on the Boltzmann model, related to polyphenol/tocopherol ratio gives a valuable insight into oil's stability [7].

Acknowledgements: The research project has been funded under the PNRR-AGRITECH-Spoke9, Missione 4, Componente 2, Investimento 1.4 – D.D.1032 17/06/2022-CN00022.

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PC8

ORGANIC DIRADICALS AS OPTICALLY ADDRESSABLE MOLECULAR QUBITS: WHAT THE PARISER-PARR-POPLE MODEL CAN TELL US?

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Recent experiments [2] and theoretical predictions [1,3] emphasize the growing importance of luminescent organic diradicals as optically addressable molecular qubits. These systems also show significant promise for magnetic sensing and quantum information science. Our objective is to develop specific π-conjugated diradical molecules for these applications by investigating the radical-radical interactions in both the ground and excited states through molecular structure tuning.

We examine the excited-state properties of these systems through a comprehensive study based on the Pariser-Parr-Pople (PPP) model. The strong electron correlation present in these systems complicates the calculation of their excited-state properties. To manage electron correlation more effectively, we diagonalize the PPP Hamiltonian within the Configuration Interaction (CI) approach and compare the results with those obtained by strategically partitioning the PPP molecular orbitals into different active spaces, adopting a restricted active space configuration interaction (RASCI) approach.[4]

Due to the multiconfigurational nature of these electronic states, we compare results with ab initio CASSCF, NEVPT2, and QD-NEVPT2. We emphasize the crucial role of the frontier orbitals and the importance of molecular structure in the radical-radical interactions. We underline that the PPP-RASCI approach combines precision and computational efficiency in accurately modelling the excited-state properties of diradical systems, enabling the mapping of excited-state properties in organic diradicals.

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PC9

EFFECT OF STRUCTURAL CONFINEMENT ON BACTERIAL DYNAMICS IN TRANSPARENT HYDROGELS WITH TUNABLE POROSITY

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Understanding the active behavior of complex living systems is crucial for both fundamental science and technological applications. Bacterial migration and proliferation in heterogeneous 3D porous networks play a key role in fields ranging from medicine to agriculture. While bacterial motility in unconfined environments like liquids and flat surfaces is well studied, tracking their motion in confined micron-scale porous matrices still represents a challenging goal.

In this work, we introduce biocompatible poly(ethylene glycol) hydrogels with tunable micron-scale porosity and high transparency[1], enabling single-cell tracking of the micro-swimmer *Bacillus subtilis*. Through laser scanning confocal microscopy the bacterial motility was related to the structural confinement imposed by the polymeric network. The characteristic run-and-tumble motion of flagellated bacteria changes into anomalous sub-diffusive movement as confinement increases. Single-trajectory analysis reveals a matrix-induced reduction in running speed and an increase in reorientation rate.

This transition from active to sub-diffusive motion is interpreted as transient trapping within the hydrogel network. A precise morphological characterization of the polymeric matrix, combined with bacterial tracking, refines the hopping-between-trapping model, whose predictions align well with experimental mean square displacements data. Moreover, the velocity of the free-diffusing bacteria can be related to the pore diameter through the relation parameter $(1 - \xi)^2$ closely matching the experimental observations.

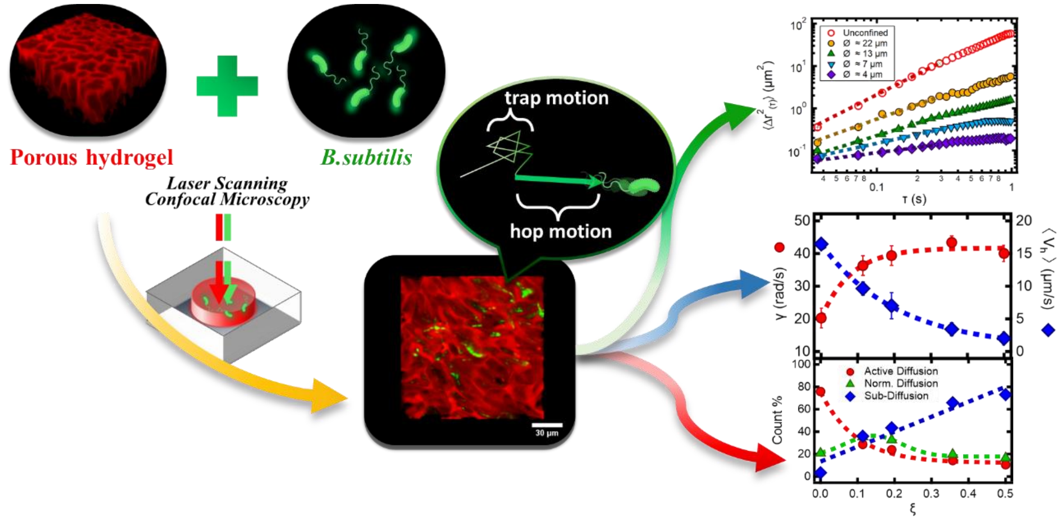

Figure 1 Porous hydrogel of PEG and B.subtilis analyzed through LSCM in order to extrapolate characteristic motility parameters with the increase of the confinement length (ξ).

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PC10

SMART OPTICAL MATERIALS BASED ON SMALL ORGANIC MIXED VALENCE SPECIES

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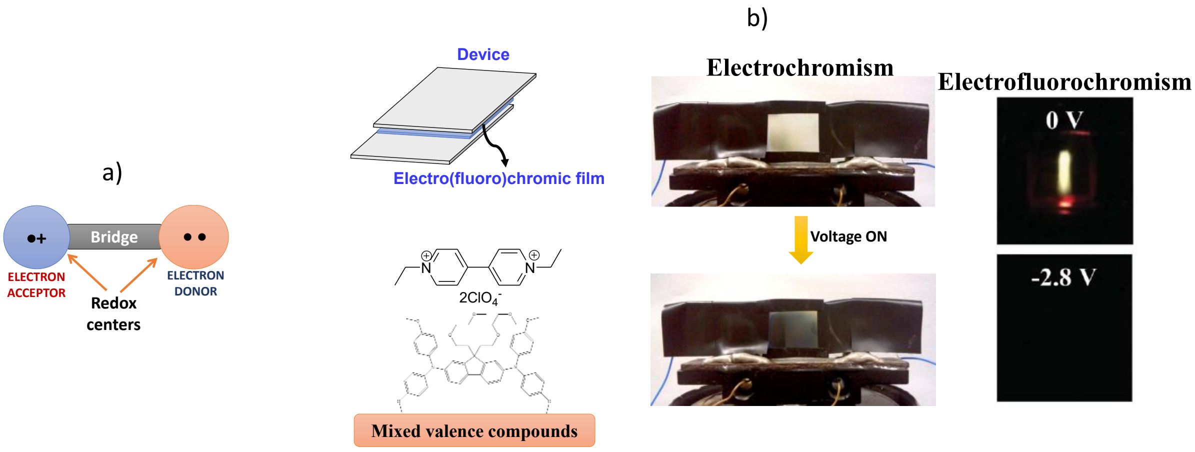

Figure 1. a) Schematic representation of the structure of mixed valence compounds, and b) example of smart device based on a mixed valence arylamine compound displaying electrochromic and electrofluorochromic properties .

Small organic molecules that can generate mixed valence species (MVs) upon electrochemical reduction or oxidation, are very attractive for the development of electroactive materials exhibiting multi-stimulus optical responsiveness [1]. A mixed valence compound possessing two redox centers, formally with different redox state (Fig. 1a), represent a versatile building block because its physical-chemical properties can be varied by changing the nature of the redox centers and the central bridge connecting them. The most important classes of MVs are those in which the redox centers are substituted arylamines [1-4] or substituted pyridinium ions (viologens) [4-7]. Here we discuss selected examples of smart optical materials based on the above two classes of compounds, where their optical properties (absorption and fluorescence) can be modulated by self-assembly (liquid crystalline properties), light, d.c. voltage, temperature, solvent, leading to systems exhibiting various types of chromisms.

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PC11

DYNAMICS OF WATER AND CARBON DIOXIDE IN AN ULTRAMICROPOROUS METAL-ORGANIC FRAMEWORK BY SOLID-STATE NMR SPECTROSCOPY

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Metal-Organic Frameworks (MOFs) are a class of crystalline porous coordination polymers built by metal ions or clusters and organic linkers [1]. Thanks to their structural and functional tunability, MOFs are of great interest for application in CO_2 separation [2,3]. Among them, the ultramicroporous MOF UTSA-280 (calcium squarate, $Ca(C_4O_4)(H_2O)$, Figure 1), possessing 1D rigid pores channels with a cross-sectional area of about 14 $Å^2$, showed a large CO_2 uptake capacity and selectivity towards CO_2 over CH_4 in CO_2/CH_4 mixtures, due to a sieving effect [4]. Water coordinated to Ca in UTSA-280 framework was found to be involved in water transport in the MOF channels through a knock-off mechanism [5], as well as in the selective uptake of ethane/ethylene mixtures [6]. Since a comprehensive understanding of molecular transport mechanisms is fundamental for successfully harnessing the potential of UTSA-280 in CO_2 separation, the state and dynamics of water and CO_2 in the MOF channels were investigated by multinuclear solid-state NMR spectroscopy, a very informative technique for the investigation of guest dynamics and guest-host interactions in solid sorbents.

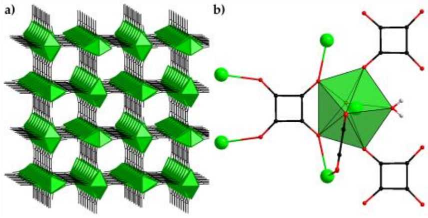

Figure 1. a) Polyhedral representation of UTSA-280 crystal structure. Atom labelling scheme: Ca, green polyhedra; squaric acid dianions, black (hydrogen atoms have been omitted for clarity); b) Local coordination environment of the squaric acid dianions and calcium cations.

By combining ^1H and ^2H Magic Angle Spinning (MAS) and static NMR experiments on activated and hydrated (with either H_2O or D_2O) samples, it was found that in the activated MOF, coordinated water undergoes local librations and π-flip motions, whereas, upon hydration, a translational hopping motion of water among Ca sites and exchange between water molecules are observed. ^{13}C MAS and static NMR spectra recorded on the MOF loaded with $^{13}CO_2$ (1 atm at room temperature) showed that CO_2 undergoes very restricted reorientational dynamics in the UTSA-280 channels.

Acknowledgements: This research has received funding from the European Union's Horizon Europe research and innovation programme, European Innovation Council and SMEs Executive Agency (EISMEA), under grant agreement No 101115488, project "DAM4CO_2".

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PC12

FLUORINATED PROBES FOR MULTIMODAL AND MULTISCALE DETECTION: SPATIALLY-OFFSET RAMAN SPECTROSCOPY FOR DEPTH-RESOLVED NANOPARTICLES DETECTION

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Molecular imaging enables non-invasive visualization of anatomical structures and physiological processes across multiple scales. Yet, single-modality techniques often face limitations in resolution, sensitivity, or depth penetration. Multimodal approaches, like the combination of ^{19}F-MRI and Raman spectroscopy, offer a powerful solution: ^{19}F-MRI provides a whole-body overview, while Raman spectroscopy delivers detailed molecular information at localized sites [1].

Building on our previous work, which demonstrated the effectiveness of the superfluorinated molecule PERFECTA as a bioorthogonal ^{19}F probe, enabling both whole-body MRI and localized Raman imaging [1], we further advanced this approach by developing innovative fluorinated PERFECTA-loaded PLGA-based nanoparticles with different surface coatings (FNPs) [2]. These FNPs were specifically designed to enhance cellular labeling and facilitate detection by both ^{19}F-MRI and Raman spectroscopy.

Here, we further optimized Raman-based approaches for detecting FNPs in complex biological environments, by refining a Spatially Offset Raman Spectroscopy (SORS) technique [3] to enable depth-resolved analysis *in-situ*. This optimization allowed us to visualize FNPs in all their components, both within cells and in specialized phantoms replicating tissue complexity. These advancements pave the way for in situ monitoring of NPs biodegradation and localization, as well as the potential intraoperative detection of ^{19}F-MRI biomarkers.

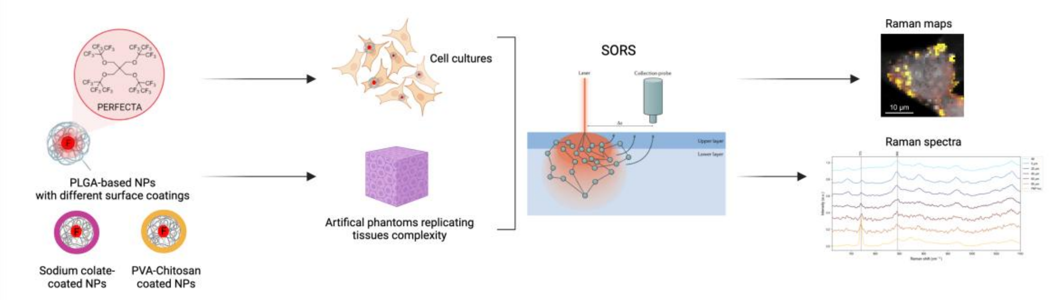

Figure 1. Schematic of the study workflow. FNPs, incubated with cells or embedded in a tissue-mimicking phantom, are analyzed by SORS to obtain Raman maps and spectra of their components.

Acknowledgements: Thanks for funding to PRIN 2022 - project 2022598YAX - BiOmimetic fluorinated nanoProbes for multIscale Tumor detection by MRI and Advanced Raman techniques (OPTIMA) - supported by Next Generation EU.

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PC13

SOLID STATE NMR AND NQR UNDER ILLUMINATION: NEW METHODS FOR CHARACTERIZING PHOTOACTIVE MATERIALS

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Light-matter interaction is an extraordinary field of the scientific research with enormous effects on everybody's day life, and its importance is central in the framework of energy transition and sustainable advances of technology. NUTSHELL is a project aimed at developing Solid State Nuclear Magnetic Resonance (SSNMR) methods to study in real time the effects of illumination on the molecular and nanoscale properties of photoactive materials, enabling the understanding of many phenomena occurring only under illumination conditions. In this contribution newly developed apparatuses aimed at the investigation of materials under illumination by exploiting high-resolution SSNMR, low-field NMR and Nuclear Quadrupole Resonance (NQR) spectroscopies will be presented, together with case-studies. Each of these spectroscopic techniques presents peculiar advantages, but also technical obstacles to the coupling with sample's illumination and, so far, only few pioneering SSNMR studies have been reported in the literature [1-5]. In this project each spectroscopic apparatus has been specifically adapted to be coupled with an illumination system; sample preparation, which resulted particularly critical, has been optimized to allow light penetration during NMR/NQR experiments. The experimental setups will be here presented together with preliminary results obtained on organic photochromic compounds, polymers and Mixed Halide Lead Perovskites.

Acknowledgements: We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title NUTSHELL: NMR Under illuminaTion SHEd Light on materiaLs– CUP B53D23013900006- Grant Assignment Decree No. 958 adopted on 06/30/2023 by the Italian Ministry of Ministry of University and Research (MUR).

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PC14

ANALYTICAL COMPLETE GRADIENT OF THE EXCITON MODEL ENERGY

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Investigating the nonadiabatic dynamics of multichromophoric systems requires the use of some form of “divide and conquer” approximations. One widely used approach is the Frenkel exciton model, where electronic excited states are expressed as linear combinations of localized excitations. In this context, Sangiogo et al. [1] proposed a Surface Hopping implementation based on the Frenkel Exciton Model. Transition energies for the localized excitations are calculated in a semiempirical framework using the floating occupation molecular orbitals-configuration interaction (FOMO-CI) method [2]. Exciton couplings are evaluated either exactly, within the semiempirical formalism, or resorting to transition atomic charges. Excitonic states, written as antisymmetrized products of individual chromophore wavefunctions, and the exciton couplings are used to construct the excitonic Hamiltonian, whose diagonalization yields the electronic adiabatic wavefunctions and energies. The gradients of the adiabatic states, considering that the derivatives of the variationally optimized excitonic coefficients give a null contribution, can be written as a combination of site energy gradients and their couplings. So far, whether transition charges or exact couplings are used, only the static part of the coupling term has been considered, which does not depend on derivatives of the CI or MO coefficients.

In this work, we introduce a method for the analytical evaluation of exciton coupling derivatives within a semiempirical configuration interaction (CI) framework. To reduce the computational cost, we directly compute the combinations of couplings with the excitonic coefficients, which can be expressed as the sum of a static term and contributions involving the derivatives of the transition density matrices for each individual chromophore. This formulation allows for the gradient evaluation to be carried out independently and in parallel for each chromophore. Computational efficiency can be further improved through the use of the Z-vector technique [3]. By using this gradient formulation, we observed improved agreement with numerical results compared to using only the static term. Additionally, in surface hopping simulations, we observed better conservation of total energy along the trajectories, especially for states with strong excitonic coupling. This approach is expected to improve the accuracy of nonadiabatic dynamics simulations, leading to more reliable and physically consistent results.

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PC15

ACTIVATED CARBONS FROM POLYSTYRENE WASTE OBTAINED BY CARBONISATION WITH KOH/KCl EUTECTIC

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The objective of this study is twofold: firstly, to study the influence of varying the washing procedure on the properties of hyper-crosslinked polymers obtained through the Friedel-Crafts reaction; and secondly, to examine the impact of the chemical activator, and the activation temperature used, on the properties of the activated carbons (AC) obtained. The target reaction involves the use of polystyrene waste as a precursor material through hyper-crosslinking in the presence of dimethyl acetal formaldehyde (FDA) and dichloroethane. After comprehensive characterisation, the HCPs were converted into activated carbons (ACs) to enhance their texturale properties using a KOH/KCl mixture as chemical activator[1], at various temperatures (650, 700 and 800°C). As reference materials, two ACs obtained using KOH and KCl were prepared. The activated carbons exhibited high specific surface area (SSA) and pore volume. Subsequently, the hydrogen uptake at various temperatures was determined. These results were then compared with those of a commercial AC (MSC30G) and ACs reported in literature[2] that achieved high performances in hydrogen adsorption (Figure 1 and Table 1). As clearly stated in the table, the AC prepared in our labs shows the highest volumetric (g/L) performances.

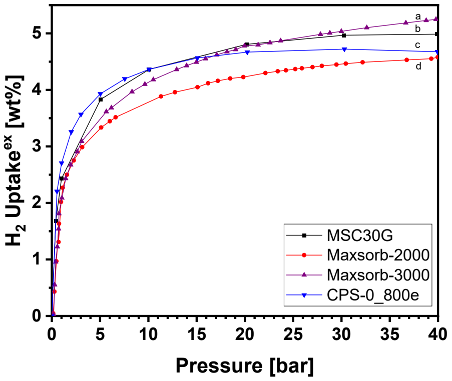

Figure 1. Excess Hydrogen uptake at 77 K of obtained material compared with commercial Maxsorb and materials reported in literature [2].

Sample	Uptake^{ex}		
	[mol/kg]	[g/g%]	[g/L]
MSC30G	25.7	5.42%	29.0
Maxsorb-2000*	22.6	4.73%	21.4
Maxsorb-3000*	26.0	5.49%	18.9
C-PS-0_800e	24.6	5.17%	31.7

*Table 1. H_2 uptake at 77 K of the MSC30G and CPS-0_800e.*Adapted from Literature [2].*

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PC16

CO_2 ADSORPTION IN METAL-ORGANIC FRAMEWORK-BASED MIXED MATRIX MEMBRANES: A MULTI-TECHNIQUE APPROACH

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Mixed-matrix membranes (MMMs) constitute a class of very promising materials for CO_2 capture in that they combine the easy processability, flexibility, low cost, and good permselectivity of the polymeric matrix with the advantageous adsorption properties of metal-organic frameworks (MOFs) [1,2]. In the framework of the *DAM4CO₂* project, MMMs for CO_2 capture are developed by exploiting polymers of intrinsic microporosity (PIMs) and MOFs based on non-critical metals and non-environmentally hazardous organic linkers and characterized using a multi-technique approach to shed light on physico-chemical properties and on CO_2 adsorption capacity and mechanism.

Here, results are shown on two MMMs prepared using PIM-1 and two different MOFs, i.e., UTSA-280 (calcium squarate, $Ca(C_4O_4)(H_2O)$) and UTSA-16 (zinc citrate, $K_2Zn_3(C_6H_4O_8)_2$), showing promising CO_2 adsorption properties [3,4]. CO_2 adsorption and separation properties from other gases (N_2, CH_4, O_2, H_2, He) were determined in comparison with the parent materials. Improved selectivity and enhanced CO_2 adsorption were found in the MMMs with respect to the neat polymer membrane. Structural properties of MOFs, polymer, and MMMs were investigated by X-ray diffraction, scanning electron microscopy (SEM) and solid-state NMR spectroscopy. Moreover, solid-state NMR gave insight into interactions between CO_2 and MMM materials at the atomic level and allowed the investigation of CO_2 reorientation dynamics in the MMMs in comparison with their parent materials.

Acknowledgements: This study has received funding from the European Union's Horizon Europe research and innovation programme, European Innovation Council and SMEs Executive Agency (EISMEA), under grant agreement No 101115488, project "DAM4CO_2".

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PC17

IMPACT OF APPLIED ELECTRIC BIAS ON OXYGEN REACTIVITY AND OXIDE DIFFUSION AT LANTHANUM STRONTIUM MANGANITE ELECTRODE SURFACES

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Lanthanum Strontium Manganite (LSM) is a widely used cathode material in solid oxide fuel cells (SOFCs) due to its stability and catalytic activity in oxygen redox reaction (ORR) [1, 2]. Although its surface properties have been extensively studied [3], the effects of electric polarization on chemical reactivity and oxide diffusion remain largely unexplored.

In this study, we employ state-of-the-art density functional theory (DFT) calculations with an applied electric field [4] to investigate the structural, electronic, and catalytic properties of the pristine and defective LSM (001) surface, focusing on oxygen migration and vacancy dynamics. We first characterize the surface geometry and electronic structure, assessing how surface reconstitution and oxygen vacancy formation energies influence catalytic activity. To simulate realistic SOFC conditions, we apply an external electric field during both vacancy formation energy calculations and climbing-image nudged elastic band (CI-NEB) simulations to model oxide ion migration. Additionally, we examine the ORR on both pristine and defective LSM surfaces under applied potentials, elucidating the role of vacancies in modulating catalytic activity. Our findings reveal how polarization and surface-specific effects influence oxygen transport and ORR kinetics, providing a more comprehensive picture of LSM's catalytic behavior. By integrating advanced computational techniques with an electrochemical perspective, this work offers valuable insights on the possible modulation of LSM electrocatalytic properties via electric bias, and contributes to the rational design of more efficient cathode materials for application in SOFCs.

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PC18

STRUCTURE–PROPERTY INSIGHTS INTO SELF-ASSEMBLED LIGNIN MICRO-PARTICLES OBTAINED BY ANTISOLVENT SYNTHESIS FOR WASTE VALORIZATION

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Lignin, a by-product of the pulp and paper industry, represents a significant resource with largely unexploited potential for valorization. The industry produces approximately 50 million tons of lignin annually, of which less than 2% is recovered for chemical applications [1]. Pulping processes such as Kraft, alkaline and Klason ones focus on extracting high quality cellulose from lignocellulose under relatively harsh processing conditions, including extensive use of inorganic salts, bases or acids [2]. The resulting lignin is a byproduct which contains approximately 6% sulfur, which increases its water solubility and facilitates further processing.

At present, two principal approaches have been proposed for the valorization of this lignin: one promotes its use without major structural changes [3], and the other focuses on the depolymerization of lignin to obtain various chemicals [4]. In this context, our approach is to valorize lignin derived from various sources, specifically those associated with pulping, agricultural processes and food production, trying to adopt eco-sustainable strategies. To this aim, I have formulated self-assembled lignin using sustainable solvents like levulinic acid, employing the anti-solvent method [5]. The resulting particles were characterized by microscopy and dynamic light scattering (DLS) to precisely determine their size distribution. Subsequently, electron paramagnetic resonance (EPR) was performed to assess modifications induced by the novel solvent used. Furthermore, all particles were examined for their capacity to encapsulate hydrophobic active ingredients. In particular, the employment of levulinic acid resulted in a positive effect, as complete dissolution of lignin and active ingredients in the solvent phase was observed. The anti-solvent procedure allowed to obtain loaded lignin particles for further applications without the need for additional steps. The loaded lignin particles were analyzed using the same physical chemical and analytical techniques described above.

This study proposes a circular green chemistry process to produce a wide variety of products from lignin waste such as pesticide or fertilizers for agricultural purposes. The physical chemical characterization of the products provides a comprehensive insight into the different types of particles that various solvents can produce and the interactions between lignin and active ingredients.

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PC19

HARNESSING NATURE'S POLYMERS: SPECTROSCOPIC AND DSC INSIGHTS INTO BIOMASS-DERIVED BIOPLASTICS

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Lignocellulosic biomass is a strategic, renewable natural resource generated by various sectors. Forests alone produce approximately 1.3 billion tons of lignocellulosic biomass annually, while agricultural biomass waste accounts for an additional 370–520 million tons per year worldwide. The polymeric constituents of lignocellulosic biomass have diverse applications, ranging from biofuels, biopolymers, and bioplastics to construction materials [1,2].

Similarly, algae are rich in natural biopolymers and find applications in industries such as bioplastics, pharmaceuticals, cosmetics, nutrition, and biotechnology. Algal polysaccharides exhibit excellent film-forming properties, contributing to the preservation and biodegradability of bioplastic materials. Additionally, algae contain valuable biomolecules such as proteins and lipids, further enhancing their applicability [3].

Given the broad potential of biomass-derived biopolymers, characterizing their composition is crucial to assess their suitability for various applications and maximize their valorization. In this context, physical chemistry provides powerful tools for analyzing both biopolymeric constituents of biomass and bio-sourced materials.

In this study, we employed various spectroscopic and thermal techniques to characterize biopolymers from different sources, including lignocellulosic biomass (cellulose, hemicellulose, lignin), microalgal residues (cell wall components), and bioplastics (cellulose acetate) synthesized from extracted cellulose.

- FTIR spectroscopy was used to analyze the biopolymeric components of lignocellulosic biomass and microalgal residues, allowing us to assess the purity of extracted polymers. Additionally, FTIR proved to be a rapid, simple, and environmentally friendly method for determining the degree of substitution in synthesized cellulose acetate (CA), where other methods had failed.
- UV-Vis spectroscopy was applied to characterize extracted lignin, evaluate the transparency and UV-shielding properties of CA bioplastic films, and determine the pigment composition of microalgal residues for potential incorporation into bioplastics.
- Fluorescence spectroscopy complemented the pigment characterization, assessing their potential use as eco-friendly colorants in bioplastic materials.
- Differential scanning calorimetry (DSC) was employed to evaluate the thermal stability of biopolymers and plasticized CA films, as well as to investigate the role of microalgal residues as additives to enhance the performance of CA-based bioplastics.

This study highlights the versatility of spectroscopic and thermal techniques in characterizing biopolymeric materials and underscores the potential of biomass waste as a valuable resource for sustainable bioplastic applications.

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PC20

COPPER BASED METAL-OXIDE CATALYSTS FOR PHOTOTHERMAL CO_2 REDUCTION

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The increase in the average concentration of greenhouse gases (GHGs) observed over the last 50 years makes it urgent to find new ways to reduce the level of CO_2 in the atmosphere.[1] Among the possible strategies, Carbon Capture and Utilization (CCU) began to attract increasing attention because of its involvement not only in the permanent storage of the captured CO_2, but also in its utilization and conversion into new sources and products such as chemicals or renewable fuels.[2]

In this respect, photocatalytic CO_2 reduction represents a more sustainable alternative to conventional thermo-catalytic approaches.[3]

A possible application of this approach is the one suggested in the EIC-Pathfinder project "DAM4CO_2" (Double-Active Membranes for a sustainable CO_2 cycle, GA 101115488), which aims to capture and convert the CO_2 into C_4-C_9 renewable fuels through the synergetic integration of two membranes.[4] The conversion component aims to develop a single photocatalyst capable of carrying out two different reactions: Reverse Water Gas Shift (RWGS) and Fischer-Tropsch (FT).

In this perspective, different catalysts based on metal-oxides of earth-abundant elements (such as Cu Fe and Ni) were synthesized and tested under photothermal conditions. The most promising ones were characterized by coupling fundamental characterization (such as X-ray diffraction and volumetry) with *in situ* IR spectroscopy to study the nature of the interactions occurring among reagent/products and the catalyst surface. Some preliminary *operando* spectroscopies were performed to correlate the catalytic performances (activity and selectivity) to the specific reaction intermediates and pathways. In addition, some first results on membranes integrating the photo-catalysts into a polymeric matrix will be shown.

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PC21

LASER ABLATION-BASED SYNTHESIS OF MAGNETIC NANOPARTICLES FROM ETNA'S VOLCANIC ROCKS

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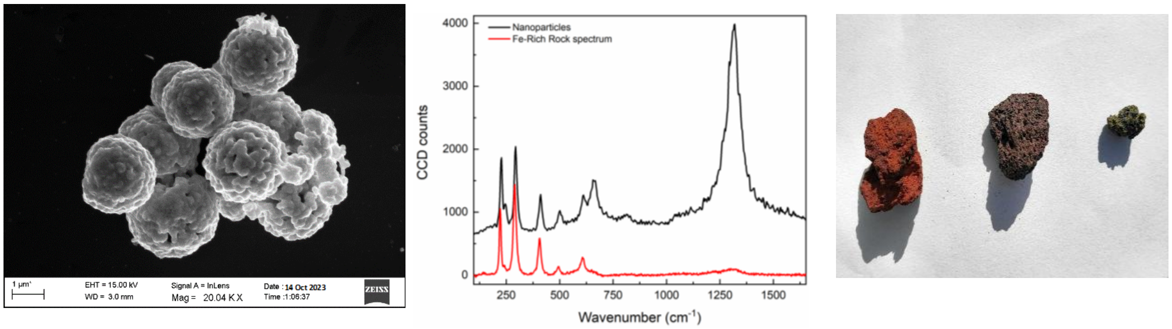
Mount Etna, Europe's highest and most active volcano, continuously deposits significant amounts of magmatic material rich in metals such as Fe, Co, V, Cu, and Zn, along with non-metals like S and B [1]. The mechanical properties of volcanic rocks make extracting these elements challenging through conventional methods. This study demonstrates the direct recovery of metallic elements from volcanic rock using Laser Ablation and their subsequent transformation into metallic nanoparticles. Before ablation, three volcanic rock samples collected at 3000 m above sea level were analyzed by Raman spectroscopy and Laser-Induced Breakdown Spectroscopy (LIBS) to determine their elemental composition. The nanoparticles synthesized via Pulsed Laser Ablation in Liquids (PLAL) exhibited distinct physicochemical properties depending on the composition of the parent rock. Notably, the Fe-richest sample led to the formation of hematite (α-Fe_2O_3) nanostructures, as confirmed by Raman spectroscopy and UV-VIS analysis (Fig. 1), with typical low-temperature magnetic properties [2]. These findings highlight the potential of volcanic rock as a sustainable source for functional nanomaterials, which can be further engineered for applications in magnetic SERS substrates or nanomedicine [3].



(a) *(b)* *(c)*

Figure 1. (a) SEM image of hematite nanoparticle obtained from Fe-rich rock, (b) Raman spectrum of the obtained nanostructure compared with that of the bulk rock. (c) The three rocks studied.

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PC22

PLASMON RESONANCE DETECTION OF WATER ADSORPTION ISOTHERMS

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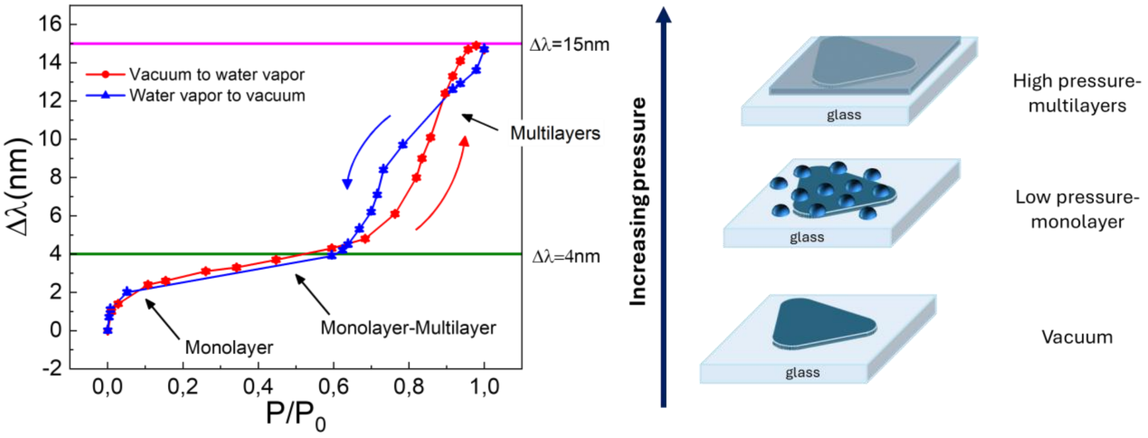
Plasmonic nanoparticles exhibit extreme sensitivity to variations in the optical properties of their surrounding environment, making them ideal candidates for sensing applications, including environmental monitoring [1,2,3]. This study investigates the localized surface plasmon resonance (LSPR) response of silver nanospheres and nanoplates chemically grafted onto transparent substrates and exposed to controlled concentrations of solvent vapours inside a vacuum chamber.
Using an *in-situ* UV-Vis spectrophotometer, we monitor the adsorption and desorption of solvent vapours on the nanoparticle surfaces, demonstrating that LSPR shifts can serve as an optical fingerprint for these interactions. Our experimental findings are supported by Finite-Difference Time-Domain (FDTD) simulations, which provide deeper insights into the plasmonic response of each nanostructure. A comparative analysis reveals that silver nanoplates exhibit the highest sensitivity to solvent vapor adsorption, highlighting their potential as highly responsive plasmonic sensors.
These results are a starting point for developing advanced optical sensors based on plasmonic nanostructures. Future research will focus on extending this approach to the real-time detection of various organic vapours.



(a) (b)

Figure 1. (a)Adsorption curves obtained by studying the variation of the main resonance peak as a function of the vapor pressure. (b) Graphical schematization of the possible adsorption mechanism on the substrate.

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PC23

MULTISCALE INTEGRATED COMPUTATIONAL APPROACHES FOR DRUG DELIVERY SYSTEMS: FROM MESOPOROUS SILICA TO CYCLODEXTRINS AND BEYOND

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Recent advancements in computational modeling have boosted the investigation of drug delivery systems, spanning from mesoporous silica to cyclodextrins (CDs). In this study, we integrate two distinct computational approaches to elucidate the atomistic details of drug interactions within these carrier materials.

Firstly, we explore the interaction between ibuprofen, a common non-steroidal anti-inflammatory drug, and a realistic model of MCM-41 mesoporous silica. Utilizing periodic Density Functional Theory (DFT) with the all-electron B3LYP hybrid functional, we elucidate the intricate interplay between ibuprofen and MCM-41. Through docking simulations, we sample different local features of the potential energy surface, revealing the exergonic and exothermic nature of ibuprofen adsorption in MCM-41, predominantly driven by London interactions. Simulated spectra align closely with experimental observations, shedding light on the dynamic behavior of adsorbed ibuprofen and highlighting the synergic H-bonding properties of the drug within the silica matrix. [1,2]

Secondly, we focus on cyclodextrin-based nanosponges (CD-NS) as carriers for various guest molecules. Employing a multiscale recently developed strategy, involving the semi-empirical xTB-GFN2 method, DFT refinements together with classical molecular dynamics, we investigate different drugs/β-cyclodextrin inclusion complexes as model systems. Our validation efforts encompass structural, energetic, and IR spectra predictions, demonstrating the accuracy and computational efficiency of our strategy. [3] By bridging the gap between density functionals and force-field-based methods, we pave the way for robust and cost-effective modeling of cyclodextrin-based nanosponges. [4]

Overall, this multiscale integrated computational approach provides valuable insights into the design and optimization of drug delivery systems, from mesoporous silica matrices to cyclodextrin carriers, offering a comprehensive framework for future studies in pharmaceutical sciences.

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PC24

PRELIMINARY CHARACTERIZATION OF A NOVEL RUTHENIUM DYE-HELICAL PEPTIDE CONJUGATED SYSTEM FOR DSSC ENHANCED PERFORMANCE

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Dye-sensitized solar cells (DSSCs) represent a promising alternative to traditional silicon-based solar panels due to their cost-effectiveness, ease of fabrication, and ability to operate efficiently under low-light conditions. Among the various photosensitizers used in DSSCs, ruthenium bipyridine complexes have gained significant attention. These complexes are favoured for their excellent photochemical stability, broad absorption spectrum, and efficient electron transfer properties [1]. Helical peptides play a crucial role in mediating charge transfer processes due to their well-defined secondary structures and ability to facilitate efficient electron transport [2]. These peptides can be engineered to enhance charge transfer mechanisms, such as superexchange and hopping, making them promising candidates for integration into DSSCs [3]. The use of helical peptides in DSSCs can potentially improve the efficiency and stability of these cells, opening the way for more advanced and sustainable solar energy technologies. In our experimental work we have explored a possible application in DSSC of a new ruthenium bipyridine dye. The dye was modified with a thymine (Figure 1) on one of the bipyridine groups, to exploit the natural hydrogen bond formation between adenine and thymine bases and create a supramolecular SAM on a flat gold surface. The SAM was composed of three layers: a lipoadenine (Lipo-A), a helical peptide functionalized with thymine and adenine, respectively, to enable Lipo-A and $[T\text{-}Ru(bpy)_3]^{2+}$ conjugation. First, the ruthenium complex was characterized spectroscopically in solution to understand its photophysical properties, with absorption, steady state and time-resolved fluorescence, quantum yield measurements. Then, the film on a flat gold electrode was studied for photocurrent generation at different excitation wavelengths (Figure 2).

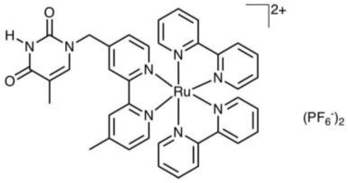

Figure 1. Ruthenium bipyridine dye linked with a thymine.

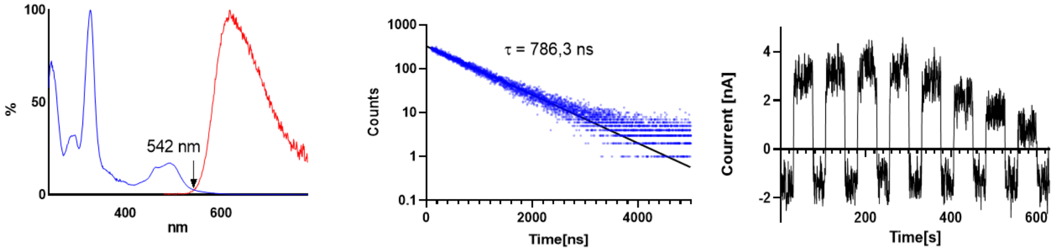

Figure 2. Dye photophysical characterization and photocurrent generation.

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PC25

SMART MESOPOROUS SILICA NANOCARRIERS FOR SUSTAINABLE CORROSION PROTECTION OF CULTURAL HERITAGE METAL ARTIFACTS AND COMPONENTS

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The corrosion of historically significant metal artifacts and structural components, such as reinforcing rebars in concrete heritage structures, poses a major challenge for conservators. This degradation process severely impacts durability, leading to complex, costly, and time-consuming maintenance efforts. Various corrosion protection strategies have been employed, with polymer coatings combined with corrosion inhibitors being a common approach. However, these conventional solutions suffer from limitations, including the UV sensitivity of inhibitors, which reduces their long-term effectiveness. A promising alternative lies in smart nanocarriers, as mesoporous silica nanoparticles (MSNs) [1]. These nanostructures offer high chemical stability and surface area, ease of preparation, and seamless integration with polymer coatings. Their porous architecture allows for the efficient loading of corrosion inhibitors, while their surfaces can be functionalized with stimuli-responsive polymers. This tailored design enables the controlled release of anticorrosive agents in response to specific degradation triggers, addressing the shortcomings of traditional inhibitors — such as UV sensitivity— and enhancing the sustainable preservation of Cultural Heritage metal components. Two distinct types of MSNs have been synthesized using a colloidal chemistry approach: spherical MSNs with hexagonal pore structure with pore sizes from 1.5-4 nm (MSNs hex) and dahlia-like morphology MSNs with pore sizes ranging from 3-4 nm up to tens of nm (MSN CR). Their surface has been intentionally functionalized by grafting two types of polyelectrolytes - polyacrylic acid (PAA) and polyethylenimine (PEI) - which respond to pH variations to regulate pore opening and cargo release. These MSNs have been loaded with caffeine, a promising green inhibitor [2] and with a conventional inhibitor, BTA as a reference. The dahlia-like morphology of MSNs has proven more effective in loading and releasing both caffein and BTA at various pH values (Figure 1c). The results highlight the potential of the proposed nanostructures for further testing in simulated pore solutions. This innovative approach offers a promising pathway toward long-lasting and sustainable corrosion protection for metal artifacts and components in Cultural Heritage conservation.

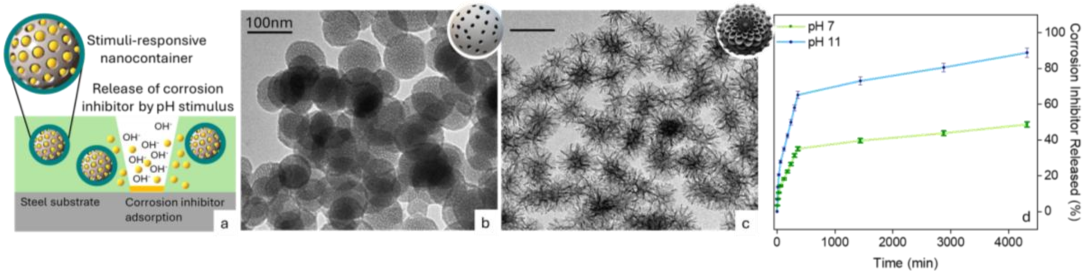

Figure 1. Sketch of the anticorrosion activation of smart nanocarriers. (a); TEM micrographs of MSNs hex (b) and MSN CR (c); Green corrosion inhibitor (caffeine) release profile from MSN CR PEI in different pH solutions (pH = 7 and 11) (d).

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PC26 PRODUCTION OF SnO_2 NANOSTRUCTURES FOR HIGH-PERFORMANCE ELECTRODES: A STUDY ON SCALABILITY AND ENVIRONMENTAL IMPACT

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The transition to a sustainable energy future requires both reducing fossil fuel consumption and developing low-impact energy systems. A crucial enabler of next-generation energy conversion and storage technologies is the scalable production of nanostructured materials, which play a key role in applications such as electrodes for photovoltaic cells, batteries, and catalytic processes. Their unique properties—tuneable through precise control over size, morphology, and composition—offer significant advantages for industrial applications. However, a major challenge remains translating laboratory-scale innovations into large-scale, commercially viable technologies [1]. Despite the availability of both top-down and bottom-up synthesis approaches, industrial-scale production of nanomaterials is still hindered by issues of reproducibility, scalability, and cost-effectiveness. Traditional three-step scale-up methods (lab-scale, pilot-scale, industrial-scale), which rely on increasing batch reactor volumes, are not directly applicable, as they risk compromising the nanostructure and functional properties of the materials.

This study addresses these challenges by focusing on the scalable synthesis of SnO_2 nanostructures using an eco-friendly, aqueous-phase approach at relatively low temperatures [2]. Key process parameters—including reaction time, temperature, precursor concentration, and process chemistry—have been systematically explored and optimized to ensure precise control over particle size and morphology. Extensive investigation into these parameters has been devoted to achieve synthesis of SnO_2 nanoparticles which could be scaled at industrial level, while preserving their critical properties such as size, morphology, crystallinity, surface features, and electronic band structure—essential for high-performance applications in energy conversion, catalysis, and storage devices. The synthesized SnO_2 nanostructures have been thoroughly characterized through morphological, structural, and spectroscopic analyses, while electrochemical studies have assessed their efficiency and long-term stability as electrode materials for hydrogen production and battery applications.

Additionally, a Life Cycle Assessment (LCA) has been conducted to evaluate the environmental and economic impact of the synthesis process, assessing both sustainability and cost-effectiveness from laboratory conditions to an industrial perspective.

This work paves the way for demonstrating the large-scale feasibility of nanostructured SnO_2 synthesis in a production environment using the explored scalable methodologies, ultimately advancing the transition to more sustainable energy technologies.

Acknowledgements: The work has been supported by “Scalable Production of Advanced Nanostructures for Electrodes” SPARKLE (PNRR NEST - NETWORK 4 ENERGY SUSTAINABLE TRANSITION”) project and by the Italian PRIN 2022 PNNR Project Hybrid ElectROchemical Energy storage in Sustainable batteries (HEROES - cod P2022AFYZX, 2023-2025).

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PC27

IR AND RAMAN SPECTRA OF GLYCEROL: A COMPUTATIONAL STUDY

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Deep Eutectic Solvents (DESs) are an emerging class of low-cost solvents based on a halide salt (organic or inorganic) and an alcohol/organic acid acting as hydrogen bond acceptor (HBA) and as hydrogen bond donor (HBD) respectively [1]. When their applicability as efficient and more sustainable electrolyte in electrochemical energy storage systems is concerned, DESs obtained by combining glycerol (Gly) and NaCl as respectively HBD and HBA should be considered [2,3]. To better characterize such system, NaCl/Gly mixtures (liquid state) at variable NaCl:Gly *ratio* were deeply investigated in the past by Raman spectroscopy, showing then a peculiar behavior of some Gly vibrational features when DES composition is reached [4]. The Raman spectrum of liquid Gly presents a very complex structure to which different Gly conformations, together with the inter-molecular hydrogen bond network, contribute. To disclose in part such complexity, we adopt a combined computational approach in which conformational search has been performed. We start our investigation from Gly molecule in the vapor phase which the experimental IR spectrum recorded at 498 K is available [5]. The conformational search has been performed by adopting the Global Optimization Algorithm (GOAT) [6] as developed in the ORCA (release 6.0.1) code [7] coupled to the GFN2-xTB method [8]. The obtained conformers have then been fully re-optimized at r^{2}SCAN-3c level [9] and both IR and Raman spectra have been computed for each conformer (IR^{conf}). The final 498 K IR^{total} spectrum (see Figure 1, red line), obtained as a combination of IR^{conf} each weighted for the relative abundance (the Gibbs Free Energy at the given temperature T has been used) of the associated conformer, showed a quite nice correspondence with the experimental one.

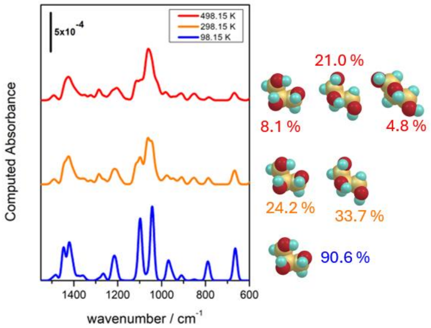

Figure 1. Computed glycerol gas phase IR spectra vs T considering the given relative abundances of its conformers.

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PC28

DYNAMICS OF LIGAND AND GUEST IN 1D COORDINATION POLYMERS WITH DIFFERENT TOPOLOGIES BY SOLID-STATE NMR

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Coordination polymers (CPs) are metal-organic materials built by metal ions or clusters bound through coordination bonds with organic ligands to give long range 1D, 2D, or 3D ordered structures [1,2]. Although previously regarded as less prominent compared to their higher-dimensional counterparts, 1D CPs have recently gained recognition for their unique advantages, such as easier design, structural flexibility, and specific adsorption capabilities, which make them well-suited for various practical applications [3]. In particular, 1D CPs have been proposed for the selective adsorption of volatile organic compounds (VOCs) [3,4], one of the main sources of air and water pollution. Since the efficiency of adsorption methods for VOC removal strongly depends on specific and stable interactions between the VOC and the CP framework, the characterization at the atomic level of host-guest interactions and guest dynamics is of particular interest for the comprehension of the adsorption properties, in view of the design of optimized CPs for VOC selective adsorption.

Solid-State NMR is one of the most powerful techniques for the investigation of structural and dynamic properties of solid adsorbent materials at the atomic scale, providing complementary structural information to long-range characterization techniques, such as X-ray Diffraction (XRD), and unique dynamic information.

In the present work [5], low- and high-resolution solid-state NMR experiments were applied to two recently synthesized 1D CPs (**1**-ClBz and **2**-ClBz with zig-zag and polycatenated topology, respectively) [6], both containing bispidine as organic ligand, Hg(II) as metal center, and chlorobenzene trapped within the framework, to acquire information on ligand and guest dynamics as a function of temperature. By combining analyses of ^{1}H on-resonance free induction decays, ^{1}H and ^{13}C longitudinal relaxation times, and ^{2}H quadrupole echo NMR spectra, it was found that chlorobenzene undergoes isotropic dynamics in **1**-ClBz, while it shows anisotropic motions in **2**-ClBz, indicating stronger interactions between framework and adsorbate in the latter. A broad distribution of correlation times was found for the guest reorientations, associated to different distances and orientations in the interactions with the CP framework. On the other hand, ligands were found to be quite rigid for both CPs in the investigated frequency scale, apart from methyl groups, which undergo fast motions about their ternary symmetry axis.

Acknowledgements: This work was supported by the MUR Project PRIN2022 CleanAir, project code 2022JB2F7H funded by the European Union-Next Generation EU, Mission 4, Component 1, CUP Master D53D23010350006, CUP B53D23015390006.

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[6] M. Lippi et al. Chem. Eur. J. *28* (2022) e202200420.

PC29 FROM LIQUID CRYSTALS TO SOFT-SOFT COMPOSITE MATERIALS WITH PHOTOACTIVE AND SHAPE-MEMORY PROPERTIES

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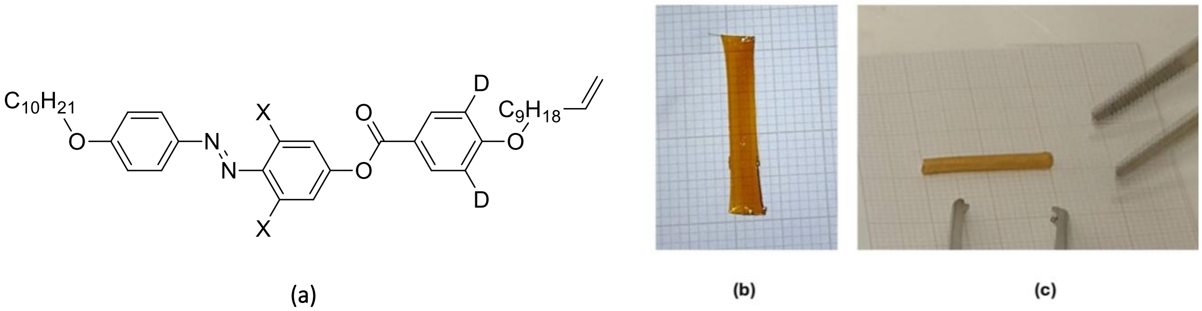
Multifunctional reactive mesogens with lateral methyl substitution in the vicinity of the azo group and selective deuteration on phenyl ring close to the reactive chain were designed and synthesized (see Figure 1a). The self-assembling and structural behaviour was established by polarizing optical microscopy, differential scanning calorimetry and X-ray diffraction techniques. Due to the presence of the selective deuteration, the reactive mesogens were studied by ^{2}H-NMR spectroscopy and the orientational order of the deuterated fragment was investigated and established in the whole mesophase range [1].



(a) (b) (c)

Figure 1: (a) Molecular structure of the designed reactive mesogens with double lateral substitution (10 DABU-D$_2$, X = CH$_3$) and without substitution (10 HABU-D$_2$, X = H) on central phenyl ring of the molecular core. (b) photographs of a monodomain LCE film and (c) a PDLCE in the form of a cylinder.

The two photo-active reactive mesogens have been used for the preparation of multifunctional photo-active Liquid Crystal Elastomers (LCEs) in the form of monodomain films (Figure 1b) and Polymer Dispersed Liquid Crystal Elastomers (PDLCEs) [2] (Figure 1c) targeted for light controlled opto-mechanical applications. The mesomorphic and structural properties as well as the thermo-mechanic / elastic and photo-active properties of the new LCEs and PDLCEs will be reported and discussed in view of possible applications.

Acknowledgments: V. Domenici & G. Romano thank the MIT-UNIPI (Partially ordered soft systems: from the prediction to the application – 2023-2025) project for financial support. The European COST ACTION CA21159 - Understanding interaction light - biological surfaces: possibility for new electronic materials and devices (PhoBioS) is also acknowledged. The co-authors from the Czech Republic greatly acknowledge the funding from the Czech Science Foundation – project 23-42944L (HOLOBLUE).

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PC30

PHOTOCATALYTICALLY REGENERABLE HYPER-CROSSLINKED MICROPOROUS ADSORBENT MODIFIED BY METAL OXIDE NANOPARTICLES

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Adsorption, recently greatly stimulated by availability of high specific surface area materials, has grabbed the attention of scientists as a versatile, cost-effective option for relatively effortless large-scale water treatment. However, adsorbent disposing may have an adverse environmental impact that should be mitigated through regeneration and reuse processes, usually employing high-cost procedures. The validation of an adsorbent cannot be limited to prove the efficiency of the adsorption process, but it must also address adsorbent lifetimes, reusability, and economic and environmental cost of regeneration treatments. This works aims at addressing this issue by proposing a new concept of smart adsorbents where enhanced adsorption is combined to in situ regeneration by heterogeneous photocatalysis for an energy-efficient removal of contaminants. Metal oxide nanoparticles, synthesized by colloidal approaches have been tested as photocatalysts and purposely combined to a hyper-crosslinked microporous adsorbent.

Solution-phase approaches under mild reaction conditions have been exploited towards the design and fabrication of metal oxide nanoparticles (TiO_2, CeO_2). Simple methodologies have been developed, including in-situ synthesis of the colloidal nanoparticles in the presence of microporous adsorbent or ex-situ approach, where pre-synthesized nanoparticles have been let to adsorb on the adsorbent, to adjoin the photocatalytic properties to a purposely synthesized hyper-crosslinked microporous adsorbent. The nanoparticle-modified adsorbent has been evaluated paying particular attention to the adsorbent structural stability, adsorption properties, nanoparticle loading and photocatalytic performance, since they will affect the adsorption and regeneration technology. Different aspects involved in the combination of large specific surface area adsorbents with nanometer-sized photocatalyst have been studied. In-depth investigation by structural, morphological, chemical and optical characterization have been exploited to assess the best photocatalyst candidate, understand the photocatalytic mechanisms involved in the contaminant degradation and, hence adsorbent regeneration, and the suitable functionalization procedure selected.

Acknowledgements: This work has been supported by the European Union through Next Generation EU, Mission 4 Component 1, from MUR within PRIN call 2022 PNRR, Project title: Photocatalytically regenerable hierarchically porous adsorbents for efficient water treatment PHOTOPAD, P2022FP2W4, 2023-2025CUP B53D23027540001) and by PNRR NEST - NETWORK 4 ENERGY SUSTAINABLE TRANSITION project “Scalable Production of Advanced Nanostructures for Electrodes” SPARKLE.

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PC31 CHEMICAL WARFARE AGENTS AND THEIR SIMULANTS FROM FIRST PRINCIPLES

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Chemical Warfare Agents (CWA) are chemical compounds unfortunately used in many conflicts, even recently.[1] CWA’s constitute a severe health risk, thus a rapid detection may help to save human lives. Due to both national and international laws, common research laboratories are not allowed to manipulate CWA’s.[1-3] Actually, researchers interested in the fabrication of CWA’s sensors have to rely on “simulants”, namely molecules that give responses similar to those of real CWA’s when contacted with an appropriate sensor.[1-4] For each type of CWA, appropriate simulant molecules have been selected on empirical bases.[3]

Chemiresistive devices are considered the sensor-of-choice for both CWA’s and their simulants. [4] While on laboratory benches real CWA’s cannot be tested by law,[3,5] in silico experiments may help to fine tune appropriate sensors via theoretical models of both CWA’s and their simulants. In this contribution, we present results obtained by modelling a series of vesicant CWA’s molecules (azoyprites) and their simulants. Several molecular properties of CWA and simulant molecules were first compared in vacuum via DFT and TD-DFT calculations. Also the interactions and the electronic properties of CWA’s and simulant molecules adsorbed on a slab model of a chemiresistive semiconductor oxide surface[4] were investigated as well.

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PC32 DIABATIC QUANTIFICATION OF THE CHARGE-TRANSFER ENHANCEMENT MECHANISM IN ELECTROCHEMICAL SERS

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SERS (Surface-Enhanced Raman Spectroscopy) has proven to be an important characterization technique, owing to both its high intensities and the large amount of information it can yield about interfaces [1]; however, this high sensibility also implies intrinsic complexity when it comes to extracting valuable information from the spectra. Electrochemical SERS (EC-SERS), in which the substrate is a nanostructured electrode for which the electrode potential (V_{el}) can be tuned, poses further challenge given the sensibility of SERS spectra of certain molecules to V_{el}. This is the case for Pyridine, the most emblematic SERS molecule, for which the interaction between Charge-Transfer (CT) states and Plasmons has been proven to play a crucial role. In this work, we have performed full diabatizations for systems consisting of Pyridine attached to different silver clusters, giving the possibility to readily define CT states, whose energy is tunable by an applied external field *E*, which acts as a microscopic analogous to V_e, as pictured in Figure 1. Nuclear wavepacket propagations on the coupled potential energy surfaces including both local excitations of the metal and CT states were performed to retrieve Resonance Raman spectra. Our results show that the population transfer from bright metal states to CT states plays a most pivotal role when it comes to both relative and absolute intensities of EC-SERS spectra of Pyridine [2].

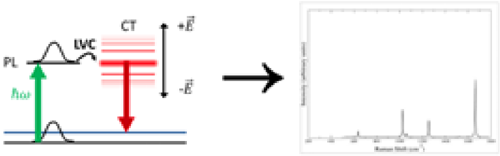

Figure 1. Scheme for a diabatic SERS mechanism.

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PC33

RESISTIVITY MAPPING OF SiC WAFERS BY RAMAN SPECTROSCOPY

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The µRaman spectroscopy measurements were used to study the resistivity in 4H-SiC samples by intercalibrating with Eddy Current measurements (eddy-current probe that accurately measures bulk resistivity of wafers). The position and line width associated with the Raman Longitudinal Optical Phonon-plasmon Coupled (LOPC) mode were used since their variation from the reference values of a material in the absence of dopant-generated defects is proportional to the amount of the free carrier concentration in the conduction band present in the semiconductor [1-4].

Using wafers of known resistivity to calibrate the model and deconvolving the individual recorded spectra, a multi-variable model was created to predict the resistivity of individual map points. Resistivity was thus predicted in a pointwise manner resulting in maps of 92 points over a 6-inch diameter area of a wafer, from which false-colour images were created showing the spatial distribution along the X and Y axes, and in the bulk, along the Z axis of the resistivity. The analysis procedure was automated by creating suitable R-language codes that extract the necessary information on the individual aspects of the analysis and create the images described above from a single dataset.

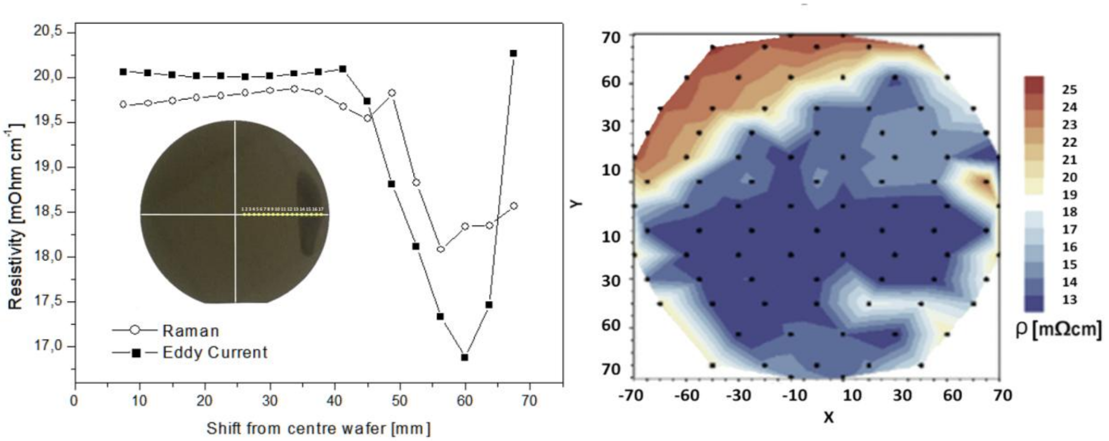

Figure 1. Left: Resistivity value vs position of the measurement with Eddy Current and Raman analysis in the wafer of the training set; Right: The 92-point false color maps of the predicted resistivity calculated with the linear regression model.

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PC34

BEYOND COVALENT CHEMISTRY: DNA-INSPIRED 3D FILMS FOR EFFICIENT LIGHT HARVESTING

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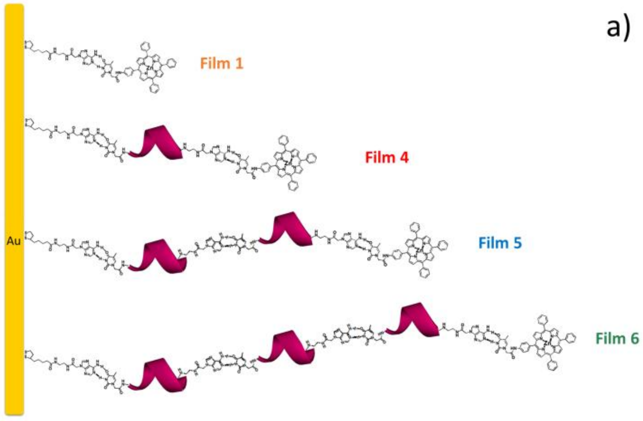
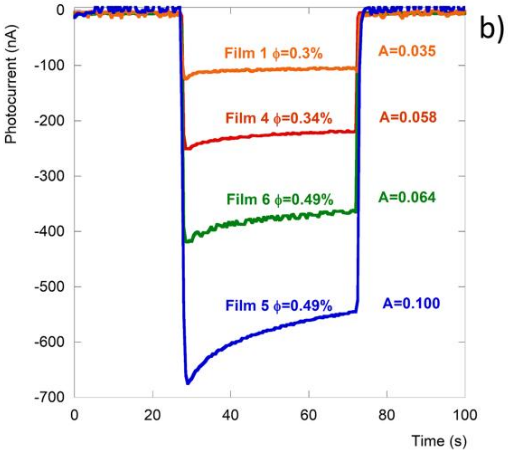
Fabrication of ordered three-dimensional nanostructures on surfaces remains an ongoing challenge in materials science. In particular, achieving molecular order and precise positioning of different redox centers is fundamental for constructing artificial photosynthetic systems capable of controlling electron flow direction. While various systems with covalently linked subunits have been reported in the literature, the synthetic effort required to obtain such multicomponent molecules is considerable. In nature, all supramolecular architectures are assembled through non-covalent interactions, including hydrogen bonds [1]. Specifically, DNA molecules are engineered using nucleobase pairing. In this lecture, we present studies on photocurrent-generating supramolecular components built using an unprecedented approach: constructing supramolecular 3D films composed of different 2D layers by exploiting thymine-adenine DNA base pairing. To this end, we engineered different types of photocurrent-generating films on gold surfaces [2]. All the films consist of multilayered systems where the light-absorbing group (ZnTPP chromophore) is non-covalently linked to the gold surface through thymine-adenine hydrogen bonding. These films are assembled by sequential deposition of each layer. In all other films, one, two, or three additional layers of helical peptides were introduced to control film length [3, 4]. Additionally, we varied the peptide orientation within the film to assess the influence of macrodipole moment direction. Each peptide was functionalized with thymine and adenine, enabling conjugation with Lipo-A and T-ZnTPP. These films were extensively characterized using electrochemical and spectroscopic techniques and exhibited remarkable long-term stability, even in solution. Moreover, under illumination, they generated photocurrent with an efficiency exceeding that of comparable systems.





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PC35

TARGETING MICRORNAS: A PHYSICOCHEMICAL STUDY

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MicroRNAs, or miRNAs, are small non-coding RNA molecules, approximately 22 nucleotides long, that play a crucial role in regulating gene expression. miRNAs regulate gene expression by binding to target mRNA, either inhibiting its translation into protein or marking it for degradation. MiRNAs bind to complementary sequences on messenger RNA (mRNA), usually in the 3' untranslated region, effectively blocking protein synthesis or leading to mRNA degradation. MiRNAs are involved in many biological processes, including development, differentiation, proliferation, and apoptosis (cell death). They also play significant roles in diseases, particularly cancer and metabolic disorders [1].

Destabilizing miRNA presents a promising approach as an anticancer strategy. To explore this potential, we employed physicochemical methodologies to investigate the thermodynamic stability of miRNAs and their interactions with two distinct classes of compounds: flavonoids and repurposed drugs.

Flavonoids are vital compounds with a wide range of health benefits and applications in nutraceutical, pharmaceutical, medicinal, and cosmetic fields. They exhibit significant biological activities, including anticancer, antibacterial, antifungal, anti-diabetic, antimalarial, neuroprotective, cardio-protective, anti-inflammatory, and anti-oxidative effects. The effectiveness of flavonoids is influenced by their absorption and bioavailability, which need enhancement for improved pharmaceutical applications. With molecular targets in cells, flavonoids can impact health positively, as demonstrated by preclinical studies highlighting their therapeutic properties, such as antioxidative, anti-inflammatory, antiproliferative, cytoprotective, genoprotective, and epigenetic restorative effects [2].

Drug repurposing, also known as drug repositioning, focuses on identifying new therapeutic applications for existing drugs. This strategy has gained significant attention due to its potential to reduce development time, costs, and risks associated with traditional drug discovery. Repurposed drugs often have established safety profiles, making them quicker to bring to market for new medical indications [3].

Preliminary findings indicate that some of the compounds examined successfully destabilize the miRNAs under investigation.

Acknowledgements: CN00000041 National Center for Gene 'Therapy and Drugs based on RNA Technology', funded by European Union-NextGenerationEU and financed by PNRR MUR-M4C2-Investimento 1.4-CUP UNINA: E63C22000940007

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NEW CONTRAST AGENTS FOR PHOTOACOUSTIC IMAGING

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Photoacoustic imaging represents a promising biomedical imaging modality, combining the contrast of optical imaging with the superior spatial and temporal resolution of ultrasound (US). It is based on the photoacoustic (PA) effect, where absorbed light energy causes an instantaneous thermoelastic expansion in tissues, generating a detectable broadband US wave. This type of imaging is non-invasive, depends on the light absorption coefficient, and achieves high contrast. Unlike optical imaging, it uses ultrasound, resulting in minimal tissue scattering and dissipation. These characteristics grant PA imaging high capabilities for deep tissue imaging.[1]

Commonly used contrast agents for PA imaging include endogenous chromophores, such as melanin, oxyhemoglobin/deoxyhemoglobin, lipids, or collagen, however, to enhance contrast, resolution, and tissue penetration, the development of externally injectable contrast agents with high PA imaging contrast is an important aspect to address.

In recent years, significant advancements in PA contrast agents have been made, essential for diagnosing and treating diseases like breast carcinoma or glioma.

An ideal contrast agent should possess specific photophysical properties, including low quantum yield, high molar extinction coefficient, and peak absorption in the near-infrared (NIR) window. Additionally, it should exhibit excellent photostability, low toxicity and immunogenicity, high affinity and specificity for the target, and biocompatibility.[2]

Organic dyes capable of absorbing in the NIR-I and NIR-II regions can be used as valid candidates for PA imaging [3]; among them, polymethine dyes are particularly interesting due to their versatile structure. In fact, by appropriately decorating the base structure of polymethine dyes, such as by inserting various substituent groups with electrondonor/electronwithdrawal properties on the polymethine bridge and/or on the indole core, it is possible to finely modulate their photophysical properties. Fluorescence yield can be reduced, making the resulting molecules promising candidates for PA imaging.

In this contribution, the preparation and photochemical characterization of three pentamethine and three heptamethine cyanine dyes is proposed. Multi Spectral Opto Acoustic Tomography (MSOT) was used to test the photoacoustic activity in agar phantoms. All the cyanine dyes exhibited high PA performances, in some cases higher then Indocyanine Green, the only FDA approved contrast agent for PA imaging.

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TAILORING DEFECTIVITY, TEXTURAL PROPERTIES AND ADSORPTION CAPACITY OF UiO-66(Ce) METAL-ORGANIC FRAMEWORKS THROUGH FLUORINE FUNCTIONALIZATION

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The strength of Metal-Organic Frameworks (MOFs) lies in the unlimited possibility of tuning their textural and electronic properties. The synthesis of fluorinated MOFs is relevant since fluorine atoms can impart excellent properties, including enhanced selectivity towards reactive species like CO_2 [1]. UiO-66 structures are characterized by very high stability when exposed to different solvents, including water, and by good mechanical resistance. Furthermore, UiO-66 MOFs find application in many different fields, like catalysis, separation and drug delivery. Here we report the investigation of the fluorination effect on the general properties of Ce-based UiO-66 MOFs [2].

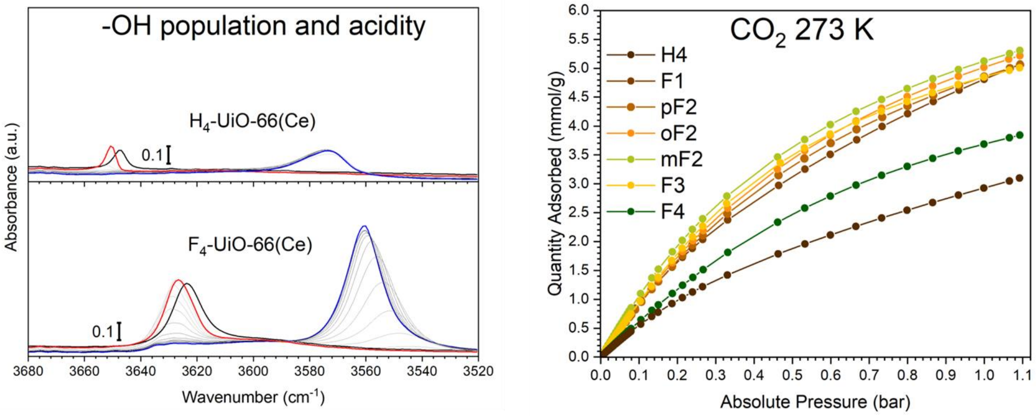

Figure 1. Left) In situ IR spectra on Fx-UiO-66 during interaction with CO at 77 K; Right) CO_2 adsorption isotherms at 273 K on F_x-UiO-66

The advanced characterization of the whole series assesses that the presence of a different number of fluorine atoms on the terephthalic linker has an impact majorly on the textural properties of the Fx-UiO-66 MOFs. Indeed, advanced analyses of the pore size distribution revealed how the substitution of bulkier fluorine atoms on the ring slightly reduces the aperture of the pores and closes the triangular windows which constitute the walls of the pores. These factors allow only very small molecules to freely enter all the cavities of partially fluorinated Fx-UiO-66 and interact with the fluorinated walls, guaranteeing a CO_2 adsorption capacity at 273 K which is almost twice the one of H_4-UiO-66. Furthermore, very interesting results were achieved by conducting *in situ* IR experiments using CO to determine the acidity of the hydroxyl groups of Fx-UiO-66(Ce). The experiment revealed some differences between the adsorption sites of H_4-UiO-66(Ce) and of the fluorinated MOFs. The first difference is related to the population of hydroxyl groups, which is comparable in the case of the Fx-UiO-66 and significantly higher compared to the hydrogenated reference. Furthermore, the experiment also revealed that fluorine atoms also affect the acidity of these groups.

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PC38 A COMPUTATIONAL APPROACH TO MODELING EXCITATION ENERGY TRANSFER AND QUENCHING IN LIGHT-HARVESTING COMPLEXES

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Light-harvesting complexes (LHCs) play a critical role in modulating energy flux within photosynthetic organisms in response to fluctuating light [1]. Under high light conditions, they activate quenching mechanisms to mitigate photodamage [2-4]. Despite their importance, the molecular mechanisms underlying these photoprotective processes remain incomplete. What is more, it is still unclear how such a mechanism can be switched on and off depending on the LHC conformation. The most accepted model for chlorophyll quenching is excitation-energy transfer to neighboring carotenoids, which quickly decay to their ground-state, completing the dissipation [5-7]. Herein, we present a computational protocol to model the energy pathways in the LHC, focusing specifically on the minor CP29 antenna complex of plants. We explore the factors that modulate the switch between the light-harvesting and quenched states. The protocol includes modeling the exciton Hamiltonian of the chlorophylls/lutein aggregate and calculating population dynamics using a kinetic model based on the Redfield-Förster approach. Our analysis reveals a highly tunable excited-state lifetime for the complex, that can switch between quenched and unquenched state depending on the excitation energy of the lutein, which acts as a final quencher, in accordance with recent experiments [5]. Moreover, we observe that the s-trans lutein conformers are more likely to exhibit characteristics of the quencher.

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PC39

SHEDDING LIGHT ON THE EFFECT OF PROTEIN-NANOPARTICLE INTERACTIONS: IMPACT ON THE INTERFACIAL BEHAVIOR OF BIO-NANOHYBRIDS

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Proteins are eco-friendly agents widely used for stabilizing fluid interfaces due to their biocompatibility, biodegradability, and unique structural properties. Their amphiphilic nature allows them to stabilize dispersed systems such as foams and emulsions effectively [1,2]. Additionally, proteins can facilitate the assembly of colloidal nanoparticles (NP) at air–water interfaces [3], leading to the development of smart interfacial systems with enhanced stability against external stimuli and variations in subphase composition, thanks to the irreversible adsorption of NP [4].

In this study, we investigate protein adsorption dynamics and their role in directing the irreversible adsorption of anionic silica nanoparticles (~25 nm diameter) at air–water interfaces, considering the influence of protein nature on interfacial properties. Using three model proteins—Bovine Serum Albumin (BSA), β-Lactoglobulin (BLG), and β-Casein (BCN)—we assess how variations in protein structure and charge distribution affect the adsorption behavior and interfacial assembly of NP. The effects of bulk composition on the formation and stability of both pure protein films and protein-NP hybrid layers were examined through a combination of experimental approaches. Specifically, Dynamic Surface Tension (DST) and compression isotherms in a Langmuir trough were employed to characterize and compare the adsorption kinetics and interfacial stability of both pure protein monolayers and protein-NP hybrid layers. Grazing Incidence Small Angle X-Ray Scattering (GISAXS) provided insights into the layers structure in static and dynamic conditions, while vibrational Sum-Frequency Generation (SFG) allowed us to capture molecular-level details in protein structure upon interaction with NP with high surface specificity.

Our findings demonstrate that protein interactions with NP significantly changes the adsorption kinetics from the bulk solution and leads to a less marked reduction of surface tension due to changes in protein conformational flexibility in a protein-dependent manner, as observed with DST and vibrational SFG. Additionally, protein-decorated NP layers exhibit complex and composition-dependent phase behavior under compression as suggested by GISAXS results, highlighting the potential of tailored protein-NP formulations for designing advanced ultrathin films with tunable interfacial properties.

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PC40

INSIDE THE STRUCTURE OF EMISSIVE 2D $(C_6H_5CH_2NH_3)_2(Pb,Mn)Br_4$ LAYERED METAL HALIDES

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In the past decade, halide perovskites (HPs) emerged as a significant class of materials for various optoelectronic applications, including solar cells, light-emitting diodes (LEDs), detectors, and lasers. Besides, an increasing interest has grown on compounds with lower dimensionality, the so called 2D structures characterized by metal-halides octahedra layers separated by organic cations [1].

Herein, we present our results on the preparation of emissive 2D (Pb,Mn)-based hybrid metal halide employing the benzylammonium ($Bz^+ = (C_6H_5CH_2NH_3)^+$) as organic cation (Figure 1). Varying the experimental conditions, we synthesized crystals with different Pb/Mn ratio. The emission ranges from the light blue of Bz_2PbBr_4 to the typical orange emission of the Mn centered at 610 nm (Figure 1b). The maximum intensity of the emission was observed for the sample with Mn composition of 8.0% (PLQY = 48%). A detailed investigation of the samples evidences a peculiar growth of the crystals with the coexisting of more than one phase if the concentration of the Mn exceeds 8% mol. Employing different characterization techniques, such as cathodoluminescence analysis, magnetic measurements and second harmonic generation we demonstrated that a maximum of the miscibility between Pb and Mn exists. Moreover, Mn rich samples present inclusions with different stoichiometry inside the synthesized single crystals.

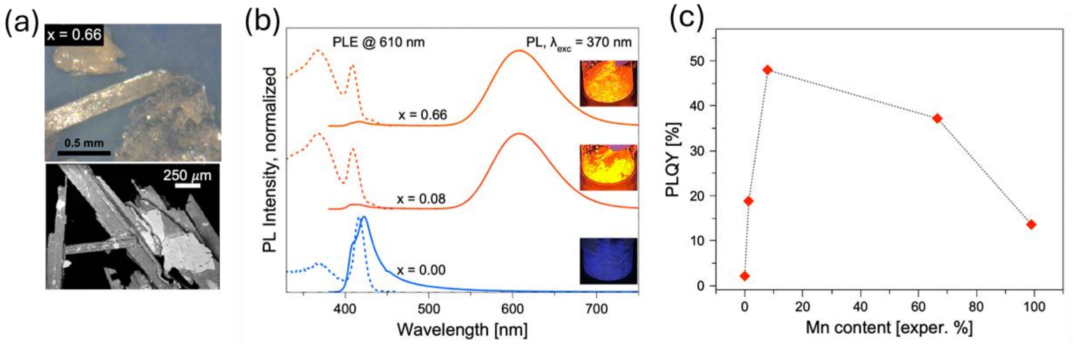

Figure 1. (a) optical microscopy and SEM images of the crystals with Mn composition of 66%; (b) PLE, PL spectra and (c) PLQY at different metal compositions.

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PC41

CALORIMETRIC STUDIES OF INTERACTIONS OF NON-WETTING LIQUIDS WITH POROUS MATERIALS

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High-pressure scanning calorimetry otherwise known as Scanning Transitiometry can be used to characterize the thermomechanical properties of solid-liquid interface development [1-5]. More explicitly it has been used to measure the heat and work of liquid intrusion into/from porous materials with a broad range of pore sizes. This is done through the simultaneous recording of three different variables which include, power, volume and pressure. Treatment of the power data provides the calorimeter curve which is used for calculating the heat of intrusion/extrusion which is combination of interface development and change in internal energy of water structure as it enters the porous structure. The work is calculated by combining the pressure and volume data to create pressure volume isotherms which can be used to determine the average pressure of filling/empting, otherwise known as the intrusion/extrusion pressure. Simultaneously this allows us to identify the volume of intruded liquid, otherwise known as the intrusion volume. These values fundamentally describe the base energetics of the intrusion of water into the hydrophobic network, however they can fundamentally be adjusted through other means such as the addition of solutes or changing the crystallite size of the material. These parameters can be used to devise energy storage system, shock absorbers or bumpers.

Acknowledgements: This project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 101017858.

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PC42 LIGHT-CONFIGURABLE LOW-DIMENSIONAL NANOSTRUCTURES AT THE AIR/WATER INTERFACE

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Molecular monolayers formed at the air/water interface serve as a fundamental model system for studying two-dimensional (2D) structures, as they allow a controlled investigation of intermolecular interactions, self-assembly processes and phase transitions in thin films.[1] Among the many molecular materials which form monolayers at liquid interfaces, photosensitive surfactants are considered a useful tool to obtain tunable liquid interfaces in a non-invasive manner, [2] enabling to modulate in real-time key properties such as surface tension, molecular organization, and monolayer stability. [3]

In this perspective, we employed a surfactant molecule containing a photoactive azobenzene group. to investigate both the stability of monolayers depending on the surfactant conformation and the role of the surfactant conformation on promoting the irreversible adsorption of nanoparticles (NPs) at the air/water interface. To achieve this, we firstly studied the desorption kinetics of spread photosensitive surfactant monolayers upon fine modulation of their cis-trans ratio. This approach allowed us to analyze how the conformation ratio affects the dynamic behavior and stability of the interface. Specifically, we will show that both the number of desorbing molecules and the desorption rate can be controlled by adjusting both the monolayer composition and density.[4] Then, we employed a cationic photosensitive surfactant to investigate with GISAXS (Grazing Incidence Small Angle X-ray Scattering) the detailed structure of the monolayers formed by negatively-charged nanoparticles. We will show that surfactant conformation greatly influences the surface activity of the surfactant-nanoparticle complex and, in turn, the NP monolayer density. Moreover, the in-situ irradiation of the aged NP monolayer allows to further modulate the interfacial structure and stability. These findings open up exciting prospects for the development of adaptive materials, smart interfaces, and light-controlled interfacial processes.

Acknowledgements: We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian MUR, funded by the European Union – NextGenerationEU – Project Title: Reconfigurable Low-Dimensional Nano-Structures at Liquid Interfaces - ReLoDS – CUP E53D23008600006 – Code 2022ZP453S- Grant Assignment Decree No. 958 adopted on 3.6.2023 by the Italian MUR.

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PC43

MAGNETIC SWELLABLE ORGANICALLY MODIFIED SILICAS FOR THE REMOVAL OF ORGANIC DYES FROM AQUEOUS MEDIA

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Organic dyes are major industrial wastewater pollutants, posing severe health risks like tissue damage and cancer disease. Their release into water disrupts ecosystems by depleting oxygen and hindering photosynthesis, leading to bioaccumulation and toxicity. Various methods exist for dye removal, but adsorption has proven to be promising due to its environmental sustainability and high removal capacity [1]. Among the different sorbents, hybrid porous silicas can offer significant advantages: large specific surface area, tunable pore structure and easy surface modification make it highly desirable adsorbents for wastewater remediation [2]. Swellable Organically Modified Silicas (SOMS) are a class of hybrid materials able to swell in organic solvents and to retain high amount of organic molecules [3]. Magnetic nanoparticles (MNPs) offer promising solution for wastewater remediation as their magnetic properties enable easy separation [4-5]. It is well-known that magnetite (Fe_3O_4) MNPs can be encapsulated in silica-based materials to improve their stability, dispersion, biocompatibility and to prevent oxidation of MNPs [5]. Here we investigate the synthesis and the characterization of magnetic nanocomposite consisting of MNPs linked to SOMS (MNPs-SOMS). MNPs-SOMS were synthesized by co-precipitation method for the MNPs, followed by a sol-gel process using bis(trimethoxysilylethyl)benzene (BTEB) to form SOMS onto MNPs (scheme in Figure 1). Morphological (SEM, TEM), structural (XRD), thermal (TGA), chemical (FT-IR) and magnetic characterization confirmed the physico-chemical properties of the synthesized material. Preliminary adsorption tests using an aqueous 1.0 x 10^{-5} M Rhodamine B (RhB) solution showed complete dye removal within 10 minutes, with retention of magnetic properties (Figure 1). These results indicate that MNPs-SOMS is a promising adsorbent for dye removal, combining high adsorption efficiency with easy magnetic separation.

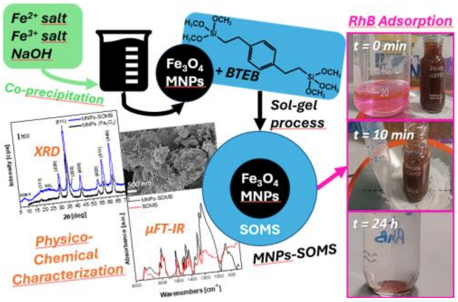

Figure 1. Scheme of MNPs-SOMS synthesis with examples of characterization analyses and images of RhB adsorption.

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[2] R. Wang et al. ChemistrySelect 9 (2024) 19.
[3] L. Maccarino et al. Micropor. Mesopor. Mat. 375 (2024) 113178.
[4] A. Shahzad et al. Sci. Rep. 14 (2024) 17674.
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PC44

LUCIFERIN-LUCIFERASE INTERACTIONS: AN ADVANCED MOLECULAR DYNAMICS STUDY

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Bioluminescence is a fascinating natural phenomenon through which living organisms (like fish, bacteria, squid, fireflies and fungi) produce light using chemical reactions [1]. The "cold light" is generated via the oxidation of a substrate, called luciferin, which is catalyzed by a group of enzymes called luciferases.

Analyzing the bioluminescence of Oplophosus Gracilirostris, the structure of the luciferase and luciferin has been characterized.[2] The luciferase is formed by two subunits, the bioluminescent active one is of ~19 kDa.[3] It is not possible to produce only the active subunit since it is unstable and poorly soluble. Therefore, the protein has been optimized and an innovative luciferase called NanoLuc has been obtained together with a novel substrate called furimazine [4]. Despite the several applications, few information are available about the interactions between NanoLuc and furimazine and between NanoLuc and the oxidated substrate, furimamide [5].

We have studied luciferase-luciferin interactions using molecular dynamics simulations. The simulations are performed on the open structure of NanoLuc with two luciferases, coelenterazine and furimazine and their products of oxidation, coelenteramide and furimamide, respectively. In addition, for the two substrates, we have considered the two tautomers, the ketonic and the enolic form. The simulations gave information about the intra-barrel pocket changes of the enzyme in the presence of the different ligands. In addition, we have shed light on the structural re-arrangements in the open and closed NanoLuc forms.

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[2] O. Shimomura et al. Biochemistry 17 (1978) 994.
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[4] M. Hall et al. ACS Chem. Biol. 7 (2012) 1848.
[5] M. Nemergut et al. Nat. Commun. 14 (2023) 7864.

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PC45 RAMAN SPECTROMICROSCOPY APPLIED TO PLANETARY FIELD ANALOGUE SAMPLES

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The search for extraterrestrial life is a key driver of planetary exploration missions, such as NASA's Mars 2020 and ESA's ExoMars and Mars Sample Return next-generation space missions. Handling samples from these missions requires rigorous protocols for sample receiving facilities and Mars sample return curation [1]. Identifying laboratory and planetary field analogues (PFA) is essential for developing effective sample collection strategies and testing scientific instruments. PFAs are terrestrial environments that mimic extraterrestrial conditions, providing valuable insights into extreme habitats where life might exist. Their study enhances our understanding of life's adaptation and preservation potential in harsh environments.

The HELENA [2] project investigates secondary volcanic geothermal phenomena at Lago Bagno dell'Acqua (Pantelleria, Italy) and the Allalobad area (Afar Region, Ethiopia). These unique ecosystems offer a window into microbial diversity and survival limits under extreme conditions. Specifically, the terraced structure of these PFAs preserves ancient lake environments, enabling comparative studies of (subfossil) biosignatures (potential traces of life preserved in rocks).

Field activities, conducted in collaboration with the National Park of Pantelleria Island and the Afar Bureau of Culture and Tourism, have facilitated the collection of representative samples from geobiofacies influenced by geothermal gradients (e.g. temperature, pH). This study presents Raman spectromicroscopy analyses of potential biosignatures within microbiologically induced structures, providing new insights into their formation and preservation.

[1] Tait et al. Astrobiology 22 (2022) S57.
[2] https://site.unibo.it/helena/it/team/bologna

PC46

UNVEILING KEY INTERACTIONS AT TiO_2-ANATASE/PEO INTERFACES: A METADYNAMICS STUDY

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Describing heterogeneous electrochemical interfaces rather than single component materials is rapidly emerging as a major challenge in advanced materials design. From the computational modelling point of view, the demanding task concerns the development of non-standard theoretical approaches required for reliably describing complex systems with different chemical nature or intricate processes on different length/time scales [1]. In this context, we propose a metadynamics study of TiO_2 anatase/poly(ethylene oxide) (*i.e.*, PEO) interfaces [2], a case-study system with technological interest in many fields, from biomedicine to energy conversion and storage [3].

By selecting the torsion angle of the polymer chain and the number of Ti-O distances below the equilibrium value (*i.e.*, 2.6Å) as collective variables, we could explore the conformational space and coordination modes adopted by PEO oligomer when interacting with the (101) anatase crystal facet. The collected 1 ns-trajectories at 300K computed at DFTB-D3BJ level of theory show that PEO will mostly assume conformations in the range of ω~40°-120° and establish two- and three-fold coordination with the anatase surface. The conformational freedom of PEO results to be significantly influenced by multiple favorable interactions with unsaturated Ti sites on the anatase surface. From these trajectories, several equilibrium structures extracted from the free-energy surface are analyzed using electronic structure calculations within density functional theory: the titania work function turns out to be largely affected by the dynamically resolved structuring of PEO on the anatase surface [4]. These findings provide the first innovative example of an affordable yet reliable computational protocol to describe a heterogeneous interface and predict the dynamics effects on physico-chemical properties of interest for electrochemical applications.

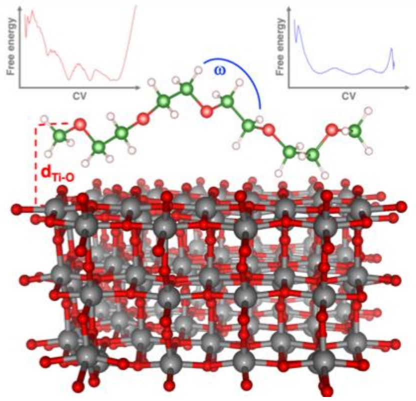

Figure 1: Configurational and conformational structuring at (101)-TiO2/PEO interfaces.

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[2] A. Barducci et al. WIREs Comput. Mol. Sci. 1 (2011) 826
[3] D. Selli et al. J. Phys. Chem. C 120 (2016) 29190.
[4] A. Massaroet al. J. Phys. Chem. C 128 (2024) 20497.

PC47

DAHLIA-LIKE MESOPOROUS SILICA NANOSTRUCTURES AND NANOSTRUCTURED LIPID CARRIERS FOR GENE TRANSFECTION IN CANCER IMMUNOTHERAPY

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Tumor immunotherapy has seen a dramatic resurgence of interest due to the development of genetically engineered T cells (Chimeric Antigen Receptor T (CAR T) cells) to express the synthetic CAR to recognize antigens directly on the tumor cells surface, allowing them to attack cancer cells with greater effectiveness. CD19 is considered a highly specific target because it is found on most B cells malignancies, so by engineering T cells to express CARs that recognize CD19, these modified T cells can selectively eliminate CD19-expressing cancer cells, leading to remission in many patients with refractory or relapsed cancers. To advance gene-modified cell therapies, lenti- or retroviral vectors are employed although these approaches are costly and characterized by residual risks such as germline transmission, immunogenicity, and insertional mutagenesis. Therefore, there is a quest for efficient strategies for non-viral transduction of synthetic receptors into primary T cells able also to protect the genetic material from the premature degradation by enzymes [1]. Synthetic nanovectors, loaded with a specific plasmid (pSLCAR-CD19-28z), have been explored to bypass chromosomal integration, reduce risks and avoid enzymes degradation. Here, nanostructured lipid carriers (NLCs) and large pores mesoporous silica nanoparticles (MSNs) were synthesized for their advantageous properties, including biocompatibility and efficient loading capability. NLCs were produced through the hot homogenization technique and loaded with the plasmid using a hydrophobic ion pairing approach. MSNs were synthesized via dynamic soft-templating and single-step sol-gel processes, respectively and were surface-functionalized with a cationic polymer polyethyleneimine (PEI) for plasmid loading. The physical-chemical characterization and in vitro studies of both nanostructures revealed an average hydrodynamic diameter lower than 200 nm, demonstrating excellent colloidal stability in physiological media, efficient plasmid release without degradation and good biocompatibility. These findings highlight the successful development of these nanoplatforms positioning them as promising candidates for potential applications in oncology.

Acknowledgements: This work was financially supported by TITAN-Tumour Immunotherapy by Nanotechnology, Bilateral Project CNR-RFBR Russia Joint research project (2021-2024) and Project PRIN 2022 PNRR (code P2022RLFZB), NHYLODEA funded by the European Union - Next Generation EU, Mission 4 Component 1, CUP H53D23007980001

[1] B. De Angelis B. et al. J. Mater. Chem. B 8 (2020) 1823.

PC48 SERS NANOSTRUCTURES WITH ENGINEERED ACTIVE PEPTIDES AGAINST AN IMMUNE CHEKPOINT PROTEIN

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PD-L1 is an immune checkpoint protein overexpressed on the surface of cancer cells and links PD-1 proteins expressed on the T-cells of the immune system. When the link occurs, the killer activity of the T-cells is depressed and the immune system fails to fight tumors. Targeting PD-L1 allows preventing the interaction PD-L1/PD-1, preserving, therefore, the activity of the T-cells.

SERS nanostructures are small clusters of gold nanoparticles in which a SERS reporter is present. These nanostructures show very intense SERS spectra which can be observed down to a single nanostructure. We functionalized the nanostructures with an engineered peptide (HS-PEG-Lys3-Gly2-CLP002-NH2 where CLP002 is Trp-His-Arg-Ser-Tyr-Tyr-Thr-Trp-Asn-Leu-Asn-Thr) to verify the targeting activity of the thousands of peptides, present on the surface of the nanostructures, against the clusters of PD-L1 proteins of the cancer cells.

Incubation of the nanostructures with MDA-MB-231 breast adenocarcinoma cancer cell line, which overexpresses PD-L1, shows, using the SERS signals of the nanostructures registered for each cell, a very good targeting activity of the nanostructures. This activity was compared to the activity of the same nanostructures, but functionalized with the peptide obtained by scrambling the amino acid (HS-PEG-Lys3-Gly2-sCLP002-NH2 where sCLP002 is Thr-Arg-Trp-Ser-His-Tyr-Asn-Thr-Leu-Trp-Tyr-Asn). Results are reported in Figure 1 [1] and show that the nanostructures with the scrambled version of the peptide (sCLP002) do not show a targeting activity, validating the results for the nanostructures with CLP002.

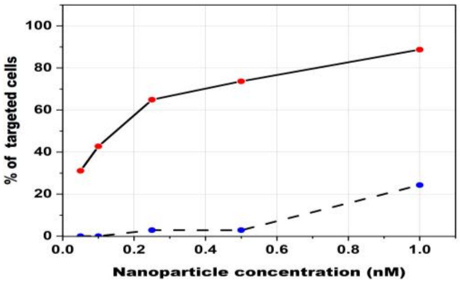

Figure 1. Activity of the SERS nanostructure for the targeting of MDA-MB-231 over-expressing PD-L1. The % of the cell with a positive targeting, obtained with SERS signals for each single cell, is plotted against the concentration of nanoparticles used for incubation (HS-PEG-Lys3-Gly2-CLP002-NH2: continuous line, HS-PEG-Lys3-Gly2-sCLP002-NH2: dashed line).

It was also previously shown that functionalized SERS nanostructures are resistant to enzymatic attack, which is one of the biggest problems for peptides with pharmacological activity [2], and that they can be used for photothermal laser treatment of the cancer at the level of single cell [3].

[1] M. Gobbo et al. Nanoscale 16 (2024) 5206.
[2] F. Biscaglia et al. Nanoscale 13 (2021) 10544.
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PC49 SILK FIBROIN NANOPARTICLES AS EFFICIENT BORON CARRIERS FOR BORON NEUTRON CAPTURE THERAPY

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Boron Neutron Capture Therapy (BNCT) is a targeted cancer treatment combining a boron-containing compound with low-energy neutron irradiation. When a ^{10}B nucleus captures a neutron, it releases Linear Energy Transfer (LET) particles (alpha particles and lithium ions),that selectively destroy boron-loaded tumor cells. Effective therapy requires a boron concentration of at least 20 ppm in the tumor and a high tumor-to-healthy tissue boron ratio to minimize collateral damage.[1]
New boron agents should exhibit strong tumor selectivity, prolonged retention, stability in the bloodstream, and reduced clearance to enhance efficacy and minimize toxicity. Currently, only sodium borocaptate (BSH) and 4-boronophenylalanine (BPA) are clinically approved for BNCT, with BPA being widely studied, while BSH suffers from poor tumor cell uptake. Nanomedicine offers promising solutions for targeted BNCT treatments,[2] as nanoparticles can enhance intracellular delivery of poorly absorbed molecules.

In this study, we present a novel formulation utilizing silk fibroin nanoparticles (SFN) capable of loading a high concentration of borocaptate ions. SFNs encapsulating sodium mercaptoundecahydro-closo-dodecaborate (or borocaptate, BSH) or tetramethylammonium BSH (hereafter N-BSH) were prepared, characterized, and tested. BSH and N-BSH differ in their counterion and, therefore, in their solubility properties.

SFNs loaded with BSH or N-BSH were extensively characterized by a multi-technique approach, including FESEM and Nanoparticles Tracking Analysis (NTA) for the assessment of morphology and size distribution, ICP-OES, EDX and FT-IR for the quantification of boron.

The formulations were then tested on U87 glioma cells, and boron uptake was evaluated using neutron autoradiography after irradiation in a thermal neutron field. Neutron autoradiography is valuable in BNCT because it provides comprehensive information on boron uptake in biological samples. This technique enables the quantification and imaging of boron distribution in cell pellets, isolated cells, and tissue sections by detecting neutron capture products without destroying the samples. The results demonstrated the significant role of the nanocarrier in enhancing boron internalization compared to BSH alone. Therefore, encapsulating BSH in silk fibroin nanoparticles offers promising potential for *in vivo* BNCT applications.

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PC50

DEVELOPMENT AND IMPLEMENTATION OF QUANTUM-CLASSICAL STOCHASTIC METHODS FOR THE CALCULATION OF KINETIC RATES OF ELEMENTARY REACTIONS IN SIMPLE AND COMPLEX CONDENSED PHASE

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This work develops a model for interpreting macroscopic kinetic constants in elementary reactions, particularly when mass transport and chemical reactions occur on comparable timescales, as in enzymatic catalysis. We focus on bimolecular exchange reactions, specifically SN2 nucleophilic substitutions in haloalkanes, using bromide and chloromethane as a case study.

Our approach employs a reaction-diffusion model inspired by Sevein and Moro [1], integrating mass transport with localized quantum-mechanical reactions.

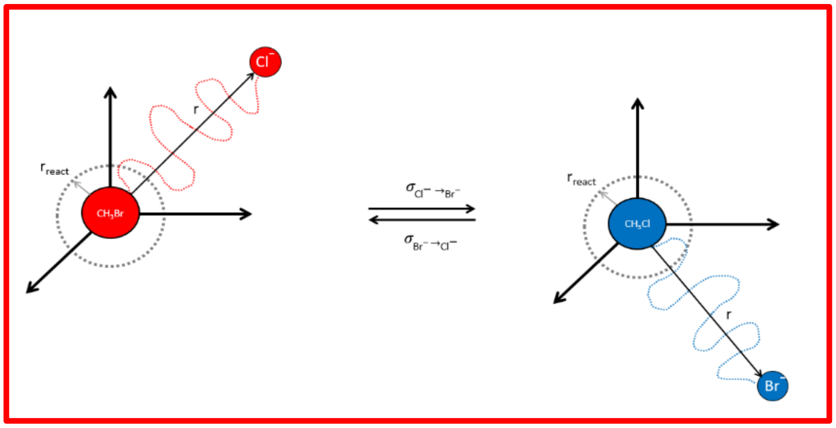

Figure 1: Schematic representing the diffusion-reaction dynamics. The system can be in the Cl^- *+* CH_3Br *or in the* Br^- *+* CH_3Cl *states. In both, the stochastic variable is the mutual distance, r, between the two reactant species. Interconversion between the two states is regulated by the rates* $\sigma_{Cl^- \to Br^-}$ *and* $\sigma_{Br^- \to Cl^-}$ *and can occur when the reactants are close enough;* r_{react} *sets the distance where a sigmoid function drops separating the reactive from the non-reactive conditions.*

The governing equations consist of (i) a diffusive term, dependent on the diffusion coefficient and mean field interaction potential determined via steered molecular dynamics [2], and well-described by a modified Buckingham potential and (ii) a reactive term, modeled through a master equation parameterized with microscopic kinetic constants [3,4].

This model establishes a continuous description of macroscopic kinetic constants by linking the interplay of reaction and transport timescales. Despite simplifications such as neglecting rotational dynamics and separating barrier crossing from other relaxation processes the method accurately captures expected kinetic behaviors across a wide dynamic range. It estimates macroscopic kinetic constants in an ab initio fashion by correlating key molecular parameters: diffusion coefficients, interaction potentials, and microscopic rate constants.

This framework enhances our understanding of reaction mechanisms in complex environments and provides a basis for future studies on reactive dynamics in liquids.

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[4] J. Campeggio et al. Phys. Chem. Chem. Phys. 22 (2020) 3455.

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PC51 CRYSTALLOCHEMISTRY AND THERMODYNAMIC PROPERTIES OF THE INTERMETALLIC COMPOUND Cu_{3-x}(As,Sb)

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Studying the ternary system Cu-As-Sb, the new intermetallic phase $Cu_{3-x}(As_ySb_{1-y})$ has been identified [1]. In this study, we present structural results based on single crystal and powder X-ray diffraction data. Both, the Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) have been performed for thermal analysis. The metallographic and chemical analysis (SEM-EDXS) has been done for providing information on the microstructure and the chemical composition of the intermetallic compound. The ternary $Cu_{3-x}(As_ySb_{1-y})$ compound has been found to crystallize in the cubic $Cu_{9.1}(TeSb)_3$-type (*cP*32, *Pm*-3*n*) [2], a ternary derivative of the Cr_3Si-type. It is the first isotypic representative of this prototype. A composition range of Cu (71.1-73.9 at%), As (5.8-24.5 at%) and Sb (2.1-23.1 at%) has been found for this ternary compound; notably, no formation of pure binaries of the Cu-As or the Cu-Sb system has been noticed. The lattice parameters have been detected in a rather wide range of 7.479 – 7.652 Å from the As-rich to the Sb-rich side. $Cu_{3-x}(As_ySb_{1-y})$ forms congruently in between 691-676 °C for compositions richer in Sb (691°C for $Cu_{72}As_7Sb_{21}$ and 676 °C for $Cu_{72}As_{14}Sb_{14}$); while the As-rich compound forms peritectically (628 °C for $Cu_{72}As_{21}Sb_7$). Some physical properties (electrical resistivity and magnetic susceptibility) have been measured on the polycrystalline bulk samples. We have found that $Cu_{3-x}(As_ySb_{1-y})$ is a good metal with electrical resistivity decreasing with increasing Sb-concentration.

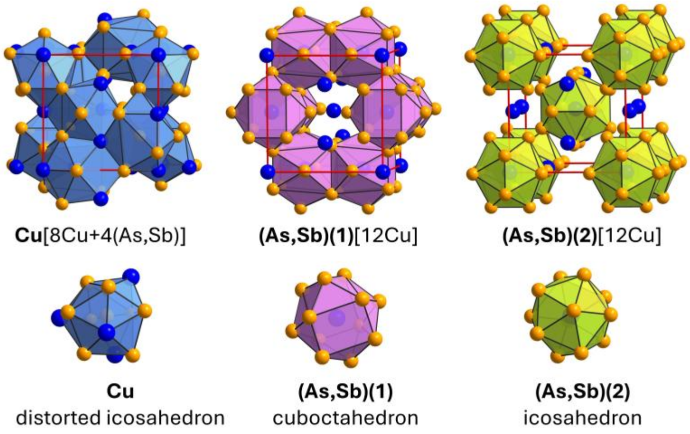

Figure 1. Perspective views of the crystal structure of the cubic compound Cu3�x(As,Sb), where the polyhedra around the Cu, (Sb,As) (1) and (Sb,As) (2) atoms [a Frank-Kasper (CN=16) and two icosahedra (CN=12), respectively] are highlighted.

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PC52

SHAPING MAGNETIC FIELDS:
ADDITIVE MANUFACTURING APPROACH FOR CUSTOMIZED NdFeB ARRAYS

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We present a methodology for creating magnetic systems with precisely controlled field configurations using additive manufacturing technologies. Our approach employs 3D-printed polylactic acid (PLA) support structures that enable accurate positioning of neodymium-iron-boron (NdFeB) permanent magnets with various geometries. The high remanence NdFeB magnets (1.2–1.4 T) enabled the generation of substantial magnetic fields even with relatively compact assemblies. We focused particularly on developing circular Halbach arrays that generate highly homogeneous magnetic fields across extended spatial regions through quasi-harmonic distributions of magnetization vectors along circular paths. Numerical simulations using the magpylib Python package were conducted to predict magnetic field topologies, which were subsequently verified through experimental mapping using a custom-built Hall probe measurement system based on a modified Anet A8 3D printer [1]. The system achieved spatial resolution of approximately 0.1 mm with field strength measurement precision of ±0.5 mT. Our research encompassed configurations with controllable field gradients—ranging from highly homogeneous fields to high-gradient systems—applicable for diverse applications, including magnetic self-assembly, recycling of the magnetic catalyst [2] and removing of heavy metals [3] upon magnetic separation from aqueous solutions.

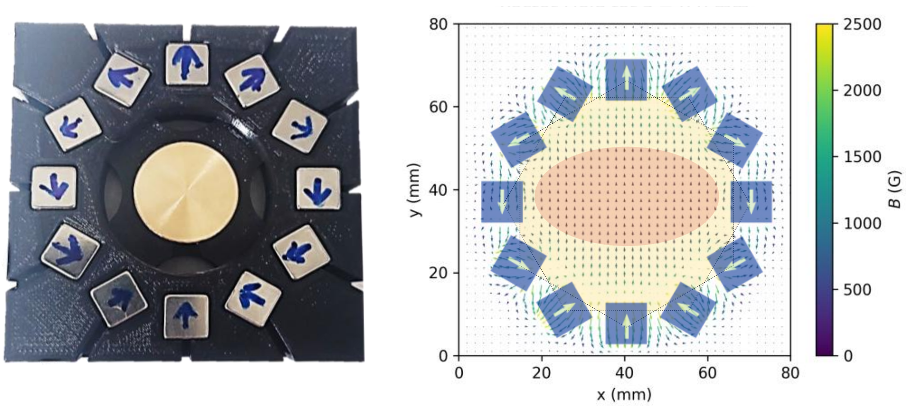

Figure 1. A picture of assembled Halbach circular array (left) and a magnetic field map obtained by a 3-axial Hall probe.

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PC53

HIGH-MOMENT FeCo NANOSYSTEMS VIA CONTROLLED REDUCTION IN MESOPOROUS SiO_2

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Metallic magnetic nanoparticles offer substantially higher saturation magnetization (M_S) compared to their oxide counterparts, making them attractive for numerous applications including data storage, sensing, and biomedicine [1]. However, these metallic systems are inherently susceptible to oxidation in ambient conditions [2,3], necessitating effective encapsulation strategies to preserve their enhanced magnetic properties. In this study [4], we investigate the synthesis and characterization of FeCo-alloy nanosystems embedded in mesoporous silica (SiO_2) matrices, with a particular focus on how matrix porosity modulates the efficiency of hydrogen reduction processes. Firstly, we optimized the reduction parameters for FeCo oxides. The equiatomic composition (50 at% Fe) emerged as optimal, offering both high M_S of ~242 A m^2/kg and superior oxidation resistance with an onset temperature of ~440°C. Subsequently, we synthesized FeCo-oxide nanocomposites within SiO_2 matrices via sol–gel self-combustion, followed by controlled thermal treatments to systematically modify the matrix porosity. As annealing temperature increased to 900°C, the matrix surface area decreased by ~30%, resulting in incomplete reduction and formation of Fe_xO_y/Co_xO_y intermediates. This decrease in matrix porosity corresponded to a ~20% reduction in saturation magnetization, confirming that restricted hydrogen diffusion impedes complete oxide-to-metal conversion. This work provides insights into the design principles for silica-embedded metallic magnetic nanosystems with enhanced stability and magnetic performance.

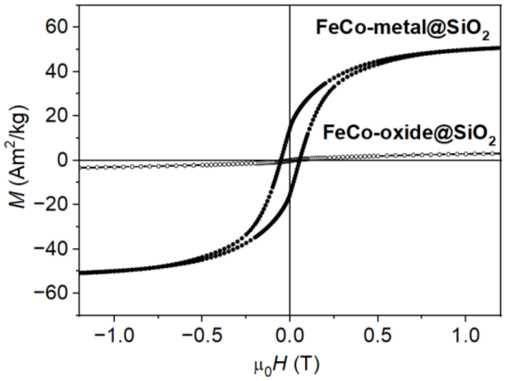

Figure 1. Comparison of magnetic hysteresis (300 K) for as-prepared and reduced FeCo nanosystems (50 at% Fe) in mesoporous matrix SiO_2.

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PC54

ULTRAFAST NONADIABATIC DYNAMICS IN REALISTIC SYSTEMS MONITORED THROUGH ENTANGLED TWO-PHOTON ABSORPTION. A QUANTUM DYNAMICAL APPROACH BASED ON ML-MCTDH METHOD

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Quantum spectroscopy which takes advantage of the quantum properties of light has come up as a potential approach to explore the properties of matter which cannot be exploited by using the classical light[1,2]. Quantum spectroscopy finds broad applications across imaging, sensing, and non-linear spectroscopic methods. Entangled two-photon absorption (ETPA), where a pair of entangled photons, known as the signal and idler, interact with a molecule, is one of the most fundamental and integral feature of the quantum spectroscopy. These photons are produced via spontaneous parametric down-conversion (SPDC) and exhibit non-Fourier correlations in their temporal and spectral characteristics. This property allows ETPA to achieve simultaneous temporal and spectral high-resolution measurements. Further, due to the photon entanglement, the rate of two-photon absorption scales linearly with pump intensity. A protocol based on time-dependent perturbation theory to describe coupled electron-vibration-photonic dynamics has been introduced by Mukamel and co-workers[3]. A model simulation around conical intersections for four electronic states and two vibrational modes demonstrated the potential of ETPA for mapping ultrafast wavepacket dynamics by tuning the signal-idler pair and pump frequency[4]. Our goal is to develop a computational protocol capable of simulating quantum dynamics near conical intersections induced by ETPA in realistic molecular systems. To achieve this, we employ an efficient approach to parameterize linear vibronic coupling (LVC) models, previously developed by our group[5]. This is combined with the multi-layer multi-configurational time-dependent Hartree (ML-MCTDH) method for wavepacket propagation. These propagations enable the computation of correlation functions necessary to reconstruct the response function, ultimately characterizing ETPA in nonadiabatic systems. The results, presented as spectra and population dynamics, demonstrate the effectiveness of our theoretical framework in capturing intricate molecular behaviour.

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Ni-DOPED LSTF AND Co-FREE Y-DOPED BSCuF AS INNOVATIVE ELECTRODES FOR INTERMEDIATE-TEMPERATURE SOLID OXIDE CELLS

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Solid oxide cells (SOC), working at temperatures in the range 800°C-1000°C, represent a class of devices considered essential to the energy transition. Since they can act both as energy production means from hydrogen or lean hydrocarbons and as hydrogen production apparatuses, these cells can be coupled to intermittent renewable resources, *i.e.* photovoltaic and wind, to constitute a reliable energy production method [1]. The current challenge to develop this technology stands in the stability and compatibility of the different materials, and in the reduction of the working temperature range.

In this work, two families of MIEC (Mixed Ionic-Electronic Conductor) materials with a perovskite structure, LSTF (Lanthanum Strontium Titanium Ferrite) [2] and BSCuF (Barium Strontium Copper Ferrite), have been studied for their potential application as electrodes in intermediate temperature (IT-SOC) cells and reversible solid oxide cells (RSOC). LSTF was properly doped with increasing concentration of Ni, and the electrochemical features in both reducing and oxidizing conditions have been investigated. This material can act both as fuel-side and air-side electrode for solid oxide fuel cells (SOFC) and solid oxide electrolysis cells (SOEC), with enhanced performances thanks to the ex-solution of Ni and Ni-based alloys in reducing conditions [3]. In particular, the effect of Ni introduction has been rationalized and the best composition for both sides of SOC systems has been identified.

Instead, BSCuF represents a promising Co-free alternative to the widely studied BSCF (Barium Strontium Cobalt Iron Oxide) as air electrode for SOC. Since cobalt substitution is crucial due to its toxicity and supply limitations, Cu has been introduced as an alternative [4]. However, this replacement typically impacts the electrochemical performance, particularly in terms of oxygen reduction reaction (ORR) activity and impedance over a wide temperature range. Given the limited data available in the literature, structural and electrochemical properties of BSCuF were explored, demonstrating its compatibility with ceria-based electrolytes and its potential as an environmentally sustainable air electrode material. Additionally, beneficial effects were observed when doping the B-site with Y, which helps preventing secondary phase formation without compromising catalytic and electrochemical performance [5].

Acknowledgements: The present work has received financial support under the projects PRIN2022-ADESSO and PRIN2022-FORCEFUL.

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ON THE PRESENCE OF MICROPLASTICS IN HUMAN URINES, KIDNEYS, AND FLUIDS FOR PERITONEAL DIALYSIS AS REVEALED BY MICRO RAMAN SPECTROSCOPY

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Microplastics (MPs) are fragments of plastic materials with sizes ranging from 1 μm to 5 mm. The presence of these particles has been demonstrated not only in environmental settings, but also in human tissues and fluids [1]. The increasing incidence of chronic kidney disease (CKD) underscores the need to assess the potential involvement of MPs in the occurrence of this condition. The present study employed μ-Raman spectroscopy, a widely utilized technique for the identification and characterization of MPs, capable of detecting fragments with dimensions below 1 μm in different matrices [2]. In the first part of the investigation, the presence of polymeric fragments, mainly constituted of polystyrene and polyethylene debris, as well as associated pigments (e.g., hematite, phthalocyanine blue), was revealed in human urine samples (from healthy donors) and renal tissue samples (from healthy portions of nephrectomies) [3]. In the second part, the identification and characterization of MPs was attempted in fluids used for peritoneal dialysis, which is a technique commonly employed in the treatment of chronic kidney failure. The presence of MPs in these liquids, due to contamination during the production process or packaging, could serve as a potential entry route for harmful MPs into patients' bodies. The preparation of samples followed this procedure: for each 2-liter sample, three 200 mL aliquots were collected, unified into a 600 mL sample and filtered through a polytetrafluoroethylene (PTFE) membrane filter with a pore size of 0.2 μm. The Raman spectra of the particles retained on the membrane were recorded and compared with reference spectra for identification. Polyethylene and polypropylene particles (Figure 1) were detected, suggesting a potential contamination deriving from the packaging of these fluids. Further investigations are required to evaluate the exposure to microplastics in dialysis patients.

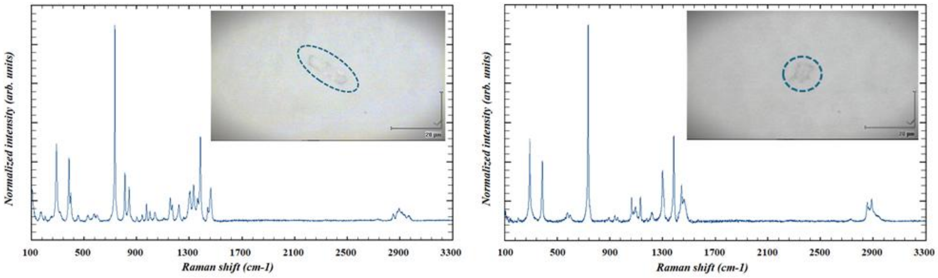

Figure 1. Polypropylene (left) and polystyrene (right) fragments detected in the samples.

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PC57

SHUTTLING PROCESSES IN MOLECULAR TUBES: A COMPUTATIONAL APPROACH

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The capability of controlling the motion at the molecular scale is fundamental for the fabrication of molecular motors and machines [1]. In liquid phases, self-assembly procedures provide viable approaches for the synthesis of *e.g.* rotaxanes and other bimolecular complexes [2,3] where the relative motion of the components could be controlled by external stimuli [1]. Calixarenes are currently adopted for the formation of bimolecular complexes [4], where a linear molecule (axle) can "enter" the tubular calixarene cavity, thus forming pseudo-rotaxanes and allowing for the molecular axle to shuttle inward and outward the molecular tube. In this respect, the knowledge of the microscopic details of the self-assembly processes of calixarene-based rotaxanes could be fundamental for a rational design of molecular motors. In order to gain atomic level insight on the transit process of molecular axles through the tubular calixarene cavity, we have simulated both the entrance (threading) and the exit (dethreading) processes of stilbazolium-based axles in and out the molecular tube. The modelling was based on a metadynamics approach [5,6] in liquid dichloromethane at room conditions. Such an approach allows for the calculation of the free energy profiles for both threading and dethreading processes. Due to the asymmetric nature of the two calix[6]arene entrances, and by using asymmetric stilbazolium axles, it has been possible to establish the kinetically preferred threading and dethreading directions, as well the most stable configuration of each pseudo-rotaxane.

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PC58 PHILOSOPHY AND PHYSICAL CHEMISTRY IN DIALOGUE: LANGUAGES AND MODELS

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In a lucid reflection on the excessive specialization of science, Chemistry Nobel laureate Roald Hoffmann emphasizes the need to make the structure and language of chemical content—whether in presentations or articles aimed at specialists—more pedagogically refined [1]. The development of this approach requires constant and fruitful interaction between the hard sciences and the humanities. This contribution presents and discusses the dialogue between the humanities and STEM disciplines with particular attention to the intersection between philosophy and physical chemistry. One of the main objectives is to explore whether, through careful use of language and engagement with various forms of communication and multimedia, it is possible to develop interdisciplinary work models that promote knowledge sharing and growth. We present and discuss some research activities carried out by 'hard' scientists and philosophers dedicated to the in-depth study of scientific topics with schools and a wider audience of non-experts. Thanks precisely to the search for common languages at the intersection of the humanities and STEM, the experience we present here has proved to be dialectically fruitful and rich in critical reflection points, capable of opening up paths of interdisciplinary training and learning and teaching models [2,3].

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PC59

BIOCATALYST MAGNETIC NANOARCHITECTURES FOR SOLVENTLESS POLYESTER SYNTHESIS

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Biocatalysis has emerged as a sustainable alternative to traditional chemical synthesis, yet its industrial adoption relies on improving enzyme stability, activity, and reusability. Immobilizing enzymes on magnetic nanoarchitectures offers a promising solution, combining enhanced catalytic performance with facile recovery and recyclability [1]. Here we investigate the design of Biocatalyst magnetic nanoarchitecture (BMN), combining Candida antarctica lipase B (CaLB) and magnetic nanoparticles. CaLB was conjugated onto 10 nm Fe_3O_4 nanoparticles under controlled conditions, followed by biochemical characterization confirming high protein loading and retained enzymatic activity. The presence of magnetic nanoarchitecture as a solid support facilitated easy recovery and reuse of the biocatalyst over multiple cycles. When applied in the polycondensation of renewable monomers (dimethyl adipate and 1,8-octanediol), the BMN achieved > 87% monomer conversion across three cycles, producing polyesters with number-average molecular weights (Mn) of 4200–5600 Da and low dispersity (<2). The high magnetic responsiveness of the nanoarchitecture to an applied magnetic field allowed efficient biocatalyst recycling via magnetic separation, demonstrating its potential for sustainable and economically viable biocatalysis [2]. In this very promising scenario, the perspective are related to some critical issues such as optimization of the magnetic properties, mass transfer limitations and low efficacy against insoluble substrates still need to be overcome. These improvements will lead to a synergistic rational design of the magnetic and biocatalytic component to produce novel magnetic nano architectures such as magnetic nano (hetero)-structure with optimized morpho-structural (e.g. size and shape) and textural (e.g. high surface area) properties .

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PC60

ELECTRONICALLY EXCITED SULFUR CHEMISTY IN COMETS

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Sulfur is one of the key elements (HCNOPS) of the molecules that support life, yet its chemistry in space remains poorly understood. In the interstellar medium, sulfur is found in icy mantles on dust grains (e.g., OCS, SO_2) and in the gas phase (e.g., SO, H_2S, CS) and may also exist in refractory material like iron sulfides. However, only about 5% of S elemental budget is accounted for [1,2], and the primary sulfur carriers in dense clouds remain unidentified.
Comets and other pristine solar system bodies provide clues about interstellar sulfur chemistry. Remote spectroscopy has revealed simple sulfur species (H_2S, OCS, SO, CS_2, etc.) in comets [3], while the Rosetta mission detected additional S-bearing molecules, including CH_3SH, S_3, S_4, and complex organosulfur species during dust storms [4,5]. The presence of these species suggests unidentified reactions involving simpler S-molecules.
S(^{1}D), a metastable electronically excited sulfur atom, plays a crucial role in cometary chemistry. Formed via photodissociation of precursors like OCS and C_S2, S(^{1}D) undergoes reactive collisions rather than mere physical quenching in cometary comae [6-8]. Our quantum chemistry simulations explore S(^{1}D) reactivity in both gas and ice phases, providing insights into cometary observations. The S(^{1}D) + H_2O gas-phase reaction produces SO + H_2, explaining additional SO sources observed in Hale Bopp [10]. Unlike previous models, our study shows this reaction is not purely a quenching process [7]. Furthermore, in an ice matrix, S(^{1}D) + H_2O stabilizes hydrogen peroxide, altering the reaction outcome compared to the gas phase [8]. Finally, S(^{1}D) + CH_3OH does not form complex organosulfur molecules in the gas phase but does on ice, yielding species like CH_2OHSH, CH_3OSH, and CH_3SOH [10]. These results help interpret Rosetta's detection of CH_4SO species following a dust emission event from comet 67P [3].
Our findings highlight the importance of excited-state sulfur chemistry in space and its role in shaping the observed sulfur inventory in comets.

Acknowledgments: This work has received funding from the Italian MUR (PRIN 2020, "Astrochemistry beyond the second period elements", Prot. 2020AFB3FX) and the Italian Space Agency (Ban-do ASI Prot. n. DC-DSRUVS-2022-231, Grant no. 2023-10-U.0 MIGLIORA).

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IS CAM-B3LYP/SMD/6-311G+(d,p)/$(H_2O)_n$ THE "ELDORADO" METHOD FOR DETERMINING PK$_A$ AND PK$_B$ OF SMALL ORGANIC COMPOUNDS?

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We have developed a method characterized by exceptional reliability, for determining the pK_a of a wide panel of organic acids, such as phenols[1] and carboxylic acids[2]. Our "easy to use methodology" returned minimum average error (MAE) lower than 0.3 for phenol pK_a, and 0.5 for carboxylic acids. Further, it can predict with great reliability the pK_a of difficult to model compounds (i.e. trichloroacetic acid) with a simple level of theory[2]. Recently, the reliability of this method was proved also on alcohols and thiols, reaping a MAE value below 0.5 in both cases. Our method exploits CAM-B3LYP as functional, the solvation model based on density (SMD) and 6-311G+(d,p) basis set[1-3]. In our approach, we draw the very first solvation shell adding two explicit water molecules at the reaction center. The pK_a is calculated applying the ionogenic equation, without using experimental energy values for H^+ nor *ex post facto* correction. We explored the possibility of applying this methodology in predicting the pK_b of primary aromatic and aliphatic amines, obtaining impressive results, i.e. MAE=0.3. Remarkable results were also obtained with secondary and tertiary amines, with a MAE equal to 0.54. Such striking result strengthens the reliability of our approach[1-3] providing, for the first time, the possibility to predict the pK_a and pK_b of small organic compounds with the same methodology, always ensuring trustworthy outputs.

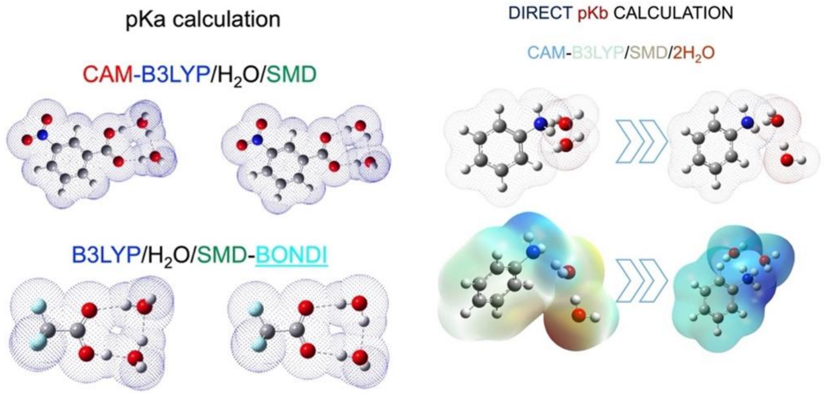

Figure 1: Accurate prediction of the pK_a and pK_b of small organic compounds in one-pot method. Geometry optimization was carried out using CAM-B3LYP/SMD/2H2O/6-311G+(d,p) or B3LYP/SMD-BONDI/2H2O/6-311G+(d,p).

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PC62 THE THERMO-OXIDATIVE BEHAVIOR OF COTTON COATED WITH POLYAMIDOAMINES: A SOLID-STATE NMR-EPR JOINT STUDY

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Cotton is not fire-resistant and therefore poses a serious hazard in the event of a fire when used in indoor furnishings. However, cotton can be made flame-retardant through treatments with additives. The development of bio- and eco-friendly treatments using different types of additives is currently a quite active research field. Polyamidoamines (PAAs) derived from α-amino acids are both bio- and eco-friendly flame retardants (FRs) and do not release smoke during combustion [1].

Aim of this study is to investigate the reactions that take place in cotton impregnated with PAAs during a fire. Given the rapidity of the process, it is difficult to follow the transformations occurring in the burning material. Thus, we adopted the strategy of thermal oxidizing the material under controlled conditions and characterizing the intermediate products. No evidence on the mechanism of thermal oxidation of cotton in the presence of the PAAs has been reported so far.

We used ^{13}C solid state NMR spectroscopy to study the products of partial combustion of cotton impregnated with different PAAs based on glycine and cystine. Figure 1 shows the ^{13}C cross polarization magic angle spinning (CP-MAS) spectra of cotton impregnated with cystine charred at different temperatures as an example. EPR spectroscopy was also used to gain insight into the mechanism of thermal oxidation.

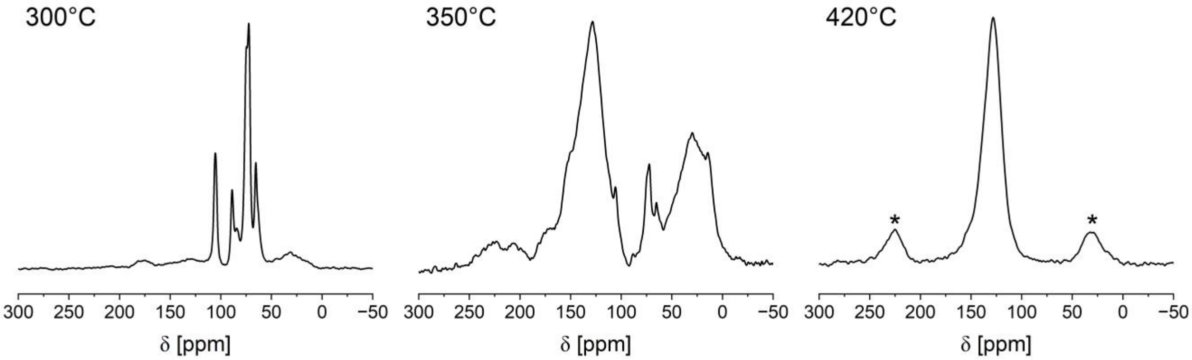

Figure 1. ^{13}C CP-MAS spectra of cotton impregnated with the cystine based PAA charred at the indicated temperatures. Side bands are marked with asterisks.

Acknowledgments: This research was funded by the Italian Ministry of University and Research (project PRIN 2022 FLARECO - Eco-friendly, washing-durable FLAme-REtardant finishing for cotton fabrics by COvalent grafting of α-amino acid-derived polyamidoamines, code 202237JYZN).

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DEVELOPMENT OF QM-DERIVED FORCE FIELDS FOR GAS MOLECULES ADSORBED IN POROUS MATERIALS

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Porous carbons, presenting a disorganised structure that includes both conjugated domains and defects, forming pores of different dimensions, represent promising candidates for gas storage systems, molecular filters, and other applications. The main challenges are given by their complex chemical structure that hinders an easy rationalization of their performance and by the necessity of combining efficiency and accuracy. Computational chemistry could act as a fundament tool to study and screen these materials [1].

Quantum-mechanically derived force-fields (QMD-FFs), tailored for a target problem, can be used to obtain accurate and predictive results, for various kinds of systems [2], exploring larger scales than electronic structure methods, both in time and in size.

In the present contribution we showcase the protocol and the tools that we developed for the automatic parametrization of an accurate adsorption potential (Fig.1). After an initial benchmarking of different density-functional and wave-function theory methods on simple models, we proceeded to analyse the behaviour of a small gas molecule (i.e. CO2) on carbon-based molecules, presenting a variety of topologies. The obtained database is then used to obtain the QMD-FF's parameters, and it is also used as a validation set for the latter, in a recursive procedure. More in detail, the parameterization procedure exploits a fitting of the intermolecular energy, expressed as a sum of Lennard-Jones and Coulombic components, to the QM interaction energy. Lastly, the resulting QMD-FFs can be employed to compute different properties for the reference system employing statistical methods such as Montecarlo or molecular dynamics methods.

Such a workflow leads to the construction of a QMD-FF specific for the system it was parametrized on, however the approach is transferrable to the study of other adsorbate-adsorbent material systems.

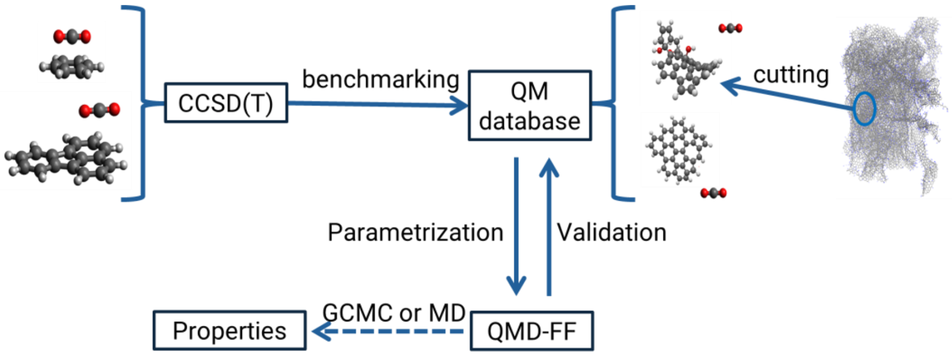

Figure 1. Schematic representation of the devised workflow.

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[2] G. Prampolini et al. J. Phys. Chem. Lett. 13 (2022) 243.

PC64

WATER CONFINED IN GRAPHENE SHEETS: A FAST FIELD CYCLING NMR STUDY

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The production of high-quality graphene sheets is crucial for their practical application in electronics, optoelectronics, energy-storage devices, and composite materials. Among the preparation methods, electrochemical exfoliation of graphite in acidic electrolytes is particularly attractive because of its easy, fast, and environmentally friendly nature [1].

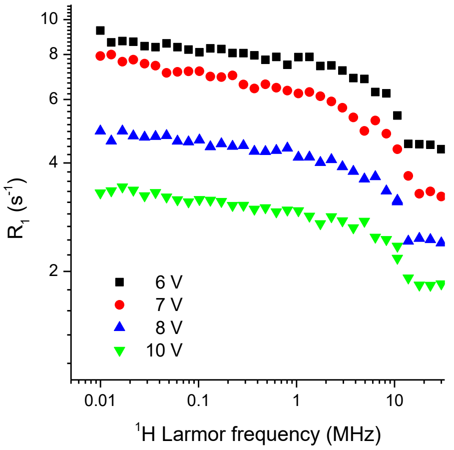

Figure 1. ^{1}H R_1 as a function of the Larmor frequency of aqueous suspensions of graphene sheets (water content equal to 66 wt%) obtained by electrochemical exfoliation of graphite at the indicated voltages.

In this work, we aim at assessing the effect of applying different exfoliation voltages on the structure of graphene sheets by using ^{1}H Fast Field Cycling (FFC) NMR relaxometry combined with X-ray diffraction and Raman spectroscopy.

The ^{1}H FFC NMR dispersion curves of aqueous suspensions of graphene sheets obtained at different voltages are reported in Figure1. The analysis of the curves enables the assessment of water accessibility to the graphene surface.

Acknowledgments**:** This research was partially funded by the Italian Ministry of University and Research (project PRIN 2022 FLARECO - code 202237JYZN).

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PC65

HAMPERING THE SELF-ASSEMBLY OF FIBROIN IN CONSOLIDANTS FOR FRAGILE SILK ARTIFACTS

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The development of sustainable biomaterials is at the forefront of the research efforts in materials science. In this regard, we proposed the use of dispersions of self-regenerated silk fibroin (SRSF) for the consolidation of fragile silk, alone [1,2] or in combination with cellulose nanocrystals (CNC) [3,4]. We have studied the response of gels formed by pure SRSF dispersions and by SRSF/CNC mixtures to shed light on the effect of nanocellulose on the physico-chemical behavior of hybrid systems. Our findings show that the addition of CNC alters the gelation kinetics, leads to stronger gels and qualitatively modifies the yielding behavior. In addition, by applying the sequence of physical processes (SPP) approach [5] to the analysis of large amplitude oscillatory strain measurements, we find evidence of a broad yielding transition which is characterized by a progressive fluidization [4]. Overall, we demonstrate that CNC speeds up the assembly of fibroin in the hybrid dispersions, leading to the formation of more compact colloidal structures at the nanoscale than the sole SRSF. When the hybrid dispersions film, the presence of CNC favors the formation of crystalline structures (most notably α-helices) even at low fibroin concentration, and the films confer optimal axial strength to aged silk fibers, surpassing the performance of single-component (SRSF or CNC) dispersions at the same concentration of consolidant, and of pure crystalline SRSF [3].

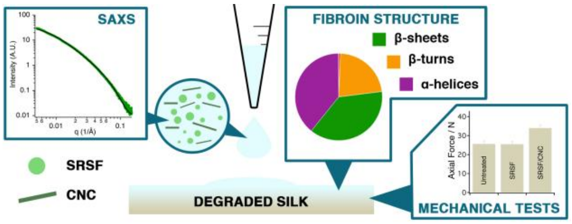

Figure 1. Hybrid systems of SRSF and CNC to be used for the consolidation of degraded silk.

Regardless the composition, the self-assembly of fibroin, which leads to the gelation of systems, must be avoided or controlled, with the aim of improving the shelf life of dispersions that are designed to be applied at the liquid state. In the framework of the European project GREENART, we have studied the effect of a protein, i.e., sericin, which is produced by silkworms in the production of silk and removed during fibroin extraction, and an amino acid, L-arginine, present in both fibroin and sericin, for hampering the self-assembly of fibroin, also in presence of CNC. Gelation times are significantly increased with increasing amount of both additives, together with a reduction of the formation of crystalline structures in dried films. Nonetheless, the consolidating effects of hybrid dispersions featuring sericin or arginine as stabilizing agents is retained, allowing for the application on aged and historical silk artifacts, such as a Japanese kimono belonging to the MET (Metropolitan Museum of Art) in New York.

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[3] C. Cianci et al. Coll. Surf. A 634 (2022) 127944.
[4] G. Poggi et al Coll. Surf. A 636 (2022) 128121.
[5] G.J. Donley et al. Non-Newton. Fluid Mech. 264 (2019) 117.

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PC66

ULTRAFAST SPECTROSCOPY ANALYSIS TO OPTICAL NANOCARRIERS IN OCULAR TISSUES

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Vesicles and liposomes are often used as nanocarriers for drug delivery. Their penetration into cells is highly influenced by their deformability, which can be altered upon drug loading. Here we used fluorescent dyes as an indirect probe to evaluate liposomes deformability by analyzing their photochemical behavior when inserted into the lipid bilayer of liposomes. In particular, we analyzed the photophysics of Nile Red (NR) inserted in liposomes and dispersed in aqueous solutions with and without the presence of surfactants. The analysis of absorption and fluorescence spectra indicates that in the liposomes NR has an optical response similar to that observed in a polar solvent. [1], [2] Room temperature excitation spectra closely matched the respective absorption profiles, indicating that only a single excited state contributes to the emission of Nile Red. Furthermore, we used transient-absorption spectroscopy to analyse the excited state photoinduced behaviour of the dye in the liposomes, exploring the effect of chromophore concentration on its photodynamics in the concentration range 10^{-6}-10^{-4} M. The measured transient absorption spectra and the kinetic behaviour of the dye were not affected by its concentration inside the liposome, excluding aggregation phenomena. The presence of surfactant did not produce notable effects as well. The observed excited state dynamics suggests that Nile red is located within the vesicles (lipid bilayer) in all cases, both with and without surfactant and that the vesicle deformability is not significantly altered in the presence of the dye within the explored concentration range.

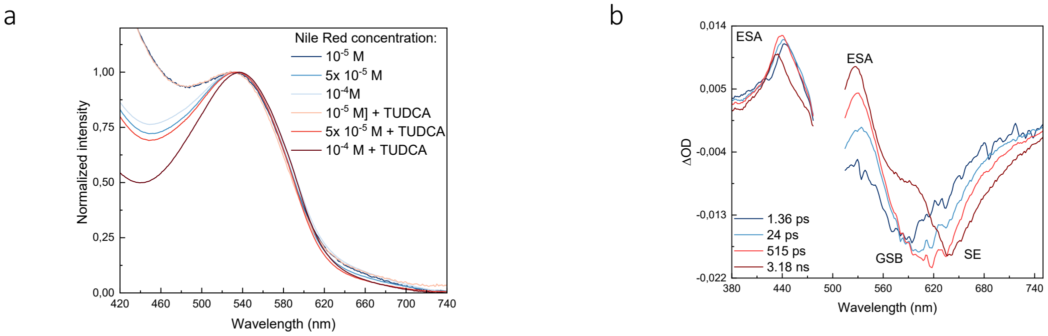

Figure 1. a) Steady-state absorbance spectra at room temperature. b) Transient absorption spectra at room temperature. Evolution-associated difference spectra (EAS) obtained from a global analysis of the transient-absorption data recorded for the sample with the Nile red at 10–4 M.

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PC67

PHASE TRANSITIONS AND INTERFACIAL MAGNETIC COUPLING IN COBALT FERRITE–HEMATITE NANOCOMPOSITES

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The development of chemical syntheses for magnetic transition-metal oxide nanoparticles has gained significant interest due to their applications in biomedical, electronic, and thermoelectric fields. Among various fabrication methods, modified sol–gel techniques have recently emerged as a powerful tool for designing multiphase nanocomposites. These materials enable the exploration of complex interfacial interactions, particularly exchange coupling between ferromagnetic and antiferromagnetic phases, leading to phenomena such as exchange bias (EB) [1].

In this work, we investigate the magnetic behavior of cobalt ferrite (CFO) nanoparticles and their composites with hematite (CFO@FO@800°C) to understand interfacial coupling and phase transitions [2]. Zero-field-cooled (ZFC) and field-cooled (FC) magnetization curves confirm a transition from a blocked to a superparamagnetic regime for CFO at ~160 K, while hematite exhibits a Morin transition at (T_M) ~257 K. In the composite, CFO dominates the hysteresis loop, showing increased coercivity and reduced remanence due to interphase interactions and particle growth during annealing.

Field-cooled hysteresis loops reveal a weak exchange bias (~1% of H_C) that vanishes above T_M. This effect is observed in an unusual scenario where the Curie temperature (T_C) of CFO is lower than the Néel temperature (T_N) of hematite, leading to a complex interplay of spin alignment across the interface. Structural analysis by X-ray diffraction and TEM confirms the absence of secondary iron oxide phases, reinforcing the role of direct CFO–hematite coupling in the observed behavior. These findings provide insights into tailoring interfacial magnetic properties in oxide nanocomposites for advanced applications in magnetism and spintronics.

[1] V. Skumryev et al. Nature 423 (2003) 850.
[2] P. Maltoni et al. J. Phys. Chem. C 129 (2025) 591.

PC68

DEVELOPMENT AND FORMULATION OF NOBLE METAL CLUSTERS

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Noble metal nanoclusters (NCs) are promising candidates for a wide range of applications in sensing, imaging, and therapeutics due to their unique photophysical properties, particularly their tunable emission that spans across the UV-VIS-NIR spectrum [1 - 4]. This project has focused on the design and synthesis of NCs, by identifying novel stabilizer sequences able to enhance the stability and photoluminescence efficiency of these nanoclusters [5]. By optimizing the radiative pathways, the quantum yield has been increased and we have observed robust emission characteristics. Additionally, encapsulation with gels has been employed to make the NCs less susceptible to environmental influences, thereby improving their practicality for real-world applications [6]. Our approach builds upon foundational studies in the field, including the exploration of sequence-dependent properties (Raman and IR spectroscopy) and the development of robust encapsulation techniques. Through this innovative methodology, we studied glutathione- and DNA-stabilized Ag NCs with enhanced performance and stability, providing significant advancements in nanomaterial applications.

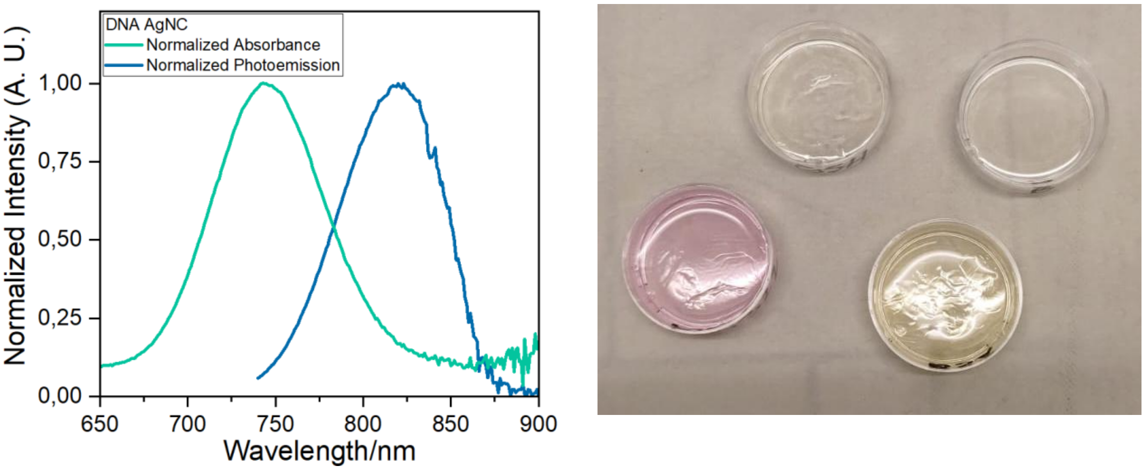

Figure 1: A) Normalized absorption and emission of a DNA stabilized-silver nanocluster; B) Palette of some DNA and peptides-stabilized noble metal nanocluster in gel.

[1] T. Vosch et al. Proc. Natl. Acad. Sci. U. S. A. 104 (2007) 12616.
[2] J. T. Petty et al. J. Am. Chem. Soc. 126 (2004) 5207.
[3] A. Gonzàlez-Rosell et al. Nanoscale Adv. 3 (2021) 1230.
[4] H. Xu et al. Adv. Mater. 22 (2010) 1078.
[5] S. L. Brown et al. J. Phys. Chem. C 121 (2017) 23875.
[6] M. Gambucci et al. Methods Appl. Fluoresc. 8 (2019) 014005.

PC69

MAPPING SELENIUM NANOPARTICLES DISTRIBUTION INSIDE CELLS THROUGH CONFOCAL RAMAN MICROSPECTROSCOPY

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Selenium nanoparticles (SeNPs) exhibit significant potential in biomedical applications due to their antimicrobial, anti-cancer, and anti-inflammatory properties [1]. In this study, we synthesized biocompatible SeNPs and employed Confocal Raman Microspectroscopy to map their distribution within Human Dermal Fibroblast (HDF) cells [2]. SeNPs possess a distinctive Raman band placed outside the cellular fingerprint region which facilitates its detection and precise Raman imaging. Viability assays revealed that SeNPs exhibit cytotoxic effects only at the highest concentrations and for long exposure times, while resulting in no harmful effects during all the other treatments. For the first time, we achieved 3D Raman mapping of SeNPs within cells, providing insights into their cellular penetration (Figure 1). Additionally, 2D Raman mapping performed at different times and at sub-lethal concentrations demonstrated dynamic uptake and confirmed internalization (Figure 1). These findings highlight the effectiveness of SeNPs for biomedical imaging and therapeutic applications, offering an additional approach to study nanoparticle-cell interactions.

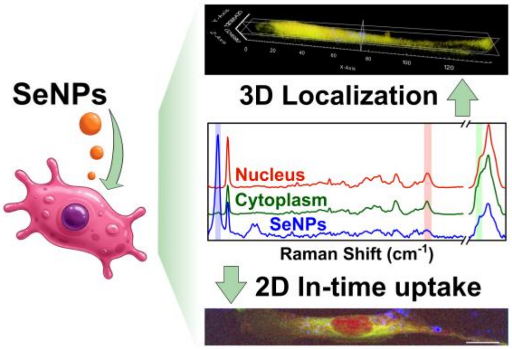

Figure 1. 3D confocal Raman image and 2D map of HDF cell treated with SeNPs

[1] N. Bisht et al. Mater. Adv. 3 (2022) 1415.
[2] D. Redolfi-Bristol et al. ACS Appl. Mater. Interfaces, accepted for publication.

* the presented research has been conducted at the Department of Molecular Sciences and Nanosystems of Ca' Foscari University of Venice (Italy), the Ceramic Physics Laboratory of Kyoto Institute of Technology (Japan) and the Department of Immunology of Kyoto Prefectural University of Medicine (Japan)

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PC70

MAGNESIUM PHOSPHATE CEMENT: A VERSATILE MATERIAL WITH MULTIFUNCTIONAL PROPERTIES FOR DIVERSE APPLICATIONS

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In the past few decades, many scientific efforts were dedicated to the formulation, characterization of the structural and physico-chemical properties and applications of magnesium phosphate cements (MPCs). This class of materials has properties that make it interesting in several diverse applications. They are particularly relevant in two main fields: the construction field (for repair applications, [1] in the containment of nuclear wastes [2] and when refractory properties are needed) and the medical field (as bone repair materials [3]).

MPCs are very different from Portland (the most used and studied type of cement), both chemically and in terms of hydration mechanisms, and for this reason a systematic investigation of their properties, in relation to the specific application, is still lacking.

Our group recently investigated formulations based on magnesium phosphate for bone repairing, trying to assess their structural and physico-chemical features and to put them in relation with the macroscopic properties. The materials were obtained by hydration of tri-magnesium phosphate (TMP) with di-ammonium hydrogen phosphate (DAHP). As a first step, a systematic study on the influence of powder to liquid ratio and DAHP concentration was performed [4], showing how these parameters impact cohesion, crystallinity, morphology, porosity and compressive strength of the final product. Then, in collaboration with the group of Prof. Baldini at IOR (Bologna, Italy) we formulated an MPC loaded with citrate, with the aim of preparing a material for bone regeneration, able to release this molecule directly on site, where citrate can fulfill its fundamental beneficial effects on the newly formed bone tissue. [5] With the same purpose of improving the MPCs' bone regeneration performances, a Sr-containing MPC was prepared and characterized in terms of chemical and structural properties, assessing also the Sr release behavior and the extrudability properties of the material, in view of practical clinical applications, with the addition of some biocompatible polymers. [6] Finally, we explored the possibility of inducing the formation of a macroporosity inside MPC (fundamental for cells permeation and bone ingrowth) by including gelatin microparticles into the matrix: upon dissolution of these microparticles, a final macroporous scaffold was obtained, endowed with a proper interconnected porosity to be percolated by osteogenic cells. [7] As the hydration times of MPC are often very rapid, retarders are usually added to the mixes. We investigated the effect of borax on TMP-based MPCs, with the aim of clarifying the retarding mechanism. [8] Finally, research was conducted on MPCs including Halloysites (natural hollow tubular clays) to improve their properties as a repair material: the Halloysites' lumen can be loaded with active molecules, thus providing for example antifouling properties. [9]

[1] A. Dabarera et al. Front. Mater. 11 (2024) 01.
[2] N. Rakhimova, Sustainability 15 (2023) 689
[3] R. Gelli et al. J. Funct. Biomater. 14 (2023) 424.
[4] R. Gelli et al. Mater. Sci. Eng. C 95 (2019) 248.
[5] R. Gelli et al. ACS Biomater. Sci. Eng. 6 (2020) 5538.
[6] R. Gelli et al. Ceram. Int. 49 (2023) 31466.
[7] R. Gelli et al. J. Mater. Sci. 57 (2022) 12994.
[8] R. Gelli et al. Constr. Build. Mater. 348 (2022) 128686.
[9] M. Tonelli et al. Constr. Build. Mater. 301 (2021) 124056.

PC71

A PHYSICAL CHEMISTRY AND MACHINE LEARNING APPROACH FOR THE IDENTIFICATION OF ROMAN SILVER COINS

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Machine learning techniques are increasingly being employed in the study and classification of ancient coins, offering new possibilities for numismatic research. This study focuses on the application of advanced algorithms to analyze Roman coins, enabling automated identification, authentication, and classification based on archeological data (weight, size, year and so on) and chemical composition.

Here, a preliminary studies on roman coins from the *A. Salinas National Museum of Palermo* is reported. A portable XRF Spectrometer was used to analyze the elements of the alloy, also in traces, in a non invasive way. A preliminary statistic data analysis was used to identify the similarities in the coins and to associate the coins in groups. Then, an algorithm was built to classify the coins based on their elemental composition and archeological features. Machine learning techniques, such as clustering and supervised learning models, were employed to distinguish patterns and correlations within the dataset.

The combination of chemical and archeological data in a machine learning framework not only enhances traditional numismatic studies but also provides a non-invasive, data-driven approach for the authentication and classification of ancient Roman coinage.

Acknowledgements: Project MML-ARCH - "Metodologie di machine learning applicate all'archeometria: una nuova frontiera per l'interpretazione materica dei Beni Culturali", Programma "CHANGES Cultural Heritage Active iNnovation for Sustainable Society" CUP B53C22003890006 - Codice Identificativo PE_00000020, finanziato dall'Unione Europea – Next Generation EU sui fondi PNRR MUR – M4C2 – Investimento 1.3 "Partenariati estesi a Università, centri di ricerca, imprese e finanziamento progetti di ricerca" Avviso pubblico per la presentazione di Proposte di intervento per la creazione di "Partenariati estesi alle università, ai centri di ricerca, alle aziende per il finanziamento di progetti di ricerca di base".

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RECOVERY OF NOBLE METALS FROM E-WASTE BY LASER REDUCED GRAPHENE OXIDE AND APPLICATION IN CATALYTIC CO_2 CONVERSION

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The recovery and re-utilization of high value raw materials, in the framework of a circular economy, is a mainstream topic. A significant portion of discarded materials comes from electronic waste, or e-waste. E-waste contains a significant fraction of noble metals like gold, silver, copper, among many others. Their recovery is thus of significant importance, both environmentally and economically. Gold recovery from e-waste by reduced graphene oxide (RGO) in solution has been recently demonstrated [1]. In this work, we demonstrate that Au^{3+} and Cu^{2}+ ions in solution (mocking a metal recovery environment) can be reduced to Au and Cu nanoparticles (NPs) by RGO surfaces. Such surfaces are then employed as photo-thermocatalytic surfaces for CO_2 conversion into CH_4.
The RGO surface, obtained by GO laser reduction, is exposed to a 10^{-4}M $AuCl_3$ or $CuSO_4$ solution for 1h. The obtained samples are characterized by scanning electron microscopy and X-Ray photoelectron spectroscopy (XPS).
SEM images show that Au or Cu NPs sized a few tens of nanometers form on the RGO surface. XPS confirms that NPs are made of purely metallic Au or Cu NPs (Figure 1a,b). Photothermo catalytic tests show that Au NP offer a significantly improved CO_2 conversion, up to 46% on both GO and RGO surfaces where NPs are not present (Figure 1c). Catalyst performance is stable upon multiple cycles. Similar performance is shown by Cu NP samples, with CO_2 conversion up to 42%.
Our results demonstrate a circular approach in which Au or Cu from e-waste can be recovered and re-used as catalyst for further processes of significant environmental impact like CO_2 conversion.

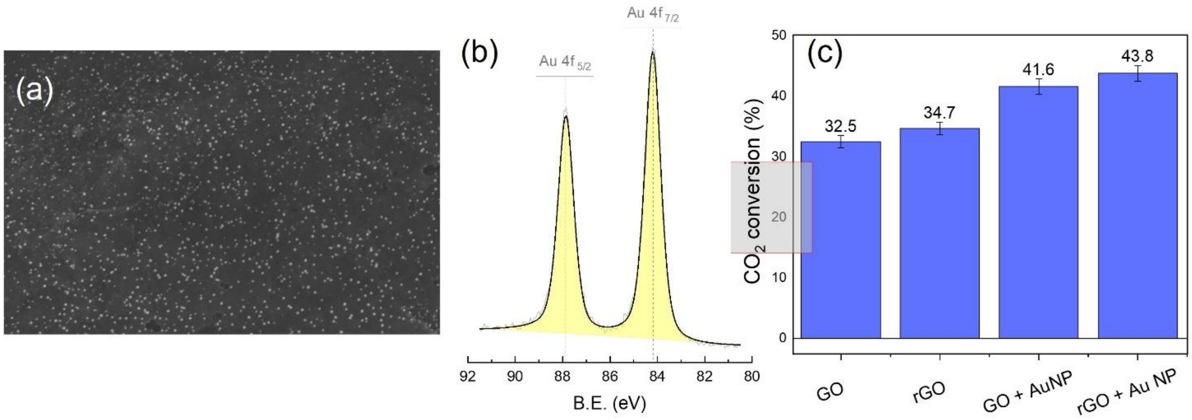

Figure 1. Characterization of Au@RGO surfaces by (a) SEM, (b) XPS. (c) CO_2 conversion yield from Au@RGO surfaces.

[1] F. Li et al. Nat. Comm. 13 (2022) 4472.

PC73

NANO-MAGNETIC FRAMEWORK: DESIGN OF MAGNETIC PROPERTIES

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The development of hybrid organic-inorganic approaches and the understanding of chemico-physical mechanisms governing the hierarchical assembly of nanocrystals into superstructures are pivotal for designing multifunctional materials [1]. This study focus on the design of magnetic properties of mesoporous spherical aggregates composed of ~7 nm spinel ferrite nanocrystals ($MeFe_2O_4$; Me: Co^{2+}; Zn^{2+}), which self-assemble into ∼50–60 nm mesoporous magnetic frameworks (MMFs) with high surface areas (~120 m^2/g). Morpho-structural characterization via X-ray diffraction (XRD), transmission electron microscopy (TEM), and N_2-physisorption confirmed the formation of well-ordered, crystalline nanocrystals organized into spherical mesoporous superstructure. Magnetic characterization of CoFe2O4 MMF reveals superparamagnetic behavior at 300K and Saturation magnetization (M_s) of 80 emu/g . Remarkably, chemical substitution of Co^{2+} with Zn^{2+} and modulation of cobalt content enhanced M_s and a decrease in the magnetic anisotropy, all while preserving the mesoporous structure. The synthetized MMFs, combining high surface area, tailored porosity, and adjustable magnetism, can show promise for applications in targeted drug delivery, magnetic separation, and sensing technologies.

[1] C. Cannas et al. Chem. Mater. 20 (2008) 6364.

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PC74

QM/MM SIMULATIONS OF GROUND AND EXCITED STATE SPECTROSCOPIC PROPERTIES OF MOLECULAR SYSTEMS IN AQUEOUS SOLUTION

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The spectral properties of isolated molecules can differ significantly from those of the same molecules dissolved in aqueous solution [1]. Multiscale Quantum Mechanics (QM)/Classical models are highly effective in simulating solvated molecules by dividing the system into two components: the solute, treated at the QM level, and the solvent, modeled classically [2-4]. Among these approaches, QM/Molecular Mechanics (MM) methods have expanded considerably in recent decades and are now widely used to study the spectroscopic properties of solvated systems [1-3]. The success of this methodology lies in its ability to retain atomistic details of the solvent while accurately describing hydrogen bonding [1-3].

In this work, we investigate various ground state and excited state spectroscopic properties of molecular systems in aqueous solution using fully polarizable QM/MM approaches [5], where the MM region is described using the Fluctuating Charges (FQ) and Fluctuating Charges and Dipoles (FQFμ) force fields [6-7].

The resulting QM/FQ and QM/FQFμ approaches are integrated with classical molecular dynamics simulations for an accurate sampling of both the ground and the excited state solute-solvent phase-space [1,8].

Computed results [9] are validated through a direct comparison with experimental data, demonstrating the robustness of our methodology.

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SULFUR SPECIES ON COSMIC ICE: INSIGHTS FROM BINDING ENERGIES AND DIFFUSION BARRIERS DISTRIBUTIONS

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Binding energies (BEs) are key parameters for understanding the evolution of molecular species in dense clouds, determining whether a species remains frozen on grain surfaces or in the gas phase. Typically, BEs are provided as single point values, but the amorphous nature of icy grains leads to a distribution of BE sites and values. The same holds for diffusion barriers (ΔE), which are often approximated as a fraction of BE ($\Delta E = f * BE$) [1]. However, these assumptions can significantly impact reaction rates due to their exponential dependence on ΔE.

While several grain models have been developed, they often lack a comprehensive and systematic physical description. Recently, ACO-FROST, an automated procedure for simulating realistic icy grains, was introduced [2], enabling the modeling of amorphous ice structures with up to 1,000 atoms and capturing a broad range of BE sites.

In this contribution, ACO-FROST was used to compute BE distributions for key sulfur-bearing species, including H_2S, OCS, and CH_3SH, addressing the long-standing sulfur depletion problem. BEs were computed at the DFT level (B97-3c) and refined using DLPNO-CCSD(T) [3]. Our results show that previous BE values [4] were overestimated compared to our new distribution. Additionally, the vibrational frequency distribution for OCS associated to each adsorbed site was compared with James Webb Space Telescope (JWST) observations, and the remarkable agreement confirms the robustness of our model [5]. By leveraging multiple energy minima on the surface, we computed the distribution of diffusion barriers for various pathways, in agreement with experimental data [6]. Kinetic Monte Carlo (KMC) simulations was also carried out to calculate the diffusion coefficient for H_2S, revealing low diffusivity and highlighting how diffusion affects the simulated TPD spectra. Our results demonstrate that pre-desorption temperature does not affect the position of the desorption peak. In the end, considering the coverage regime usually applied in the laboratory setup, the effect of the lateral interaction is considered to explain the discrepancy between computational and experimental BEs.

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PC76

SYNTHESIS AND CHARACTERIZATION OF CLAY MINERALS-PERPHENAZINE COMPOSITES

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Perphenazine (PPZ) is a BCS class II drug used to treat psychoses, including anxiety and schizophrenia. BCS class II drugs are characterized by low and pH-dependent solubility in gastrointestinal fluids, affecting their bioavailability [1,2].

Clay minerals are widely applied in the biomedical field thanks to their biocompatibility, suitable properties, as high surface area and porosity, non-toxicity, and cheapness.

In this work, we selected laponite, saponite (both natural and synthetic), and halloysite nanotubes as carriers for PPZ to enhance its dissolution rate.

Synthetic saponite was obtained via a sol-gel route [3]; hybrids were synthesized using a solution method [4].

FT-IR and XRPD characterizations were carried out to qualitatively assess the drug loading. In the case of layered clays (laponite and natural saponite), by analyzing the shift of the (001) reflection and the increase in the interlayer distance, the arrangement of perphenazine molecules between the layers can be assessed: in natural saponite, they align parallel to the layers, whereas in laponite, they adopt a perpendicular orientation.

Quantification of PPZ in the composites was carried out through UV-Visible spectroscopic analysis and thermogravimetric measurements. TG measurements were combined with DSC analysis to assess the crystallinity percentage by comparing the enthalpies of fusion peaks. In synthetic saponite and halloysite nanotubes, the loaded perphenazine is present in both crystalline and amorphous forms, as further indicated by ^{13}C CPMAS spectra. FT-IR results put into evidence weak interactions between the perphenazine molecules and the clay minerals supports.

All the analyzed hybrid systems demonstrate improved dissolution rates and enhanced wettability at neutral pH compared to perphenazine, although complete dissolution of the drug is not achieved within a short period. The most promising formulation utilized natural saponite as a carrier, for which a tablet containing 8 mg of the drug and appropriate excipients was developed. This formulation enabled full drug release within one hour. A key advantage is that the drug's dissolution remains unaffected by the pH variability in the gastrointestinal tract, thereby enhancing its bioavailability.

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PC77 DESIGN OF TITANIUM-BASED METAL-ORGANIC FRAMEWORKS FOR ENVIRONMENTAL INTEREST APPLICATIONS

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Metal-organic frameworks (MOFs) are porous materials consisting of metal nodes and organic linkers that organize themselves into rigid crystal structures. The properties of both metal ions and linkers determine the physical, structural, and morphological features of MOF. The aim of this study was the synthesis of titanium-based metal-organic frameworks (Ti-MOF) based on poly-oxo titanium cluster (PTC) functionalized with a multidentate organic ligand. Ti-MOFs represent one of the most promising subclasses of MOFs owing to their promising optoelectronic and photocatalytic properties. These features make them suitable for a wide range of interesting applications ranging from energy to environmental protection, such as the fields of photocatalytic redox reactions like water splitting or organic pollutant degradation. Unfortunately, the synthesis of Ti-MOF has to face several problems mainly due to the high reactivity of commonly used titanium sources, such as titanium alkoxides or inorganic salts (e.g. $TiCl_4$), which generally causes fast and uncontrollable nucleation and irregular framework growth leading to the formation of amorphous coordination polymers [1]. In this work Ti-MOFs were prepared through a building block approach, which involved the preliminary synthesis of the zero-dimensional cluster $[Ti_6O_4(OiPr)_{10}(O_3P\text{-}Phen)_2]^{2+}$(OiPr = isopropyl group, O_3P-Phen = phenylphosphonic acid), functionalized with isonicotinic acid. This structure, known in the literature with the code PTC-3 [2], was successively subjected to a ligand exchange reaction, during which isonicotinic acid was replaced with a polycarboxylic ligand in order to extend the dimensionality of the structure (Figure 1). Several variables involving the synthesis process, such as solvent, cluster to ligand ratio, temperature, time, and amount of a crystallinity modulator were investigated through a multivariate approach in order to identify the conditions which best promote the crystals growth's process. All the synthesized compounds were characterized by means of powder X-Ray diffraction (PXRD), Fourier-transformed IR spectroscopy (FTIR), Brunauer-Emmett-Teller method (BET), and UV-Vis diffuse reflectance spectroscopy (DRS).

The most promising T-MOF were tested towards the adsorption and the catalytic or photocatalytic degradation of methylene blue (MB) in aqueous solutions. As future developments, we aim to verify the potential applicability of T-MOF for the removal particularly hazardous contaminants of emerging concern (CECs).

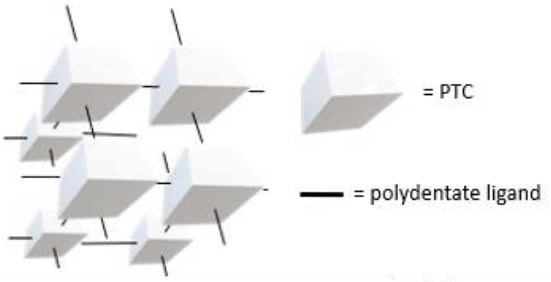

Figure 1. Schematic representation of Ti-MOF structure

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EXPLORING THE EFFECTS OF DEEP EUTECTIC SOLVENTS ON BACTERIAL PHOTOSYNTHESIS

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Deep eutectic solvents (DESs) are innovative two-component sustainable solvents characterized by melting points much lower than those of individual components [1]. The formation of an eutectic solution descends from the strong interaction between the components, leading to a less ordered structure that maintains them liquid at room temperature and sustains chemical stability of molecules that are solved into. DESs are formed by a mixing of hydrogen bond acceptor and hydrogen bond donor or Lewis acids and bases. Most DESs are not toxic, generally low-cost, and their preparation is easy and straightforward.

DESs have been shown to maintain the catalytic activity of the membrane photosynthetic enzyme – known as reaction center (RC) – obtained from the purple non sulphur bacterium *Rhodobacter (R.) sphaeroides*. Nine different DESs were tested and all but one showed full compatibility with the membrane protein [2].

In this study, we extended our investigation to evaluate the compatibility of DESs toward photosynthetic membrane vesicles containing whole photosynthetic apparatus, RC and light-harvesting complexes, called chromatophores that are isolated from the mutant strain R26 of *R. sphaeroides*. Three different DESs were studied, namely TBAB:Gly (1:3), ChCl:EG (1:3) and ChCl:U (1:2) and their effect on the integrity of vesicles was analysed by UV-Vis-NIR spectroscopy.

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PC79

OPTICAL COMMUNICATION BETWEEN NEURONAL SURROGATES

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Artificial intelligence (AI) profoundly influences our modern society by driving advancements in economics, medicine, security, and both basic and applied sciences. One promising approach to AI development is neuromorphic engineering [1]. This innovative field seeks to replicate the characteristics of human intelligence by designing artificial neurons (ANs) and their networks in both software and hardware. Our research contributes to the progress of neuromorphic engineering by using solutions of specific nonlinear chemical systems implemented in wetware. These systems are capable of simulating the dynamics of biological neurons [2-4].

By leveraging chemical processes maintained under non-equilibrium conditions, we demonstrate how certain brain-like functionalities can be reproduced. In particular, our study explores the use of ultraviolet and visible radiation as a signal to establish optical communication between the Belousov-Zhabotinsky (BZ) reaction and either photochromic or luminescent materials. This study demonstrates that UV-visible radiation can be exploited as a signal for communication among neuronal surrogates in oscillatory, chaotic, and photo-excitable regimes. The achieved optical communication is reflected as a synchronization phenomenon either in-phase or out-of-phase or phase-locking, between the transmitting element and the receiving compound. These phenomena closely resemble the mechanisms by which neurotransmitters enable chemical communication within biological neuronal networks [5].

Inspired by natural brain processes, such as the transport of molecules and signals via interstitial and cerebrospinal fluids, this method reflects the dynamic and adaptable nature of the brain's operations. This innovative approach emulates the brain's liquid state and uses diffusion and convection as mechanisms for transmitting messages. By harnessing UV/visible radiation to encode information, it ensures rapid propagation of messages and offers easy intensity modulation, enhancing communication efficiency.

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