Università degli Studi di Bari Aldo Moro

Politecnico di Bari

IPCF

Società Chimica Italiana
Divisione di Chimica Fisica

51st Congress of the Physical Chemistry Division Società Chimica Italiana

Book of abstract

Bari, 7 – 10 July 2026

Politecnico di Bari, Campus Universitario

Società Chimica Italiana
Divisione di Chimica Fisica

51 CDCF BARI 2026

51st Congress of the Physical Chemistry Division
Società Chimica Italiana
Bari, 7–10 July 2026

Exploring Fundamentals, Driving Innovation,

Advancing Sustainable Future

Book of Abstracts

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Foreword

It is a great pleasure to welcome you to the 51st Congress of the Physical Chemistry Division of the Società Chimica Italiana, CDCF51, held in Bari, Italy.

This Congress continues the long-standing tradition of the Division as a forum for scientific exchange, discussion, and collaboration within the physical chemistry community. Under the theme "Exploring Fundamentals, Driving Innovation, Advancing a Sustainable Future", CDCF51 aims to highlight the central role of physical chemistry in connecting fundamental understanding with technological progress and societal impact.

The contributions collected in this Book of Abstracts reflect the breadth and vitality of our discipline. They cover a wide range of topics, spanning spectroscopy, kinetics, thermodynamics, electrochemistry, catalysis, surface science, materials and nanoscience, polymers, quantum chemistry, biophysical chemistry, machine learning, and data-driven approaches. Together, they demonstrate how theoretical, computational, and experimental physical chemistry contribute to addressing key challenges in renewable energy, climate action, sustainable and circular materials, clean water, environmental protection, and health.

CDCF51 brings together researchers from universities and research institutions and gives particular attention to the participation of young scientists. Through plenary and invited lectures, oral communications, and poster sessions, the Congress offers an opportunity to share recent results, discuss new ideas, and strengthen collaborations across different areas of physical chemistry.

On behalf of the Organizing Committee, I would like to thank all participants, speakers, contributors, sponsors, and supporting institutions for making CDCF51 possible. I also wish to acknowledge the members of the Scientific and Organizing Committees for their valuable work and commitment.

We hope that this Book of Abstracts will serve not only as a guide to the scientific program of the Congress, but also as a record of the ideas, achievements, and perspectives shared by our community in Bari.

Alongside the scientific program, CDCF51 will create moments for participants to connect, exchange ideas, and build new relationships, while discovering the unique charm, history, and Mediterranean character of Bari.

M. Lucia Curri — *Conference Chair*

Mariano Venanzi — *President of the Physical Chemistry Division*-SCI

Welcome to the 51st Congress of the Physical Chemistry Division (PCD) of the *Società Chimica Italiana* (CDCF51). The Physical Chemistry Division is committed to promoting physical chemistry as a comprehensive and interdisciplinary scientific discipline, fostering the advancement of both fundamental research and chemical education. To pursue this mission, the Division organizes conferences, schools, and, starting this year, the new Physical Chemistry Symposia, conceived as less formal forums for in-depth discussion on focused and timely scientific topics.

The 51st Congress, hosted in Bari, continues the Division's tradition of recognizing excellence within the physical chemistry community. Alongside the Bonino Prize, honoring researchers who have made outstanding and long-lasting contributions to the discipline, the Conference will present the Semerano Prize for the best PhD thesis, the Distinguished Scientist and Young Scientist Prizes for the best conference lectures, and the Senatore Prize for the best poster presentation. We are also delighted to introduce, for the first time, the Califano Prize, established to recognize young researchers who have already demonstrated an original and well-established scientific profile.

We thank all the participants for their scientific contributions and active engagement, which make this Conference a valuable opportunity for exchanging ideas, fostering collaborations, and strengthening our physical chemistry community. We are also grateful to the Organizing Committee for their commitment and efforts in making this event possible.

We wish you a stimulating and enjoyable CDCF51.

The Board of the Physical Chemistry Division

Società Chimica Italiana

09:15–10:00 Registration

10:00–10:30 Coffee break

10:30–11:00
Aula Magna "A. Alto"
Opening: Prof. M. Venanzi *(President DCF SCI)*, Prof. U. Fratino *(Rector, Polytechnic University of Bari)*, Prof. R. Bellotti *(Rector, University of Bari)*, Prof. L. Armelao *(Director, DSCTM-CNR)*, Prof. G. Palazzo *(Director, Chemistry Department University of Bari)*, Dr. O. Maragò *(Director, CNR IPCF)*, Dr. R. Comparelli *(Head of Bari Unit, CNR IPCF)*, Prof. A. Agostiano *(President, EuChemS)*.

11:15–11:45
Aula Magna "A. Alto"
Plenary lecture
I. Pastoriza-Santos, *Colloidal Plasmonic Nanomaterials as Platforms for (Bio)Sensing* – Chair: A. Agostiano

12:00–13:00

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A O1 D. Ranieri Enhancing the Optical Response of Gold and Silver Nanoclusters via Rigid Embedding in High-Refractive Index Polyacrylamide Matrix	**D O1 R. Oliva** Modulating Disease-Related Biocondensates with Small Bioactive Peptides	**F O1 S. Garroni** Low-Temperature Formation of BCZT Piezoceramics: Kinetic Pathways and Structure–Property Relationships
A O2 A. Mercedi Spectral Reshaping of Porphyrin Excitation by Plasmonic Nanostructures	**D O2 D. Roversi** Membrane Interactions of Antimicrobial Peptides: a Kinetic Perspective	**F O2 S. Slimani** Spin Disorder in Hollow Nanoarchitectures: Beyond Geometric Surface Effects
A O3 G. Cappelletti Turning Waste into Value: Sustainable Bio-Emulsifiers from Agro-Food By-Products	**D O3 M. Roggio** Aerosol-Assisted Atmospheric Pressure Plasma Jet Deposition of Antimicrobic Zinc-Based Nanocomposite Thin Film	**F O3 G. Ragusano** Enhanced Physico-Chemical Characterization of Complex Hybrid Nanocomposites: an O_2-GCIB TOF-SIMS Depth Profiling Approach
A O4 A. Grandolfo Chemical Affinity-Driven SERS Response of Histidine-Functionalized RGO/Ag Nanowire Nanocomposites on Hydrophobic Paper		**F O4 V. Spampinato** Physico-Chemical Insights into the Stepwise Assembly of Copper-Based Metal-Organic Frameworks Thin Films on Functionalized Silicon Oxide

13:00–14:40 Lunch

14:40–15:25
Room A
Plenary lecture
C. Giannini, *Deciphering the Hierarchical Structure of Natural and Engineered Materials - A Multiscale X-ray Scattering-Based Approach* – Chair: L. Marchese

15:25–15:35
ROOM A
Sponsor presentation - G. Gariano, ALFATEST

15:35 - 16:05

Room A	Room B	Room E
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A O5 F. L. Damiani Crystal Structure Refinement of New Organocatalyst: Benchmarking Between Independent Atom Model (IAM) Refinement and Hirshfeld Atom Refinement (HAR)	**C O1 V. La Gambina** Exact Stoichiometry Far-Off Neutrality Catanionic Nanotubes: Unconventional Self-Assembly of Oppositely Charged Surfactants	**F O5 D. Peddis** From Cultural Heritage to Fundamental Magnetism: Insights from Nanostructured Hematite
A O6 L. Evangelisti Decoding Molecular Structure with Rotational Spectroscopy	**C O2 G. Li Destri** Macro- and Nanoscale Electrostatics Govern the Static and Dynamic Behavior of Charged Aqueous Interfaces	**F O6 M. L. Saladino** The NanoLuBC Project: a Join Chairs on Innovative Nanostructured Materials with Luminescent Properties for Cultural Heritage

16:05–16:45 Coffee break

16:45–17:30

Room A	Room B	Room E
Fundamental Physical Chemistry: Structure, Dynamics, and Spectroscopy | Chair: A. Panniello	**Soft Matter, Interfaces, and Complex Systems |** Chair: G. D'Errico	**Electrochemistry, Catalysis, and Energy Conversion |** Chair: E. Fanizza
A O7 G. Sambucari Integrating Twisted and Push-Pull Structural Motifs for Efficient Dual-Functioning Near-Infrared Bodipy Photosensitizers	**C O3 S. Napoletano** Soluplus® Micelles Characterization and Application in Drug Delivery	**E O1 R. Del Sole** Combined Atomic Layer Deposition and Sputtering of ZnO/Cu Coatings for CO_2 Electroreduction
A O8 P. Sassi Spatially Resolved Biochemical Signatures of Cardiorenal Syndrome Revealed by FTIR Imaging	**C O4 R. E. Camerini** Bio-Based Polyglycerol Esters for LLPS-Driven Soft Microencapsulation	**E O2 N. Iuliano** Spectroelectrochemical Insights into Heterogeneous Catalysts for the CO_2Reduction Reaction
A O9 S. Massardo SpeComp: a User-Friendly Tool for Spectral Comparison to Facilitate Microplastics Detection in Complex Biological Matrices	**G O1 P. Lasala** Cellulose-Based Nanocomposites Embedding Metal Oxides Nanoparticles for Dye Removal from Wastewater by Synergistic Adsorption and Photocatalytic Processes	**E O3 F. Panagini** Structural Insights on FeZnCuK Catalysts for Mild Photothermal CO_2-to-Hydrocarbons

17:30–18:00
Room A
Invited lecture
P. P. Abis (Acquedotto Pugliese S.p.A.), *Ensuring Drinking Water Quality in Acquedotto Pugliese through the Digitalization of the Water Safety Plan* - Chair: L. Curri

18:00–18:15
Room A
L. Marchese, RisPA CENTER: *The Research and Development Center for Environmental Remediation and Protection*

18:30–20:30 Welcome event at Caffè Vergnano Via Amendola

09:15–10:00 **Plenary lecture**
Room A **G. M. Pavan,** *The Information Contained in Self-Assembling Systems* – Chair: M. Pavone

10:00–11:15

Room A	Room B	Room E
Theory, Modelling, and Data-Driven Physical Chemistry | Chair: M. Pavone	**Physical Chemistry for Health and Life Sciences |** Chair: C. Giancola	**Electrochemistry, Catalysis, and Energy Conversion |** Chair: M. Trotta
B O1 F. Avanzini Coarse Graining Photo-Isomerization Reactions: Thermodynamic Consistency and Implications for Molecular Ratchets	**D O4 P. Maltoni** Magnetic Response of Giant Unilamellar Vesicles Embedding Functionalized Magnetite Nanoparticles	**E O4 M. Grattieri** Tuning Bacteria-Electrode Interfaces for Biohybrid Electrochemical Systems
B O2 G. Bocchinfuso Multiscale Molecular Dynamics for Probing Second-Timescale Protein Conformational Changes: the SHP2 Activation Case	**D O5 G. Quaglia** Photothermal Effect of Gold Nanostructures on Amyloid Aggregates: Role of Shape and Size in the Optical Response	**E O5 M. Viviani** Stability and Electrochemical Properties in Multi-Doped Sr Ferrates
B O3 N. Tuccitto When Molecules Communicate: Entropy Production as the Thermodynamic Cost of Molecular Information Transfer	**D O6 F. Cardoni** Plasmonic Au NP-Derived Thin Films for Monitoring Cardiac Cells and Their Biomarkers	**E O6 A. Astengo** The Gilded Cage: Towards High Thermoelectric Efficiency in Single-Filled Skutterudites
B O4 S. Pezzola The Perfect Couple: a Critical Analysis of CAM-B3LYP/SMD for Alcohol pKa Prediction	**D O7 G. Mandriota** Functionalized Petal-Like ZnO as a Promising Nanoplatform for Gene Delivery	**E O7 V. Ferrara** Interference and Plasmonic Effects in Dielectric/Metal/Dielectric Multilayers for Semi-Transparent Perovskite Solar Cells
B O5 D. Tatini Machine Learning and Data Fusion Strategies for the Investigation of Hofmeister Effects in Polysaccharide Systems Combining IR Spectroscopy and Thermal Analysis	**D O8 V. De Leo** Liposomal Co-Encapsulation of Curcumin and Quercetin Enhances the Protective Effect on Endothelial Cells from TNF-α-Induced Inflammation, Oxidative Stress, and Apoptotic Damage	**E O8 C. Zonno** Controlling Energy Flow in *Rhodobacter Sphaeroides* Chromatophores via Selective Electron Transfer Inhibition

11:15–12:00 **Coffee break**

12:00–12:30 **Keynote lecture**
Room A **P. L. Gentili,** *The Contribution of Photochromic Materials in the Development of Chemical AI* – Chair: F. Mavelli

12:30–13:30

Room A	Room B	Room E
Fundamental Physical Chemistry: Structure, Dynamics, and Spectroscopy | Chair: F. Mavelli	**Soft Matter, Interfaces, and Complex Systems |** Chair: F. Ridi	**Environmental Physical Chemistry |** Chair: L. Catucci
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A O10 A. Scarperi Multinuclear Solid-State NMR Investigation of Adsorption-Induced Structural Changes and CO_2 Dynamics in CALF-20	**C O6 G. Palazzo** The Empirical HLD-NAC Model of Microemulsion Can Be Rationalized on the Basis of Random Field Description of Oil/Water Domains	**G O3 M. Baratta** Synthesis and Preparation of Cyclodextrin Modified Carbon Nanotube Buckypapers for the Efficient Removal of Carbofuran from Water
A O11 A. Ghelardi Molecular Motions of Active Pharmaceutical Ingredients Investigated by Solid-State NMR Spectroscopy	**C O7 A. Del Giudice** Complex Coacervation Between Sodium Decanoate and Cationic Inulin: Structural and Deposition Studies of Bio-Based Polymer and Surfactant Mixtures	**G O4 S. Nanan** Magnetic Fe_3O_4/BiOBr for Sunlight Degradation of Tetracycline Antibiotic
A O12 S. Melandri The Halogen Advantage: the Role of Halogen Atoms in Architecting Novel Non-Covalent Interactions	**C O8 M. Tancredi** Microfluidic Production of Rhamnolipid Coacervates: Linking Droplet Formation to Internal Organization	**G O5 F. Secci** Probing Aluminum Speciation and Surface Acidity in Mesostructured Aluminosilicates: Structure–Acidity Insights for CO_2-to-DME Conversion

13:30–15:15 **Lunch**

15:15–16:00 **Plenary lecture**
Room A **R. Marcilla,** *Unlocking the Potential of Organic Materials for Energy Storage: The Fascinating Journey Toward Sustainable Batteries* – Chair: M. Striccoli

16:00–16:30 **Keynote lecture**
Room A **A.B. Muñoz-García,** *Addressing Complexity in Energy Materials and Interfaces: Predictive Modelling Strategies Beyond DFT* – Chair: M. Striccoli

16:45–17:30

Room A	Room B	Room C
Theory, Modelling, and Data-Driven Physical Chemistry | Chair: M. Cossi	**Physical Chemistry for Health and Life Sciences |** Chair: L. Latterini	**Electrochemistry, Catalysis, and Energy Conversion |** Chair: M. Striccoli
B O7 M. A. Zambrano Angulo Atomistic Insights into Hole Injection at Multi-Cation Perovskite/HTL Interfaces	**D O9 I. Miletto** Advanced Yb^{3+}/Er^{3+}-TiO_2 Architectures: Mastering Upconversion for NIR-to-Visible Light Harvesting	**E O9 F. Murgia** Boosted Ionic Conductivity in $Na_2B_{12}H_{12}/SiO_2$ Nanocomposite Electrolyte for Solid-State Sodium Batteries
B O8 A. Landi From Electronic Structure to Nonradiative Pathways in INVEST Emitters: a Combined Electronic-Structure and Quantum-Dynamics Perspective	**D O10 L. Fabiano** Tuning Physicochemical Properties of PEDOT:PSS/HNTs Nano Composites for Smart Bioactive Interfaces	**E O10 U. Mattia** Enhanced Biophotocurrent Generation via Tailored Nano-Biointerfaces in *Rhodobacter Capsulatus* Biohybrids
	D O11 V. Piscopo Development of Dielectric/Metal/Dielectric (DMD) Architectures for Optical Biosensing Applications	**E O11 S. Brutti** The SIGNE Project: Composite Silicon Nanowire on Graphite Anodes with Ni-Rich Cathodes and Safe Ether Based Electrolytes for High-Capacity Li-Ion Batteries

17:30–19:00 **Poster session and refreshment**

19:30–on **Social event: Guided tour following the "Di Arco in Arco" itinerary in Bari's Old Town**

09:15–10:00 **Room A**

Plenary lecture
R. Mezzenga, *Amyloid-Metal Supramolecular Hybrids for Health and Environmental Remediation Technologies* – Chair: E. Selli

10:00–10:30 **Room A**

Keynote lecture
E. Gianotti, *Confined Spaces, Boundless Opportunities: Controlling Confinement in Porous Materials from Catalysis to Nanomedicine* – Chair: E. Selli

10:30–11:15

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Theory, Modelling, and Data-Driven Physical Chemistry | Chair: A. Massaro	**Physical Chemistry for Health and Life Sciences** | Chair: L. Petraccone	**Environmental Physical Chemistry** | Chair: E. Selli
B O10 M. Corno Atomistic Modelling of Hydroxyapatite Surfaces: from Biomolecular Adsorption to Environmental Catalysis	**D O12 P. Albanese** Photomodulation of Vesicle Dynamics Using Fluorescent Photoswitchable Amphiphiles	**G O6 G. Ancora** A Sequential Probe Adsorption Approach for the Characterization of Acid Sites in Hierarchical Zeolites
B O11 V. Palumbo A New Method to Characterize the Porosity of Materials: Distribution of Nanoporous Volume, Specific Surfaces and Prediction of Gas Adsorption	**D O13 N. Depalo** pH-Responsive Dendritic Large-Pore Mesoporous Silica Nanoplatforms for 5-Fluorouracil Delivery in Colorectal Cancer	**G O7 G. Mulas** Valuable Waste for CO_2 Conversion and H_2 Evolution Induced by Mechanical Energy
B O12 S. C. Sarnataro Computational Exploration of Derivatized Cyclodextrin-Based Drug Delivery Systems	**D O14 A. Auditore** Decoding Molecular Information via Mass Transport–Electron Transfer Coupling	**G O8 V. Ancona** Use of Vis-NIR Spectroscopy for Environmental Monitoring: Potential and Applications

11:15–12:00 Coffee break

12:00–12:45 **Room A**

Plenary lecture
D. Berti, *Engineering Nano-Bio Interfaces: from Self-Assembly to Functional Hybrid Nanosystems*
Chair: G. Palazzo

12:45–13:15

Room A	Room B	Room E
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A O14 R. Lettieri Structure-Property Relationships in Cellulose Acetate Composites Containing Microalgal Residues	**C O10 P. Tordi** Ion-Programmed Biopolymer Organohydrogels for Multiresponsive Soft Electronics	**F O8 G. Rando** Next-Generation Sustainable Membranes: Nanostructured Platforms for Environmental and Energy Challenges

13:15–14:45 Lunch

14:45–15:15 **Room A**

Kenote lecture
C. Milanese, *The C Treasure in Biomasses for Energy and Analytical Applications*
Chair: G.P. Suranna

15:15–16:00

Room A	Room B	Room E
Fundamental Physical Chemistry: Structure, Dynamics, and Spectroscopy | Chair: G.P. Suranna	**Soft Matter, Interfaces, and Complex Systems** | Chair: N. Depalo	**Electrochemistry, Catalysis, and Energy Conversion** | Chair: D. Peddis
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A O16 M. C. Di Gregorio Engineering Metal-Organic Frameworks for Highly Nonlinear Photonics	**C O12 M. Trotta** Repurposing Bacterial Photosynthesis	**E O13 D. Conelli** Photoinduced Surface-Driven Bromination of Electron-Rich Arenes on Lead-Free $Cs_2AgBiBr_6$ Microcrystals under Sustainable Conditions
A O17 T. Gentili Infrared-Activated Dynamic Crystals: Remote Motion in a Metal-Organic Framework	**B O9 R. Sarkar** First-Principles-Based Insights into Adsorption and Reactivity of Na^+ Salt and Room-Temperature Ionic Liquids at Sodium Metal Surface	**E O14 G. Manca** Ultrafast Piezo-Assisted Engineering of Metal-ZnO Interfaces for Catalytic Applications

16:00–16:45 Coffee break

16:45–19:00 **Room A**

Assembly of the Physical Chemistry Division and Medals Ceremony

20:30 – on **Social dinner at Villa Romanazzi Carducci**

09:15–09:45 **Keynote lecture**
Room A
M. R. Plutino, *Innovative Hybrid Materials for a Sustainable Future: Bridging Circular Resources, Nanotechnologies, and Green Transition* – Chair: S. Melandri

09:45–11:00

Room A	Room B	Room E
Fundamental Physical Chemistry: Structure, Dynamics, and Spectroscopy | Chair: S. Melandri	**Soft Matter, Interfaces, and Complex Systems |** Chair: D. Berti	**Materials and Nanoscience for Sustainable Technologies |** Chair: B. Pignataro
A O18 F. Locardi Persistent Luminescence Nanocrystals	**C O13 F. Sarnelli** A Physicochemical Approach to Surfactant-Mediated Deposition of Volatile Compounds from Detergent Formulations onto Fabrics	**F O9 C. Ingrosso** Innovative Hybrid Nanocomposites based on Soot Carbon Nanoparticles Decorated with Au Nanoparticles for Electroanalytical Sensors
A O19 R. Gelli Bisphosphonates and Polyacrylates Control the Size and Assembly of Amorphous Magnesium-Calcium Phosphate Particles	**C O14 C. Adamo** Controlling Fibroin Self-Assembly in Sustainable Consolidants for Fragile Silk Artifacts	**F O10 C. Carandente Coscia** Modulating the Morphology of Lignin Microparticles via Green Solvent-Shifting
A O20 A. Mangolini Structural and Magnetic Properties of Iso-Oriented Assemblies of Co–Zn Ferrite Nanoparticles	**C O15 M. Baglioni** Influence of Surfactants on Industrial Cheese Sauces	**F O11 F. Morari** Activated Carbon Derived from Agro-Industrial Waste for H2 Storage
A O21 V. Scardaci Study and Characterization of the Gold Nanoparticle's Formation Mechanism by Re-Irradiation of Linear Bromide Induced Gold Nanoparticle Chains	**C O16 G. Ballabio** Interfacial and Emulsifying Properties of Potato Protein Hydrolysates Obtained by Enzymatic Processing	**F O12 M. Tonelli** 3D-Printable Bioreceptive M–S–H Cements Containing Large Quantities of Marble Dust Waste
A O22 C. N. Dibenedetto Assembling Colloidal Emissive Nanocrystals into 3D Super-Architectures	**C O17 J. Costa** Physicochemical Characterization of High-Performance Chitosan Based Adhesives: a Sustainable Approach to Enhance Interfacial Adhesion	**F O13 L. Viacava** Flexible Synthesis of Copper, Iodine – Based Coordination Polymers with Modulable Luminescent Emission

11:00–12:00 **Coffee break**

12:00–13:00 **Conference awards ceremony**
Room A

13:00–13:30 **Closing remarks**
Room A

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Poster Contributions

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Poster Contributions

Plenary Lectures

-PL 1-

Colloidal Plasmonic Nanomaterials as Platforms for (Bio)Sensing

Isabel Pastoriza-Santos

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The physical chemistry of plasmonic nanomaterials provides a powerful foundation for connecting nanoscale structure–property relationships with innovative sensing technologies addressing pressing societal challenges. In this talk, I will first discuss the colloidal synthesis of plasmonic metal nanoparticles, highlighting how controlled nucleation, growth kinetics, and surface chemistry enable precise tailoring of size, morphology, and optical response. Particular emphasis will be placed on chiral growth strategies that introduce symmetry breaking at the nanoscale, leading to plasmonic nanostructures with well-defined optical activity [1].

Building on these fundamental concepts, I will show how both achiral and chiral plasmonic nanoparticles can be engineered as efficient platforms for (bio)sensing and imaging based on surface-enhanced Raman scattering (SERS) [2-6]. Recent advances will be presented in pushing the limits of lateral-flow immunoassays through SERS readout, enabling ultralow detection of targets such as SARS-CoV-2 virus and allergens. Morever, additional examples will include the use of plasmonic-based nanoprobes for multiplex immunophenotyping, as well as the design of chiral nanoparticles for the enantioselective SERS detection of biologically relevant molecules.

[1] B. Ni et al. Adv. Mater. 2023, 35, 2208299.
[2] A. Serrano et al. ACS Nanosci. Au 2026 , 6, 313.
[3] L. González-Cabaleiro et al. Nano Lett. 2025, 25, 17911.
[4] T. Serra et al. Sens. Actuators B Chem. 2025, 428, 137249.
[5] C Fernández-Lodeiro et al. ACS Appl. Nano Mater. 2023, 7, 498.
[6] L. González-Cabaleiro, et al. Small Sci. 2024, 4, 2400259.

-PL 2-

Deciphering the Hierarchical Structure of Natural and Engineered Materials – a Multiscale X-Ray Scattering-Based Approach

Cinzia Giannini

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The organization of hierarchically ordered materials, from the nanometric scale of molecular building blocks to the assembly of functional structures, dictates their extraordinary properties. Deciphering this complexity requires advanced experimental and analytical tools capable of bridging multiple length scales. This lecture will review a comprehensive multiscale approach based on X-ray scattering techniques (SAXS/WAXS) to uncover the structural features of diverse hierarchical systems.
Drawing from extensive research on natural and engineered fibers—such collagen, silk, cellulose, and peptide base fibers—we demonstrate how X-ray scattering provides unique insights into their sub-molecular and supra-molecular structures. Furthermore, the discussion extends to the burgeoning field of colloidal nanotechnology, focusing on the self-assembly of nanocrystals into highly ordered superlattices and analyzing their translational and orientational order within these assemblies.
The integration of state-of-the-art laboratory instrumentation with synchrotron radiation and advanced data modeling allows for a precise description of these materials' morphology, crystallinity, and hierarchical connectivity. This multiscale perspective not only enhances our fundamental understanding of engineered systems but also provides a robust framework for the rational design of the next generation of smart materials.

Acknowledgments. Potentiating the Italian Capacity for Structural Biology Services in Instruct-ERIC", acronym "ITACA.SB" (Project No. IR0000009, CUP B53C22001790006), funded by the European Union's NextGenerationEU under the MUR call 3264/2021 PNRR M4/C2/L3.1.1

-PL 3-

The Information Contained in Self-Assembling Systems

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Nature uses self-assembly to generate complex molecular systems such as, e.g., microtubules, protein filaments, or lipid assemblies, that are innately dynamic and express complex functions. Learning how to design artificial systems with similar behaviors would be a breakthrough, but the key factors controlling them are typically difficult to ascertain. Molecular models [1], simulations [2] and machine learning [3] are fundamental to this end.
In this talk, I will describe methods that we have developed to model supramolecular self-assembling systems of different types on multiple scales [1-2,4] and to resolve, from the data extracted from their trajectories, their structural and dynamic complexity [5-7]. I will show how tracking dominant fluctuations allows understanding how collective properties emerge in it [8-10]. These data-driven methods are general and can be applied also to study experimentally resolved trajectories of higher-scale complex dynamical systems whose physics is unknown a priori [8-12]. This opens fundamental questions, such as, e.g., at what levels/scales do complex behaviors emerge in self-organizing systems. The results that we are obtaining are challenging, broadly, how we look at a variety of phenomena central in physics and materials science [9-14].

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-PL 4-

Unlocking the Potential of Organic Materials for Energy Storage: the Fascinating Journey toward Sustainable Batteries

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The expected growth of the battery sector over the coming years is enormous, with approximately 7 million tons of new batteries projected per year. This growth is mainly driven by the development of electric vehicles and energy storage systems coupled with renewable energy generation (wind and photovoltaic). However, the massive expansion of the sector could become an environmental issue, since most commercial batteries are based on inorganic materials such as lithium, nickel, and cobalt in lithium-ion batteries, or vanadium in flow batteries. These materials are scarce, their production is in some cases unsustainable, and some are even toxic.

In this context, replacing these materials with organic compounds based on abundant elements such as C, H, O, and N has become a highly promising alternative. In this talk, I will present the enormous structural and synthetic possibilities offered by redox-active organic materials and their application in different types of batteries. I will present our recent advances in developing organic electrode materials (OEMs), including both linear and hyperbranched designs [1], with a particular focus on redox-active conjugated microporous polymers (CMPs) as versatile candidates for next-generation batteries [2]. CMPs offer key advantages—such as enhanced electrolyte infiltration, short ion/electron diffusion paths, and robust mechanical stability—that enable high capacity utilization, rapid charge/discharge kinetics, and outstanding cycling stability [3].

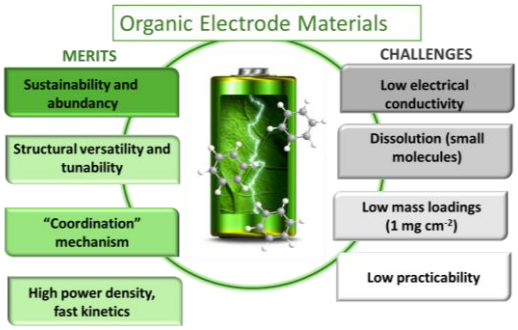

Figure 1. Merits and Challenges associated to redox-active organic compounds as electrodes for batteries.

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[3] a) R. Grieco, et al. Mater. Today Energy 2022, 27, 101014; b) R. Grieco, et al. Batter. Supercaps 2024, e202400346; c) R. Grieco et al. Faraday Discuss. 2024, 250, 110.

-PL 5-

Amyloid-Metal Supramolecular Hybrids for Health and Environmental Remediation Technologies

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Amyloid fibrils interact with metal ions via metal-ligand supramolecular interactions whose energy is of the order of tens to hundreds of K_BT [1]. The occurrence and abundance of the 20 essential amino acids in food-based amyloid fibrils derived from inexpensive animal and plant proteins, including from food waste and agricultural side streams, combined with the extreme aspect ratio of the amyloids, allow for an affordable, yet universal toolbox to produce multifunctional hybrids which can serve in a multitude of applications and technologies. In this talk I will provide several examples of food amyloid fibrils interacting with metal ions and nanoparticles for both health and environmental remediation, some of which have made it into real technologies. Taking β-lactoglobulin amyloids as a model amyloid system derived from whey, a by-product of cheese making process, I will show how metal ions can be adsorbed from water and wastewater solutions by amyloid-based filters for water purification purposes [2], or how gold ions can be adsorbed and processed from amyloid aerogels to recycle gold from e-waste [3] (Figure 1); I will also show how iron atoms can be coordinated to β-lactoglobulin amyloids to deliver highly bioavailable Fe(ii) for iron fortification [4-5], or to design hydrogels capable of performing cascade enzymatic reactions for alcohol detoxification in vivo [6].

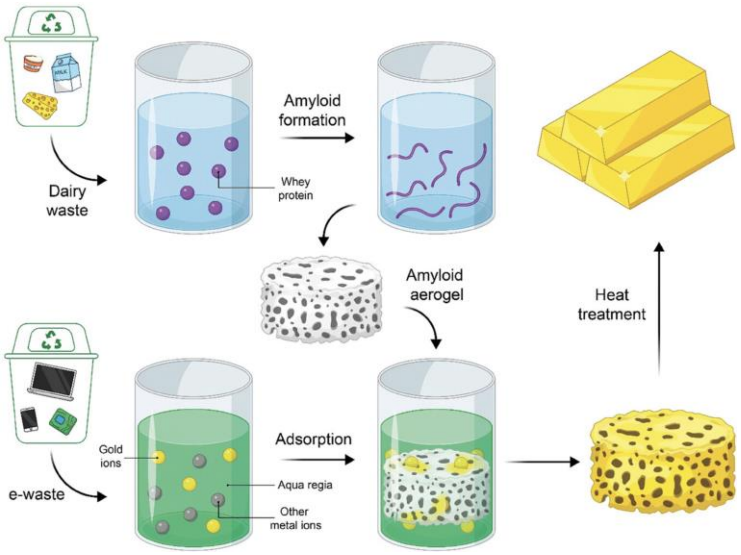

Figure 1. An example of environmental remediation technology enabled by amyloid-metal supramolecular interactions: Gold Recovery from E-Waste by Food-Waste Amyloid Aerogels (reproduced from ref. 3).

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-PL 6-

Engineering Nano–Bio Interfaces: From Self-Assembly to Functional Hybrid Nanosystems

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The role of interfaces in governing structure, dynamics, and function in complex systems is central in modern physical chemistry, with broad implications for soft matter, colloidal systems, nanomedicine, and complex formulations.
In this contribution, I will discuss recent progress from our group on the design of hybrid nanosystems arising from the interplay between inorganic nanoparticles, biomacromolecules and soft, self-assembled synthetic lipid structures.
We show that lipid membranes can act as active templates for nanoparticle organization, directing mesoscale assembly and emergent optical properties. In particular, recent results demonstrate how collective plasmonic responses can be quantitatively correlated with interparticle spacing, providing new insight into structure–function relationships in soft–hard hybrid systems enabling non-invasive probing of nanoscale mechanical properties.
Extending to biologically relevant environments, I will present recent findings on lipid nanoparticles interacting with biomolecular environments, highlighting how the formation of protein and lipoprotein coronas can induce not only surface modifications but also profound internal structural remodeling. These results redefine the concept of biological identity of nanomaterials as an emergent property of coupled interfacial and bulk processes.
Finally, I will discuss recent strategies to engineer structurally defined hybrid systems combining synthetic lipid nanoparticles with biological components such as extracellular vesicles, enabling controlled integration of functionality while preserving structural integrity.
Altogether, these examples illustrate how core concepts from colloid and interface science, self-assembly, and soft matter physics converge to enable the rational design of complex formulations with programmable properties.

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Keynote Lectures

-KN 1-

Ensuring Drinking Water Quality in Acquedotto Pugliese through the digitalization of the Water Safety Plan

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This case study focuses on how digital transformation being applied to guarantee safe drinking water in a large utility, highlighting the example of Acquedotto Pugliese (AQP) in Italy. AQP, one of the biggest water companies in Europe, has embraced an innovative, digital Water Safety Plan (WSP) to manage water quality risks across its vast supply network. Water Safety Plan is a comprehensive risk assessment and management approach covering every step from source watershed to consumers' taps, as recommended by WHO. Traditionally, WSPs could be paper-based checklists. AQP instead developed a dynamic digital integrated platform that incorporates GIS mapping of infrastructure, hydraulic models, several datasets and a central control room – dubbed the "digital brain" of AQP – that consolidates all signals of possible water safety issues and coordinates action. AQP's approach also involves stakeholders like local health and environmental authorities that will have access to the platform for transparency and to collaborate actively in the risk assessment evaluation, and the public can be quickly informed of any preventive boil notices through integrated communication tools. On the innovation side, AQP implemented new water treatment technologies and advanced monitoring tools to minimize harmful by-products while ensuring microbial safety. Yet, the case study demonstrates clear benefits of digitalizing water management i.e. greater resilience to contamination events, identification of measures to mitigate risks and enhanced trust from consumers and regulators. AQP's digital WSP serves as a blueprint for utilities worldwide striving for excellence in water quality under the imperatives of the green transition and climate adaptation.

-KN 2-

THE CONTRIBUTION OF PHOTOCHROMIC MATERIALS IN THE DEVELOPMENT OF CHEMICAL AI

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Chemical Artificial Intelligence (CAI) is an emerging research field focused on designing chemical systems in wetware—that is, liquid-phase environments—that emulate competencies typical of biological intelligence [1]. UV–visible radiation is a key resource in this endeavor, as it maintains chemical systems out of equilibrium, enables their responsiveness to optical and physicochemical signals, and enables their monitoring.
As in all kingdoms of life, photochromic compounds play a central role in these processes. Many organisms rely on photochromic molecular switches to generate diverse responses to environmental light. This work offers a plausible justification for their significance by showing how each photochrome can be viewed as a simple form of a Markov blanket, capable of implementing (i) forward, (ii) final, and (iii) circular causalities [2].
Beyond their biological relevance, photochromic materials are also well suited for chemical information processing. They can perform Boolean and fuzzy logic operations and exploit chemical reactivity, chaos, and quantum effects for computation [3]. Additionally, photochromic molecules constitute promising components for neuromorphic engineering in wetware environments driven by optical signals [4, 5].
Altogether, CAI provides inspiration for the development of adaptive, active, and autonomous chemical systems that may empower humanity to navigate and master the molecular world in tackling challenges such as disease, pollution, and poverty.

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-KN 3-

Addressing Complexity in Energy Materials and Interfaces: Predictive Modeling Strategies beyond DFT

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Establishing a quantitative and predictive link between atomistic-level theory and experimental observables remains a critical bottleneck in the rational design of sustainable energy technologies. One central difficulty is that key processes in energy materials and interfaces often involve electronically complex states that challenge standard density functional theory (DFT).
In this talk, we present recent results from our group showing how complementary beyond-DFT approaches help bridge the theory–experiment gap across a range of energy-relevant systems. In photoactive interfaces, including perovskite solar cells and dye-sensitized photoelectrochemical systems, we show how diabatization enables a quantitative description of interfacial electronic couplings and carrier injection timescales [1,2]. In Na-ion batteries, atomistic simulations of P2-type cathodes reveal the mechanisms of structural phase transitions during charge and discharge, with variable-cell nudged elastic band (VC-NEB) calculations providing details on their pathways and kinetics [3,4]. As for interfacial reactivity, we first probe to what extent the inclusion of electric fields shapes reaction energetics and pathways, using CO_2 activation on defective Bi_2O_3 surfaces as a test case. We then show how multireference embedded-cluster and QM/MM approaches are needed to capture the role of strong electronic correlations in processes such as oxygen evolution in Li–air batteries [5].
Overall, these results suggest that the main limitation is not the lack of methods, but how they are combined and applied across different regimes of complexity, choosing the right description for the physics at play

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-KN 4-

Confined Spaces, Boundless Opportunities: Controlling Confinement in Porous Materials from Catalysis to Nanomedicine

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The traditional paradigm of materials science has long prioritized the solid framework; however, the transformative potential of porous materials is ultimately defined by the architecture of the void and the accessibility of active sites. The evolution of porous materials science reflects a profound shift in molecular engineering, from the foundational role of zeolites in petrochemical processing to the advanced design of nanovectors for personalized medicine. Central to this progress is the ability to tailor pore size, shape, topology, and surface chemistry with molecular precision. In this context, porous materials have emerged as a cornerstone of modern physical chemistry, enabling fine control over molecular organization, transport, and reactivity within confined environments. From zeolites to mesoporous silica, the rational design of porous architectures has opened new frontiers toward more sustainable and greener chemical processes.

In this contribution, nanoconfinement is presented as a unifying principle governing reactivity across conceptually connected systems, spanning zeolite-based catalysts and organic–inorganic mesoporous silica hybrids for applications in catalysis and nanomedicine. Selected examples will demonstrate that pore architecture, surface chemistry, and host–guest interactions collectively dictate reactivity and efficiency, and that their full understanding requires multi-technique approaches for comprehensive physico-chemical characterization.

In zeolites, Brønsted and Lewis acid sites embedded within well-defined microporous frameworks promote shape-selective catalysis, with high activity and selectivity [1]. In parallel, hybrid mesoporous silicas provide versatile and tunable environments in which molecular functionality and structural confinement are intimately integrated, enabling cascade catalytic transformations as well as the incorporation of photosensitizers with improved light harvesting and efficient singlet oxygen ($^1O_2$) generation for nanomedical applications (Figure 1)[2,3].

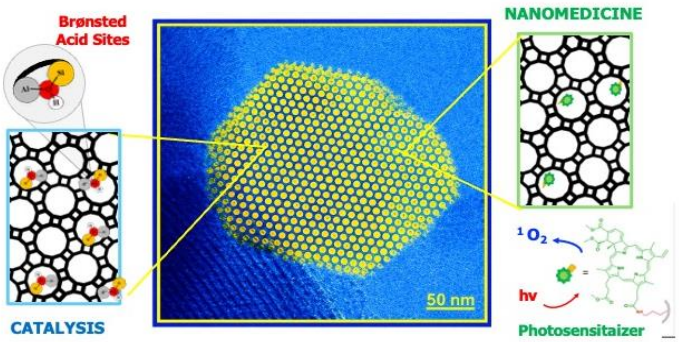

Figure 1. Pictorial representation of confined catalytic sites and a photosensitizer for singlet oxygen generation.

From this perspective, confined spaces are no longer merely containers but active environments where chemistry is shaped, offering boundless opportunities to design next-generation catalytic and nanomedical systems for more sustainable and resource-efficient processes.

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-KN 5-

The C Treasure in Biomasses for Energy and Analytical Applications

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The implementation of environmentally green materials is essential in materials chemistry to ensure a fair and ethical transition to net zero. Carbon-based materials play a fundamental role thanks to the versatility of the different allotropes, and the possibility to tune their porosity, surface area and chemistry, making them suitable as adsorbents for water purification, analytical determinations, electrodes materials for supercapacitors and batteries, as well as active phases in storing gasses like H_2 and CO_2. In the last years, in the frame of the circular economy concept and of CIRCOLARE project (RSH2A_000015, funded by MASE) we devoted to the preparation and characterization of C-based materials from different kind of (common or less studied) agri-food biomasses, tuning their characteristics based on the different applications. In this frame, we optimized the pyrolysis conditions (time, temperature) in dependence on the biomass nature, obtaining the C solid phase, namely biochar, with good yields. Biochar samples obtained from orange and pumpkin peels [1,2] and from olive pomace [3] were successfully tested for analytical applications. More in detail, these materials were used as the adsorbent phase in innovative miniaturized settings (VWSE, SBSME) for the determination of steroid hormones at the trace levels in complex matrices, namely environmental waters and wastewater (environmental monitoring), and in human saliva (bioanalysis). The adsorbents showed a satisfactory sorption/desorption behavior for the target compounds allowing for streamlined sample preparation procedures with improved greenness, before instrumental quantification. The biochar immobilized in the extraction devices exhibited excellent physico-chemical stability, assuring reusability for repeated uses with no efficiency loss.

The chemical activation of biochar by KOH followed by *ad hoc* thermal treatments (up to 650°C), allowed to obtain C materials with specific surface area up to 2500 m^2/g, presenting high H_2 storage efficiency (up to 5wt% at 77K and 8 bar for rice bran biochar, with the US DoE target fixed at 5.5wt% for the storage systems) coupled with a very promising kinetics (less than 1 minute for full adsorption and maximum 3 min for desorption).The decoration of the activated C surface with metals nanoparticles (Ni, Pd) by chemical impregnation in a salt solution, followed by a thermal treatment under reducing atmosphere, allowed to obtain materials with good catalytic activities towards metallic hydrides dehydrogenation and re-hydrogenation reactions.

Finally, char obtained via hydrothermal treatment of the biomasses in autoclave and subsequently activated with KOH were used as electrodes in supercapacitors standard coin cells assembled with different electrolytes (KOH and Na_2SO_4 aqueous solutions) to find those better matching the pore size of the carbon matrix [4]. An almost ideal electrical double layer capacitance and electrochemical performance in accordance with that of state-of-the-art materials were obtained, with specific capacitance up to 220 F/g and high stability upon cycling.

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-KN 6-

Innovative Hybrid Materials for a Sustainable Future: Bridging Circular Resources, Nanotechnologies, and Green Transition

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The transition toward a sustainable society requires the development of materials and technologies capable of minimizing environmental impact while maximizing resource efficiency. In this context, research is increasingly focused on the recovery and valorization of secondary resources obtained from waste streams, industrial and agricultural residues, and renewable biomass, gaining attention as sustainable precursors to produce innovative materials with reduced environmental footprint. Converting these underutilized materials into functional products represents a key strategy to reduce landfill disposal, decrease the consumption of primary raw materials, and promote circular material cycles [1]. In this regard, hybrid organic–inorganic materials represent a versatile class of advanced materials capable of integrating the flexibility and functionality of organic components with the robustness and stability of inorganic structures. This combination enables the design of multifunctional systems with tailored mechanical, chemical, and surface properties, which are increasingly explored in technological fields that address major global challenges, including renewable energy systems, environmental remediation, water treatment technologies, and biomedical applications [2].
At the nanoscale, hybrid materials can exhibit enhanced reactivity, improved catalytic behavior, and controlled interaction with molecules and ions. At the same time, the incorporation of bio-based polymers and recycled components into hybrid matrices contributes to reducing the environmental footprint of the materials themselves, aligning their production with circular economy principles and climate action goals [3]. The synthesis route also plays a crucial role in determining the sustainability of advanced materials. Among the available techniques, the sol–gel process offers a flexible and relatively low-energy pathway for producing hybrid coatings and bulk materials with high compositional uniformity, controlled nanostructure and improved performances [4].
This work presents the design and development of hybrid and bio-inorganic materials obtained also through sustainable synthesis strategies. The study focuses on their preparation, structural and physicochemical characterization, and evaluation of their potential applications in areas related to green transition and climate mitigation, circular materials and resource recovery, water monitoring, purification and environmental protection, as well as emerging applications in health, well-being, and several application fields related to material sciences. Overall, the results will highlight how these advanced hybrid materials can contribute to the development of environmentally responsible technologies and support the transition toward a more sustainable future.

Acknowledgments. MICS Extended Partnership (PE00000004) and Ecosistema SAMOTHRACE (ECS00000022) PNRR projects are gratefully acknowledged.

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-SKN-

RisPA CENTER: the Research and Development Center for Environmental Remediation and Protection

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The RisPA Center is the result of a collaboration between the Department of Science and Technological Innovation (DISIT) of the University of Eastern Piedmont and the Syensqo company, with the scope of creating a *Joint-Lab* dedicated to research and development (R&D) of advanced and sustainable solutions for environmental remediation and protection.

With a five-year agreement signed on February 9, 2024, the Center represents a concrete model of integration between academia and industry, in an open collaborative model, with the aim of:
- developing new technologies applicable to real-world contexts;
- accelerating the technology transfer of research results;
- contributing to environmental sustainability through scalable solutions.

The activities are supported by:
- new laboratories and research spaces;
- advanced scientific instrumentation managed by dedicated technologists;
- multidisciplinary teams composed of academic and industrial researchers, technicians, and young talents.

The Center also provides an advanced training environment for undergraduate and graduate students, doctoral students, and young researchers, with access to cutting-edge technologies.

The RisPA Center develops activities in several complementary areas:
- Development of polymers, carbons, and advanced **porous materials** for the **removal of contaminants**;
- Development of **phytoremediation** technologies;
- Use of **computational modeling** assisted by AI and machine learning for advanced simulations;
- Analysis of environmental and economic impacts throughout the entire life cycle.

Session A

Fundamental Physical Chemistry:

Structure, Dynamics, and Spectroscopy

-A O1-

Enhancing the Optical Response of Gold and Silver Nanoclusters via Rigid Embedding in High-Refractive Index Polyacrylamide Matrix

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Biomolecules-stabilized metal nanoclusters (NCs) are promising emitters formed by gold and/or silver atoms and cations encapsulated in strands of small peptides, oligonucleotides or bigger proteins[1,2,6]. In this work we propose an innovative strategy to enhance their extraordinary optical and luminescent properties, making them excellent candidates for new smart materials. Some fully characterized NCs have been inserted into a polymer to preserve their fine characteristics, making them independent from the environment, thereby enhancing the practical applicability of NCs in real-world scenarios[3,4]. The chosen gel is highly transparent, with a high refractive index and very easy to obtain: the results confirm the success of our approach, as the NCs absorption and excitation spectra do not undergo significant variations even after several months, while the luminescence quantum yield and decay time have been significantly increased. Moreover, while some of these NCs, once placed inside the polyacrylamide matrix, only improve their photophysical performances (Figure 1), others undergo a remarkable emission change, activating important long-lived emission components[5](Figure 2).

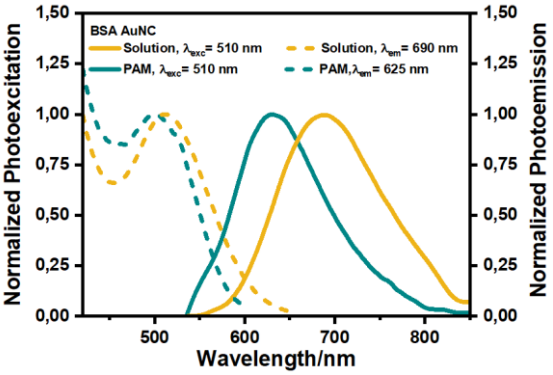
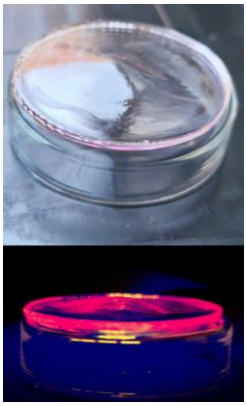


Figure 1, Excitation and Emission spectra of BSA Au NC in solution and in PAM matrix.



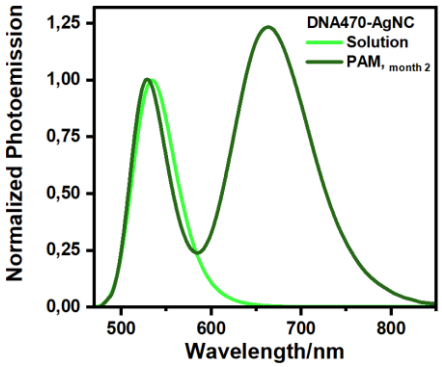


Figure 2, Excitation and Emission spectra of DNA-Ag NC in solution and in PAM matrix.

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-A O2-

Spectral Reshaping of Porphyrin Excitation by Plasmonic Nanostructures

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The interaction between plasmonic nanostructures and molecular chromophores has attracted significant attention because localized surface plasmons can strongly modify the optical response of nearby molecules. While these effects are often discussed in terms of fluorescence enhancement or quenching, plasmonic near-fields can also modify the relative contribution of different molecular absorption bands, owing to their wavelength-dependent field enhancement [1].

In this work we investigate how plasmonic nanostructures affect the excitation behaviour of tetraphenylporphyrin (H_2TPP), a well-known chromophore whose absorption spectrum is characterized by an intense Soret band and weaker Q-bands. Electromagnetic BEM simulations [2] were first performed to evaluate wavelength-dependent near-field enhancement in different plasmonic architectures, including Au and Ag nanosphere aggregates, Au nanorods, and Au nanostars [3]. These calculations highlight how the spectral overlap between plasmonic resonances and molecular absorption bands can lead to selective amplification of specific transitions.

To experimentally explore these effects, H_2TPP molecules were covalently attached to plasmonic nanoparticles through a rigid α-helical peptide spacer [4] that fixes the dye at a controlled distance from the metal surface. Optical spectroscopy measurements reveal reproducible changes in the relative contribution of porphyrin excitation bands, with an increased role of the Q-bands compared to the Soret band. The observed trends are consistent with the wavelength-dependent field enhancements predicted by the simulations.

These results provide insight into how plasmonic near-fields influence molecular spectroscopy and contribute to a deeper understanding of light–matter interactions in hybrid metal–molecule systems.

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-A O3-

Turning Waste into Value: Sustainable Bio-Emulsifiers from Agro-Food By-Products

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Agro-food waste streams represent a significant environmental and economic burden due to their large volumes and elevated chemical oxygen demand (COD) and biological oxygen demand (BOD). Nevertheless, these residues constitute valuable reservoirs of bioactive and functional compounds, including polyphenols, carbohydrates, proteins, lipids, and fatty acids, thereby offering considerable potential as renewable feedstocks to produce value-added biobased materials [1,2]. This study investigates the synthesis, characterization, and performance evaluation of novel bio-based emulsifiers derived from agro-food byproducts, specifically cheese whey permeate (CWP) and soybean meal (SBM). CWP, a major byproduct of the dairy industry, was utilized as a substrate for the synthesis of sugar fatty acid esters (SFAEs), a class of non-ionic surfactants recognized for their superior interfacial activity, biodegradability, and low ecotoxicity [3]. In parallel, SBM, a protein-rich residue generated during soybean oil extraction, was explored as an alternative renewable source for the development of high-performance emulsifying agents [4]. In both cases, a chemoenzymatic synthetic strategy was employed, and the reaction parameters were systematically optimized using chemometric methodologies.

The synthesized bio-emulsifiers were comprehensively characterized and assessed for their surface-active properties, including their ability to reduce static and dynamic interfacial tension. Their emulsification performance was further evaluated through the preparation and stabilization of water-in-sunflower oil (W/O) emulsions, both in model systems and in more complex formulations, with stability monitored over extended storage periods. Furthermore, computational modeling and interfacial rheological analyses were conducted to elucidate the structural and mechanical properties of the oil–water interface and to predict long-term emulsion stability.

The findings demonstrate the feasibility of valorizing agro-food waste as a sustainable source of bio-based emulsifiers, thereby contributing to the development of environmentally benign industrial formulations and supporting the implementation of circular economy and green chemistry principles.

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-A O4-

Chemical Affinity-Driven SERS Response of Histidine-Functionalized RGO/Ag Nanowire Nanocomposites on Hydrophobic Paper

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Hybrid nanocomposites combining graphene derivatives with plasmonic metal nanostructures represent an effective strategy to synergistically combine the intrinsic properties of pristine components for surface-enhanced Raman spectroscopy (SERS) [1]. Here, we investigate the physicochemical origin of the SERS response of a colloidal hybrid nanocomposite composed of histidine-functionalized reduced graphene oxide (His-RGO) sheets decorated with silver nanowires (AgNWs), synthesized through a scalable *in situ* polyol approach and processed into flexible substrates by drop-casting onto hydrophobized chromatographic paper. Structural characterization confirms the formation of micrometric AgNWs anchored onto His-RGO sheets, generating a hybrid architecture where plasmonic hotspots produced by AgNWs coexist with the adsorption capability and fluorescence quenching properties of the His-RGO platform [2,3]. This configuration enables investigation of the interplay between electromagnetic enhancement, charge-transfer contributions, and analyte–substrate chemical affinity. The SERS performance was evaluated using probe molecules with distinct chemical structures and interaction mechanisms, namely rhodamine 6G (R6G), 1-naphthalenethiol (1-NAT), and benzo[a]pyrene. The results demonstrate that analyte–substrate affinity governs both sensitivity and stability of the SERS response. The nanocomposite exhibits strong enhancement for R6G, with a limit of detection of 10^{-7} M, attributed to synergistic electromagnetic amplification and aromatic π–π stacking interactions with the His-RGO basal plane, which promote analyte capture and fluorescence quenching [4]. Conversely, 1-NAT, interacting primarily through Ag–S bonding, shows higher sensitivity on pristine AgNWs, indicating that the spatial separation of nanowires induced by the His-RGO scaffold partially reduces nanowire coupling and hotspot density. No detectable SERS response is observed for benzo[a]pyrene, highlighting the importance of effective chemical interactions for signal enhancement. SERS spectra monitored over time reveal improved signal stability for R6G on the hybrid substrate compared to AgNWs alone, attributed to π–π interactions and the protective barrier effect of His-RGO against nanowire oxidation [5]. The applicability of the hybrid substrate was demonstrated through detection of propranolol hydrochloride (PRNL), a β-blocker of pharmacological and anti-doping relevance, achieving a limit of detection of 10^{-4} M, below cytotoxicity limits and antidoping thresholds. These results provide insight into the interplay between electromagnetic enhancement and chemical interactions and demonstrate the potential of His-RGO/AgNWs nanocomposites on paper as portable platforms for molecular detection [6].

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-A O5-

Crystal Structure Refinement of New Organocatalyst: Benchmarking between Independent Atom Model (IAM) Refinement and Hirshfeld Atom Refinement (HAR)

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The structural refinement is a process through which the obtained structural model is improved with the aim of achieving the best possible agreement between the experimental data and the calculated model. The majority of structural refinements are based on approximation of the independent atom model (IAM), in which the electron density of the atoms is considered spherical; however, in this way the atoms are treated as non-interacting spherical entities, neglecting the fact that electrons are not only localized on the atoms but also participate in chemical bonding[1]. Thus, this model leads to an inaccuracy in the model. To avoid this issue, an alternative refinement approach known as Hirshfeld atom refinement (HAR) is based on quantum mechanical calculations and applied within NoSpherA2 procedure, considering the electrons involved in the chemical bonding during the refinement. After calculating a molecular wavefunction for the structural model, the electron-density functions of the so-called Hirshfeld atoms are extracted through a partitioning process[1], and a Fourier transform is then performed to provide non-spherical scattering factors for each individual atom. More accurate structure factors are calculated during the least-squares refinement, and the entire process is iterated until convergence. Aspherical refinements yield more accurate and precise information on chemical bonding, non-covalent interactions, lone pairs, partial charges, and hydrogen atom positions [2].
We performed the structural refinement of a novel organocatalyst [3] (Figure 1) with the two procedures, i.e. considering the IAM and the NoSpherA2 approach. In this work we compare the results and discuss the advantages of the new method.

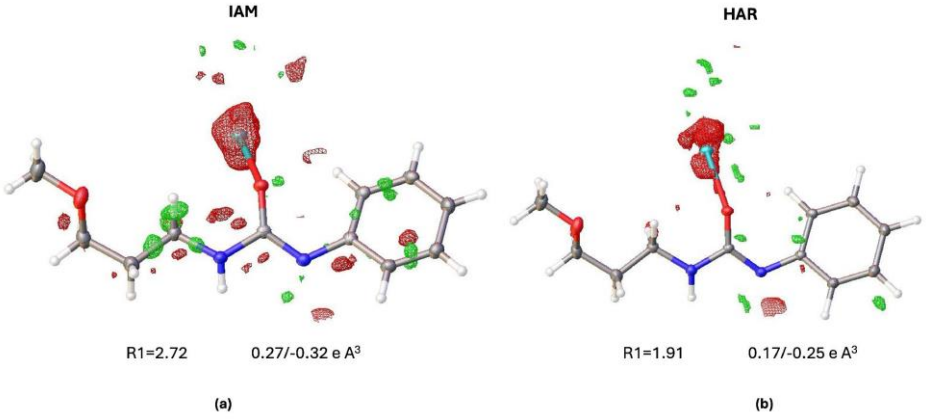

Figure 1. Comparison of the refinement results for (a) Spherical and (b) Non-Spherical Model.

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-A O6-

Decoding Molecular Structure with Rotational Spectroscopy

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Molecular rotational resonance spectroscopy has recently developed into a powerful analytical technique for the precise determination of molecular structure. Its high spectral resolution and intrinsic sensitivity to molecular moments of inertia allow closely related species—including regioisomers, stereoisomers, conformers, and isotopic variants—to be distinguished unambiguously, even in complex mixtures and without the need for prior separation.

In this contribution, the application of rotational spectroscopy to structural and chiral analysis of small molecular systems will be discussed. Particular attention will be given to the synergy between high-resolution spectroscopy and computational chemistry for the assignment of experimental spectra. Automated conformational search tools such as CREST or GOAT are essential for identifying low-energy structures and predicting spectroscopic parameters, enabling reliable interpretation of rotational spectra.

The role of high-performance computing (HPC) resources will also be highlighted, both for large-scale conformational exploration and for the implementation of dedicated analysis workflows. In particular, the use of in-house algorithms for automated spectral analysis and fitting will be presented, illustrating how the integration of spectroscopy, computational methods, and advanced data analysis enables robust structural identification in challenging molecular systems.

-A O7-

Integrating Twisted and Push-Pull Structural Motifs for Efficient Dual-Functioning Near-Infrared Bodipy Photosensitizers

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Cancer treatment is moving beyond traditional approaches like chemotherapy and radiation therapy, with photodynamic therapy (PDT) offering a targeted and less invasive alternative. PDT relies on light-activated photosensitizers (PSs) to generate reactive oxygen species (ROS) that kill cancer cells. A promising strategy for designing heavy-atom-free PSs with high triplet formation is relying on a mechanism called Spin-Orbit Charge-Transfer Intersystem Crossing [1]. For theragnostic applications, PSs must balance ROS generation with sufficient fluorescence for imaging (Figure 1).

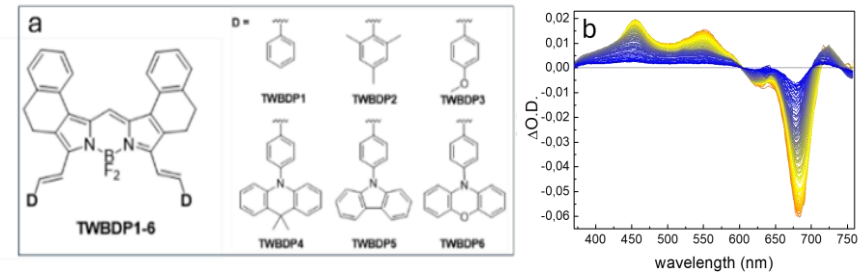

Figure 1. a) Structures of the BODIPYs b) Transient absorption spectra of TWBDP4 in $CHCl_3$.

In this work, three new twisted push-pull BODIPYs with different electron-donating groups were synthesized and studied (Fig. 1a). These dyes exhibit strong absorption and emission in the red region (600–800 nm), combining high fluorescence quantum yields (up to 50%) with excellent singlet oxygen generation (up to 69%). Transient absorption spectroscopy (Fig.1b) shows ultrafast charge separation, influenced by solvent polarity and donor strength. Computational studies (DFT/TD-DFT) confirm that donor substitution modulates HOMO–LUMO separation and electronic properties [2]. These new BODIPY derivatives exhibit balanced photophysical properties, highlighting their potential in cancer theragnostics.

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-A O8-

Spatially Resolved Biochemical Signatures of Cardiorenal Syndrome Revealed by FTIR Imaging

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Cardiorenal syndrome (CRS) is a multifactorial disorder characterized by a bidirectional interaction between cardiac and renal dysfunction, driven by hemodynamic, neurohormonal, inflammatory, and metabolic mechanisms. Early detection of CRS progression remains challenging, highlighting the need for sensitive molecular biomarkers. Vibrational spectroscopy techniques, such as Fourier-transform infrared (FTIR) spectroscopy, offer label-free approaches for probing biochemical alterations in biological tissues; however, their application to cardiorenal disease remains limited.

In this study, FTIR micro-imaging was used to identify molecular signatures associated with cardiorenal pathology and to evaluate their modulation following treatment with Entresto, the first approved angiotensin receptor–neprilysin inhibitor. Cardiorenal interactions were modeled in male Wistar rats through uninephrectomy followed by cardiac ischemia–reperfusion injury. Molecular alterations were primarily investigated in the left ventricular myocardium, a key contributor to CRS progression. Renal tissue changes were analyzed separately within the cortical, medullary, and vascular compartments (Figure 1).

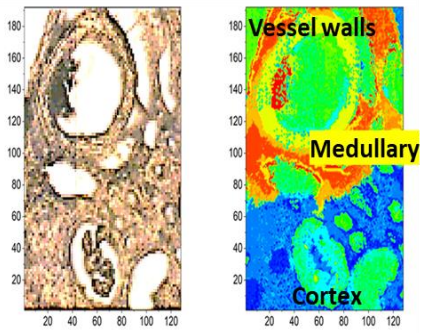

Figure 1. Optical (left) and FTIR (right) image of renal tissue.

By integrating hierarchical clustering–based anatomical segmentation with compartment-specific PCA marker extraction, the analysis revealed that disease-related spectral variance is not uniformly distributed across tissues but is concentrated within discrete anatomical microenvironments. Disease-associated biochemical changes were related to fibrosis, protein remodeling, and metabolic imbalance. After Entresto treatment, a partial normalization of tissue chemical composition was observed. Overall, the present work demonstrates that compartment-resolved FTIR imaging, combined with targeted multivariate analysis, provides a powerful framework for quantitative characterization of spatially heterogeneous tissue remodeling in experimental disease models.

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-A O9-

SpeComp: a User-Friendly Tool for Spectral Comparison to Facilitate Microplastics Detection in Complex Biological Matrices

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Microplastics (MPs, 1 µm–5 mm) are pervasive environmental contaminants originating from either the intentional production of small plastic particles or the degradation of larger products. Due to their ubiquitous presence, human exposure is continuous, and MPs have been detected in multiple human bodies compartments (e.g., lungs, blood, liver), suggesting systemic uptake and distribution. Their potential health implications, however, remain poorly understood. Our group conducted a comprehensive study on urine and kidney samples from healthy individuals, identifying for the first time MPs and their additives in these matrices using micro-Raman spectroscopy [1]. The study was then extended to other biological fluids (e.g., exhaled breath condensate, dialysis fluid).

These analyses were enabled by SpeComp [2], a Python program developed in-house to identify unknown substances by comparing their Raman spectra to self-created databases (Figure 1). The need for such a program arose from the complexity of real biological samples, where MPs often come from everyday objects and undergo human digestion, and where different matrices are pretreated and analyzed under different conditions. SpeComp performs spectral comparison using six statistical algorithms: Normalized Correlation, Hit Quality Index, Convolution, Fast Fourier Transform Convolution, Correlate Correlation, and Difference Metric, allowing the selection of the most suitable method for each scenario. The software also supports pre-processing (noise filtering, baseline correction, normalization, smoothing) and subtraction of known spectra (e.g., substrate signals).

The presentation will cover the methodologies for MP detection in the studied biological samples and an overview of SpeComp's main functionalities.

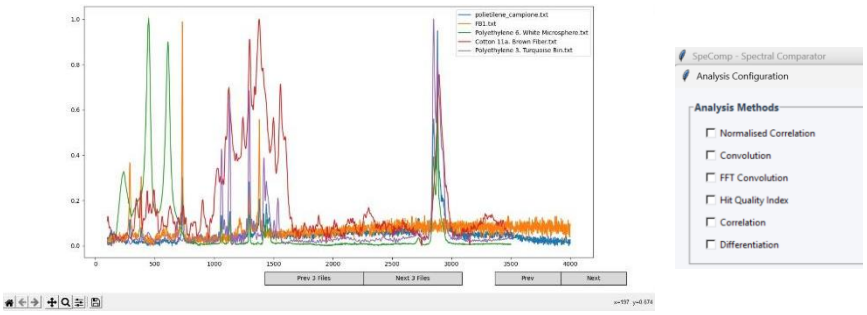

Figure 1. GUI of the SpeComp software showing the results from a spectral comparison (left) and the window for the selection of statistical methods (right).

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-A O10-

Multinuclear Solid-State NMR Investigation of Adsorption-Induced Structural Changes and CO_2 Dynamics in CALF-20

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Metal-organic frameworks (MOFs) are a versatile class of porous materials with high surface areas and tunable pore architectures, making them attractive for gas capture and separation [1]. However, their practical deployment is often limited by poor hydrothermal stability. CALF-20 (Calgary Framework-20, [Zn_2(1,2,4-triazolate)$_2$(oxalate)]) represents a notable exception, combining high CO_2 uptake under humid conditions with remarkable stability and demonstrated industrial scalability [2-4].

Despite extensive investigation, its hydration behavior remains debated, with discrepancies arising from differences in sample history, experimental conditions, and structural assignments of hydrated phases. Current understanding converges toward a reversible transition between an open-pore, weakly hydrated state and a contracted, water-stabilized phase at intermediate humidity, involving significant structural reorganization [3, 5, 6, 7].

In this work, we employ multinuclear solid-state NMR spectroscopy to gain atomic-level insight into the structural evolution of CALF-20 upon hydration and CO_2 adsorption. By monitoring changes in local environments under controlled hydration levels, we clarify the nature of the phase transition and its reversibility, as well as the role of framework-water interactions in stabilizing distinct hydration regimes.

A key aspect of this study is the investigation of CO_2 behavior in the CALF-20 framework. While previous studies have proposed possible adsorption sites [2,3,5], experimental information on molecular dynamics remains scarce. Here, we analyze the temperature dependence of static ^{13}C lineshapes of adsorbed CO_2 in differently hydrated CALF-20 to probe its reorientational dynamics within the pores, revealing a strong dependence on both temperature and hydration state.

Acknowledgments. 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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-A O11-

Molecular Motions of Active Pharmaceutical Ingredients Investigated by Solid-State NMR Spectroscopy

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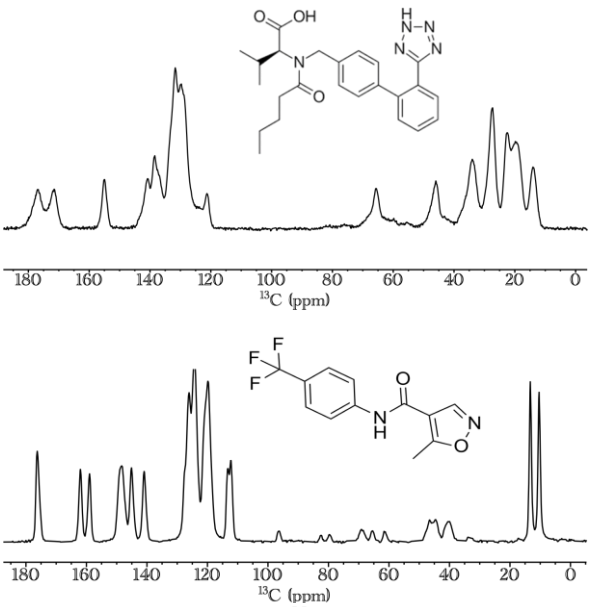
The molecular dynamics of active pharmaceutical ingredients (APIs) can play a key role in determining important macroscopic properties of solid drug products, particularly solubility and dissolution rate. A thorough understanding of these dynamics is therefore essential for selecting the most suitable solid form for final formulation.

Solid-state NMR (ssNMR) spectroscopy is a highly versatile technique for probing molecular dynamics, providing access to motions over an exceptionally wide timescale, from picoseconds to seconds [1]. This sensitivity arises from the anisotropic nature of nuclear spin interactions, which depend on molecular orientation with respect to the external magnetic field and thus encode its temporal fluctuations.



The investigation of different nuclei offers complementary insights: low-abundance nuclei, such as ^{13}C and ^{15}N, provide localized, site-specific information, while abundant nuclei, typically ^{1}H, probe the collective behavior of the molecular framework. This combined approach enables a comprehensive characterization of both local and long-range motional processes. Molecular motions affect ssNMR spectra in multiple ways and govern nuclear relaxation phenomena. By combining high-resolution ssNMR experiments with spin-lattice relaxation time (T_1) measurements, it is possible to extract both qualitative and quantitative information on the dynamics of solid samples.

Here, we present dynamical studies on different solid forms of two APIs, Valsartan and Leflunomide (Figure 1). Valsartan, an antihypertensive compound exhibiting polyamorphism [2], shows distinct dynamic behaviors across its amorphous forms, which can be qualitatively discriminated by ssNMR. In contrast, Leflunomide, a disease-modifying antirheumatic drug (DMARD) used primarily for rheumatoid arthritis, exists in two known polymorphs [3] whose molecular motions have been fully and quantitatively characterized. In this case, activation energies and correlation times were determined, enabling a detailed comparison of the underlying dynamical processes [4].

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-A O12-

The Halogen Advantage: the Role of Halogen Atoms in Architecting Novel Non- Covalent Interactions

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Experimental observations conducted via rotational spectroscopy in cold, isolated free-jet expansions have recently uncovered novel behaviors in non-covalent interactions (NCIs). Specifically, ring perfluorination in arenes and aryl halides has been shown to significantly enhance regions of depleted electron density [1-4]. This technique has also characterized a divergence from established new trends in the complexes of fluoro-alcohols with water, while revealing substantial shifts in the conformational landscape of halogen-substituted carboxylic acids.

These high-precision findings are crucial for the interpretation of complex molecular systems, as they allow for a direct and synergistic integration with high-level quantum chemical calculations performed under identical isolated conditions. In this context, the experimental data serve as a fundamental benchmark, providing the necessary ground truth to test the accuracy of different theoretical models and functional treatments in describing subtle electronic effects. Such a rigorous comparison is essential to confirm the existence of regions of electron depletion classified as σ or π-holes which enable certain atoms or fragments to replace the traditional bridging proton in attracting electron donors.

Ultimately, the interplay between experimental evidence and theoretical validation advances our understanding of NCIs, which remain fundamental to a vast array of physical, chemical, and biochemical processes, as reflected in the extensive and growing body of literature in the field.

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-A O13-

Acid-Induced Plasticization on Cellulose Thin Films

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This study investigates the influence of coagulation bath pH on the structural and mechanical properties of microcrystalline cellulose (MCC) thin films prepared via a tetrabutylammonium hydroxide (TBAH) sol-gel route [1]. By modulating the bath pH between 3 and 5 using organic acids (Oxalic, Citric, and Acetic acids), we achieved control over the material's mechanical response.
As illustrated in the dynamic mechanical analysis (DMA) data (Figure 1), decreasing the coagulation pH leads to a significant increase in ductility. Notably, films regenerated at pH 3 exhibit an elongation at break of 9.4 ± 1.0%, a value comparable to nanocellulose papers [2]. This behavior is attributed to the entrapment of organic acid molecules within the cellulose matrix, which act as molecular plasticizers by increasing chain mobility. Structural analysis performed via X-ray scattering (SAXS/WAXS) shows slight variations in the crystallinity index at different bath pH. ATR-FTIR measurements confirm the entrapment of the organic acids in the matrix. Finally, the films were rinsed in water and measured via ATR-FTIR again, demonstrating the physical nature of this interaction. Despite their currently limited mechanical properties, these pH-tuned MCC thin films represent a prospective platform for sustainable aerospace coatings or substrates, where ongoing advances in nanofibrillation, cross-linking, and densification will unlock strengths competitive with composites, enabling future lightweight, low-CTE applications in space structures.

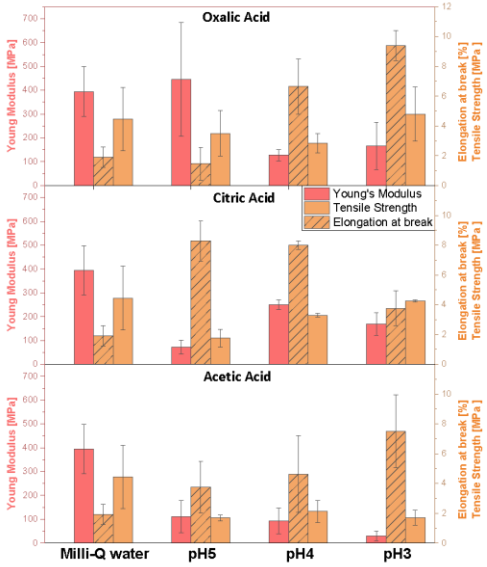

Figure 1. DMA measurements of different cellulose films fabricated in different coagulation baths.

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-A O14-

Structure-Property Relationships in Cellulose Acetate Composites Containing Microalgal Residues

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The development of bio-based polymeric materials from renewable waste streams represents an important challenge for sustainable materials science. In this work, cellulose acetate obtained from grapevine lignocellulosic residues was used as a polymer matrix for composite films incorporating exhausted microalgal biomass (*Chlamydomonas reinhardtii*) as a biofiller. The study builds on previous work of our group on cellulose acetate derived from grapevine waste and on the valorization of exhausted microalgal biomass in bio-based materials [1,2]. Films were prepared by solvent casting using glycerol as plasticizer and investigated to elucidate structure-property relationships in the resulting composites. Mechanical analysis shows that microalgal incorporation increases the breaking stress while maintaining Young's modulus and elongation at break essentially unchanged, indicating improved resistance without loss of flexibility. FTIR-ATR spectroscopy reveals intermolecular interactions involving cellulose acetate, glycerol, and biomolecular components of the microalgal residues, while UV-vis spectroscopy highlights the contribution of lignin chromophores and algal pigments to the optical properties of the films. DSC analysis shows a significant shift of the main degradation events toward higher temperatures, indicating enhanced thermal stability. SEM-EDX observations reveal that microalgal residues induce a more compact microstructure compared to the porous morphology of microalgae-free films. This structural organization results in increased surface wettability, reduced bulk water absorption, and higher water vapor and oxygen permeability, properties suitable for packaging applications requiring gas and moisture exchange. The results demonstrate that microalgal residues act as multifunctional biofillers capable of modifying intermolecular interactions, microstructure, and mass transport properties of cellulose acetate composites derived from biomass waste.

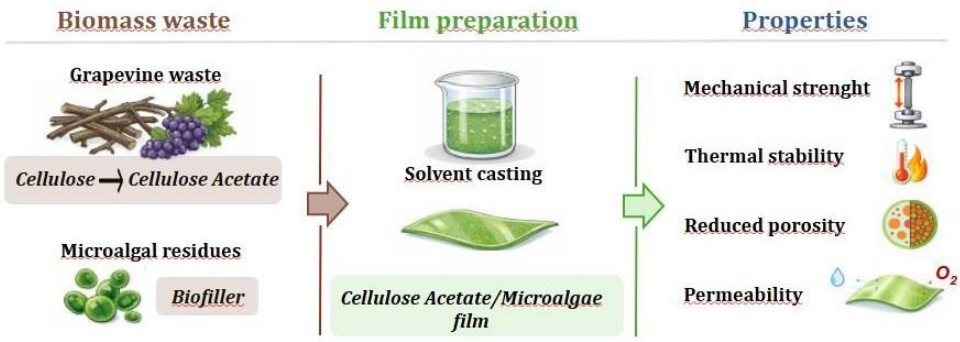

Figure 1. Microalgal biofillers tailor microstructure and mass transport in cellulose acetate films derived from lignocellulosic waste.

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-A O15-

Doping Strategies in Lead-Free Double Perovskites for X-Ray to NIR Photodetection

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Lead-free halide double perovskites are semiconductors that combine compositional tunability, solution-processability and improved stability with lower toxicity as compared to the Pb-based counterpart [1,2]. $Cs_2AgBiBr_6$ is a promising platform for radiation detection from visible light to X-rays. In this presentation, site-selective doping is discussed as a general strategy to tune charge generation, defect landscapes and carrier transport. Bi-site lanthanide doping and Cs-site substitution with small organic cations first demonstrate the broader potential of cation engineering: Eu-rich/Bi-poor growth and imidazolium incorporation markedly enhance X-ray sensitivity, while ammonium improves the photo-to-dark current ratio [3]. The focus is then shifted to noble-metal cations doping of $Cs_2AgBiBr_6$ single crystals with Au^{3+}, Pd^{2+} and Ir^{3+}. Low-level dopant incorporation preserves the cubic double-perovskite framework while modifying the electronic structure and extending the absorption edge from the visible region into the near-infrared (NIR). Optical characterization reveals redshifts up to ca. 1100 nm for Au- and Ir-doped crystals and up to ca. 1600 nm for Pd-doped crystals. Photodetection measurements show that Au doping provides the most balanced response, enabling stable NIR, visible and X-ray detection, including a fourfold increase in X-ray sensitivity compared with pristine crystals; Pd doping instead offers the broadest NIR coverage, but with a defect-mediated less efficient response [4]. Overall, these results show how controlled doping can transform $Cs_2AgBiBr_6$ from a visible/X-ray absorber into a broad-spectrum photodetection platform, with enhanced all-around properties while retaining structural and operational stability [3-4]. This will open new avenues for hybrid interfaces with organic functional dyes in (in)organic dye-perovskite composites.

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-A O16-

Engineering Metal-Organic Frameworks for Highly Nonlinear Photonics

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Upconversion is a process where two or more low-energy photons are converted into a single higher-energy photon. Among upconversion mechanisms, photon avalanche (PA) is the most nonlinear one, producing a sharp burst of emission once the excitation power exceeds a critical threshold. To date, PA has been observed only in lanthanide-doped inorganic crystals, where emission originates from electron accumulation in the 4f levels of lanthanide ions [1].

Metal-organic frameworks (MOFs) have been widely studied for their adsorption and catalytic activities [1]. Nonlinear optical properties of MOFs are more recent areas of research, so far mainly focused on second harmonic generation. Here, we show that lanthanide-based MOFs actively enable PA upon IR irradiation, unexpectedly generating a broad band/white emission. (Figure) The PA mechanism is fundamentally different from previously reported ones: the avalanche develops within the organic ligands. In this process, IR photons are first absorbed and upconverted through the cooperative action of lanthanide ions. The excitation energy is then funneled into a long-lived ligand state that acts as a reservoir, enabling electron accumulation and subsequent avalanche-like re-emission [2]. The observed nonlinearity is comparable to that of state-of-the-art inorganic PA crystals.

The synthetic strategy is highly versatile and generalizable, allowing the PA process to be coupled with diverse MOF [3-4]. This work vastly expands the family of materials capable of nonlinear optical responses. Moreover infrared-triggered photon upconversion in porous materials presents intriguing prospects for combined functionalities such as molecular sponge, energy harvesting and conversion.

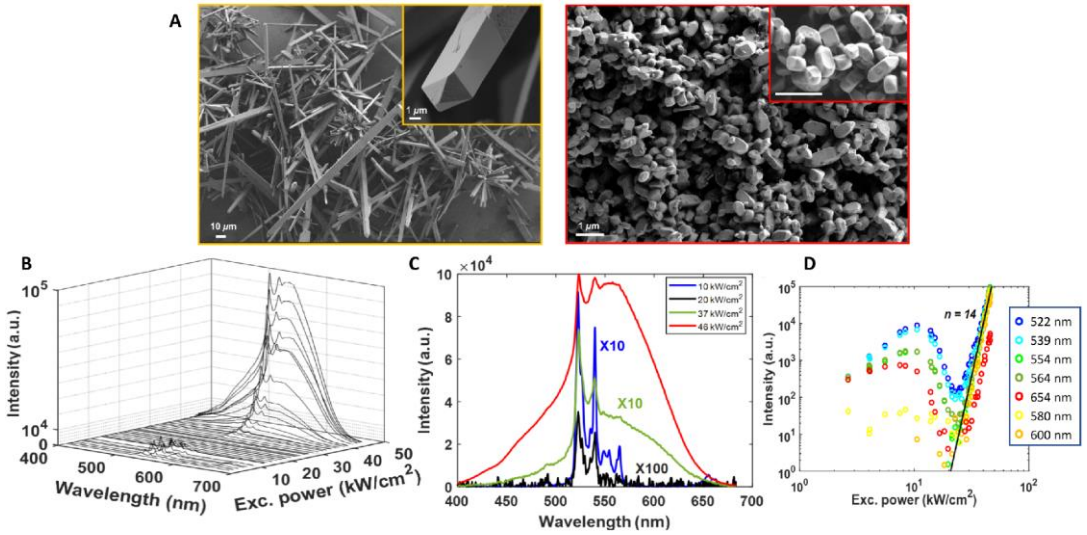

Figure. SEM images of PA MOFs(A); emission spectra upon IR irradiation (B, C); Intensity vs density power plot showing non- linear emission.

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-A O17-

Infrared-Activated Dynamic Crystals: Remote Motion in a Metal-Organic Framework

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Dynamic crystals are smart materials that respond to external stimuli with structural transformations that translate into shape and size changes, producing motion at the micrometer scale. They are promising candidates for soft microrobotics and memory devices and can be built from organic, biological or inorganic components [1,2]. Metal-Organic Frameworks (MOFs) are porous crystalline materials that have demonstrated structural and morphological flexibility [3-7].
Here we demonstrate the actuation of MOFs triggered by low-energy infrared (IR) radiation from a low-power laser (~100 mW) (Figure 1).

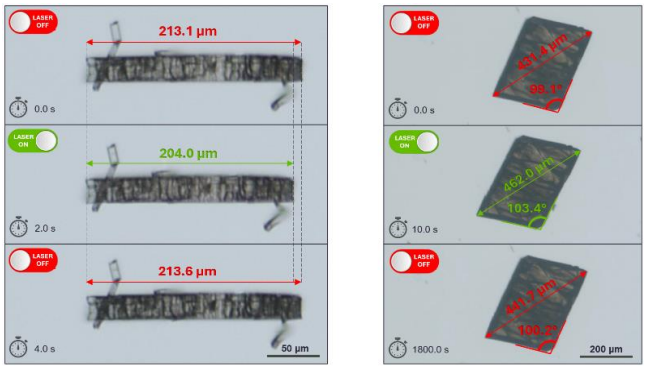

Figure 1. Optical microscopy images of lanthanide-based Metal-Organic Frameworks with and without IR laser irradiation.

The stimulus is user-tunable, spatially addressable, and potentially tissue-penetrating compared with commonly employed triggers. IR absorption arises from lanthanide ions forming the coordination nodes, producing a temperature increase that drives the phase transition. Notably, the introduction of additional lanthanide dopants enables upconversion energy transfer that activates non-radiative relaxation pathways, generating further localized heating and allowing the phase transition to occur at lower IR power densities.
The phase transitions induce microscopic motions, including crystal contraction, morphology changes, and jumping. These responses are reversible and repeatable over multiple cycles. The structural transformations underlying the dynamics were elucidated using complementary spectroscopic techniques, including in situ single-crystal X-ray diffraction under irradiation.
This strategy can be integrated into several MOF architectures, opening new opportunities for remotely controlled, low-energy crystal actuators.

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-A O18-

Persistent Luminescence Nanocrystals

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Persistent luminescence (PeL) is a peculiar optical phenomenon in which a material continues to emit light after the excitation source has been removed, i.e., it glows in the dark following proper excitation. Interest in PeL materials significantly increased in the 1990s after the discovery of $SrAl_2O_4:Eu^{2+}$, Dy^{3+}. To date, hundreds of different compositions are known to exhibit PeL, ranging from oxides to sulfides and fluorides. Some of these materials display intense and long-lasting emission, persisting for days or even weeks. Notably, several PeL materials have already found practical applications in everyday objects (e.g., toys, watches) and emergency signage. However, their widespread use is still limited by suboptimal emission performance. Moreover, from a fundamental perspective, the mechanisms governing PeL—especially in nanomaterials—remain poorly understood. Here, we present our results on the study of PeL nanomaterials, focusing in particular on halide perovskite nanomaterials and zinc–gallium–germanate compounds. The materials were prepared via a hot-injection method and hydrothermal processes, respectively. The as-synthesized compounds were first structurally characterized by X-ray diffraction and synchrotron analysis, and subsequently investigated through detailed spectroscopic measurements.
The results demonstrate that the decrease of the particle sizes induce changes in trap density, leading to either a decrease or an increase in PeL intensity. These changes may be induced by modifications in the oxidation state of the constituent elements (particularly the dopant) or by local structural distortions. Our findings contribute to a deeper understanding of how compositional and size tuning influence the PeL mechanism, suggesting possible strategies to enhance performance and thus improve practical applicability.

Acknowledgements. FL acknowledge the financial support by *Ministero dell'Università e della Ricerca*, bando FIS 3, Progetto FIS-2024-03509 – DELPHI, CUP: D53C25002460001.

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-A O19-

Bisphosphonates and Polyacrylates Control the Size and Assembly of Amorphous Magnesium-Calcium Phosphate Particles

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Calcium phosphate-based particles represent attractive materials for biomedical applications owing to their biocompatibility, sustainability, pH-responsive dissolution behavior, and compositional similarity to mineralized tissues [1]. Despite these advantages, precise control over particle size, colloidal stability, and crystallinity remains a significant challenge. This is especially relevant for amorphous calcium phosphate systems, which exhibit a pronounced tendency to aggregate from nanometric into micrometric assemblies and to undergo phase transformation toward more crystalline, thermodynamically stable forms [2,3]. Size control is indeed a crucial parameter as it influences biodistribution, cellular uptake, *in vivo* fate, dissolution kinetics and drug release profile.

In this contribution, we describe two strategies developed in our group to control the aggregation and stability of Amorphous Magnesium-Calcium Phosphate (AMCP) particles during synthesis, exploiting either molecular or polymeric stabilizers, *i.e.,* bisphosphonates and polyacrylates.

Bisphosphonates represent a promising molecular tool due to their strong affinity for calcium ions and phosphate-rich surfaces [4]. We investigated the effect of four different bisphosphonates -alendronate, zoledronate, neridronate, and ibandronate - during AMCP synthesis. These molecules, which differ in alkyl chain length and side-chain functionality, were selected to systematically evaluate how structural variations influence particle formation and the resulting physicochemical properties. Concerning polyacrylates, we explored the effect of polymer's molecular weight on the assembly of AMCP-based nanoclusters [5].

A common characterization approach was applied to both systems: particle size, morphology and phase evolution were analyzed through multiple physico-chemical techniques, including dynamic light scattering, electron microscopy, X-ray diffraction, infrared and Raman spectroscopy. The amount of stabilizing agent present within the particles was determined, along with particle redispersibility and stability over time under different conditions.

Taken together, the results show that both molecular and macromolecular stabilizers are effective in tuning the size and stability of AMCP, enabling reproducible solution processing and providing a rational, controllable platform for nanoparticle assembly.

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-A O20-

Structural and Magnetic Properties of Iso-Oriented Assemblies of Co–Zn Ferrite Nanoparticles

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Spherical assemblies of iso-oriented cobalt ferrite nanoparticles with high surface area were synthesized via a normal micelle approach [1]. First, a systematic variation of the cobalt content in cobalt ferrite (25%, 50%, and 75%) was investigated to assess its impact on structural organization. Subsequently, Co–Zn ferrites with varying Zn contents (20%, 50%, and 70%) were studied to further explore compositional effects on both structure and magnetic properties [2]. The primary $CoFe_2O_4$ nanocrystals (~7 nm) self-assemble into spherical, nanoporous aggregates with an average size of 50–60 nm.

Morpho-structural properties were investigated by X-ray diffraction (XRD), transmission electron microscopy (TEM), and N_2 physisorption, confirming the formation of highly crystalline nanocrystals organized into well-defined spherical mesoporous superstructures. Variations in cobalt content strongly affect the structural organization: decreasing cobalt content leads to a progressive loss of the iso-oriented order. In contrast, Zn-doped samples preserve both the spherical assembly and the overall structural organization, although noticeable changes in magnetic behavior are observed.

Magnetic characterization reveals that Zn incorporation primarily affects the saturation magnetization (M_s), due to modifications in cation distribution within the spinel lattice. Conversely, variations in cobalt content mainly influence the coercive field (Hc), reflecting changes in magnetic anisotropy, as further supported by Mössbauer spectroscopy.

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-A O21-

Study and Characterization of the Gold Nanoparticle's Formation Mechanism by Re- Irradiation of Linear Bromide Induced Gold Nanoparticle Chains

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One of the main characteristics of metal noble nanoparticles is the Localized Surface Plasmon Resonance (LSPR) which is strictly dependent on the morphology and environmental factors such as refractive index of the medium or the presence of halide ion that can lead to the formation of aggregates that can disrupt the plasmon resonance properties. In this work we present the study and characterization of gold nanoparticle's formation mechanism implied in the re-irradiation of bromide induced gold nanoparticles chains.
We start by producing Au nanoparticles (NPs) by pulsed laser ablation in liquid, and aggregating them using a bromide salt. Through UV-Vis absorption spectroscopy and electron microscopy, we observe the formation of aggregates made by particles larger than the initial ones [1]. As such aggregates are irradiated in resonance (532 nm) with their LSPR, at high fluence we observe fast aggregate disruption along with fragmentation, while at lower fluence we only observe slow aggregate disruption. Interestingly, by ceasing irradiation the NPs begin aggregating again (Fig. 1). By studying the kinetics of such process, using UV-Vis spectra, we determined a threshold fluence separating the two regimes. Irradiating far from resonance causes a much slower aggregation process, suggesting a plasmon driven phenomenon [2].

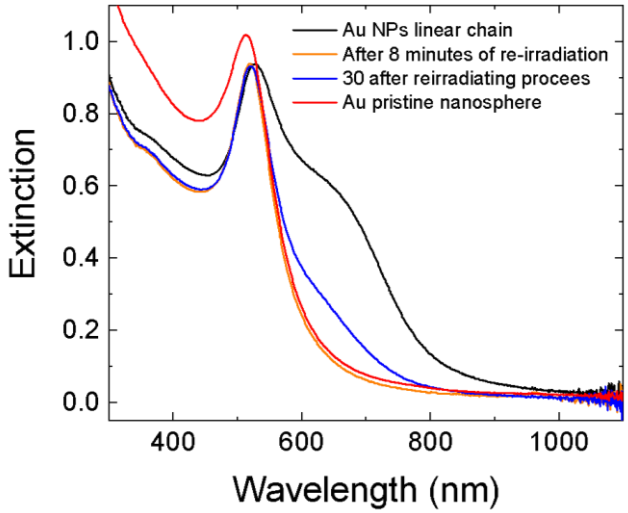

Figure 1. Absorption spectra from each step of our process: initial Au NPs (red line), aggregated NPs (black line), irradiated NPs (green line), aggregated NPs after ceased irradiation (blue line)

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-A O22-

Assembling Colloidal Emissive Nanocrystals into 3D Super-Architectures

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Progresses in colloidal synthesis enable the fabrication of metals nanoparticles (NPs), semiconductors quantum dots (QDs), and perovskites nanocrystals (NCs) with designed optical and electronic properties and promising implications across multiple technological domains. QDs and NCs are particularly interesting owing to their tunable electronic structure and photoemission behavior, making them ideal nano-building blocks for next-generation optoelectronic devices and quantum information systems [1]. One compelling approach to bridging the gap between individual nano-objects and functional devices lies in organizing them into ordered microscale assemblies called supercrystals (SCs), which preserve the nanoscale properties of their constituents while enabling collective phenomena [2]. Like atoms arranging themselves into a crystalline lattice, QDs and NCs can spontaneously organize into highly-ordered, periodic, 3D architectures during the assembly [3]. In the process, the organic ligands coating the QD/NC surface act as key mediators, with their mutual interactions guiding the geometry of the final assembly [3].
Here, slow destabilization approach in presence of an antisolvent is used as a bottom-up strategy for growing ordered assemblies of nanoparticles directly on solid substrates. The approach aims at producing macroscopic crystalline structures with well-defined facets and high internal order. CdSe QDs and $CsPbCl_xBr_{3-x}$ perovskite NCs, also doped with Mn, are used as nano-objects in model systems. The assembled structures are thoroughly characterized using confocal microscopy, electron microscopy, X-ray diffraction, and time-resolved optical spectroscopy, among other techniques, revealing pronounced differences in their assembly behavior, morphology, and optical response [4]. These findings provide key insights into how nanoparticle structure and capping ligands influence self-assembly pathways and the resulting optical behavior in supercrystals, establishing a foundation for the rational design of functional nanomaterial-based architectures with tailored properties for next-generation optoelectronic devices.

Acknowledgements. The Project “Network 4 Energy Sustainable Transition - NEST” (code PE0000021), funded under NRRP by the European Union - Next Generation EU; the PRIN 2022 project "SUPERNANO" (code 2022C7Z2RA) funded by the MUR, concession Decree No. 966 of 30.06.2023 of MUR and the COST Action CA21101 COSY supported by COST (European Cooperation in Science and Technology) are gratefully acknowledged.

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-A P1-

Bottom-Up and Top-Down Strategies for Emissive Silicates Nanocrystals

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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. These materials are characterized by an intense blue color and high stability over time [2]. Besides historical interest, the peculiar layered crystalline structure and their emission in the near infrared region (NIR), makes them interesting new compounds for optoelectronic applications [3]. The chromophore group is based on$[CuO_4]$ 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 [5].

This work presents our recent progress in the preparation of copper silicate-based 2D nanosheets with excellent colloidal stability. The synthesized nanoplates exhibit a well-defined morphology, with an average lateral diagonal of 30 nm and a thickness of 7 nm (Figure 1a). The homogeneity of the dispersions is further confirmed by cuvette absorbance measurements, where the nearly total absence of scattering demonstrates the high stability of the resulting suspensions (Figure 1b). In addition, the nanosheets retain the optical properties of the bulk material, featuring an excitation maximum at 618 nm and an emission peak at 950 nm (Figure 1c, 1d). This innovative synthetic protocol paves the way for a new class of 2D nanomaterials with promising applications: from biomedical imaging and photovoltaic energy conversion to IR light-emitting devices.

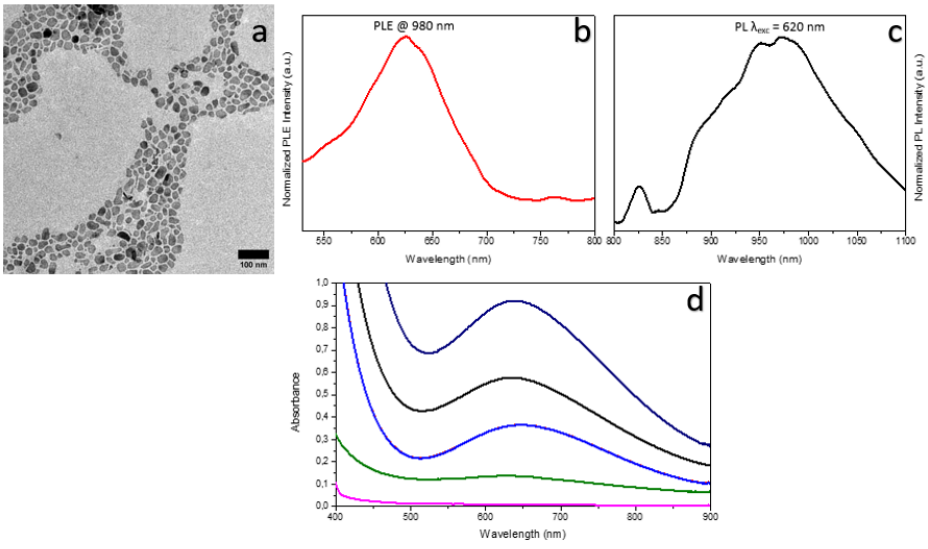

Figure 1. (a) TEM image, (b) PLE, (c) PL and (d) ABS spectra of $BaCuSi_4O_{10}$ nanoplates.

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-A P2-

Exploring Red/NIR TADF Emitters: the Effect of Different Donor Substituents

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Thermally activated delayed fluorescence (TADF) is a fascinating phenomenon observed in systems where the energy level of the lowest triplet states closely aligns with those of the lowest excited singlet state. When the dark triplet state becomes populated, either via intersystem crossing (ISC) following photoexcitation or directly via the injection of charges in a device, thermal energy may be sufficient to allow for a reverse ISC (RISC) process where population is transferred upwards from the triplet to the singlet. This TADF process yields long-lived (delayed) fluorescence, typically with lifetimes in the microsecond range [1]. TADF materials have attracted considerable attention for organic light-emitting diodes (OLEDs), as they can in principle achieve near-unity internal quantum efficiency by utilizing both singlet and triplet excitons [2]. Beyond optoelectronics, the long-lived TADF emission is of interest for time-resolved fluorescence imaging (TRFI), where lifetime-based contrast can improve detection sensitivity. In this context, developing TADF emitters operating in the red and near-infrared (NIR) spectral regions is particularly important. Red/NIR emission is highly desirable for biological imaging due to reduced light scattering, lower autofluorescence, and deeper tissue penetration [3]. However, achieving efficient TADF in this spectral range remains challenging, as the reduced energy gap is often associated with increased non-radiative decay pathways. Consequently, the design of red/NIR TADF materials represents a critical and actively evolving area of research [4]. In this study, three donor-acceptor-donor systems (*Figure 1*) were synthesized and spectroscopically characterized to examine how the nature of the donor units influences their emissive properties and their potential to act as red/NIR TADF emitters. UV-Vis absorption, steady-state and time-resolved fluorescence are collected at room and low temperature in solvents and matrices of different polarity. While BTZ-DMAC clearly exhibits TADF behavior, BTZ-AZ and DMAC-BTZ-AZ act as efficient emitters, particularly in the solid state, but show no experimental evidence of TADF. The experimental findings are supported by DFT/TDDFT calculations, which indicate that the singlet–triplet energy gaps of BTZ-AZ and DMAC-BTZ-AZ are too large to enable the TADF mechanism.

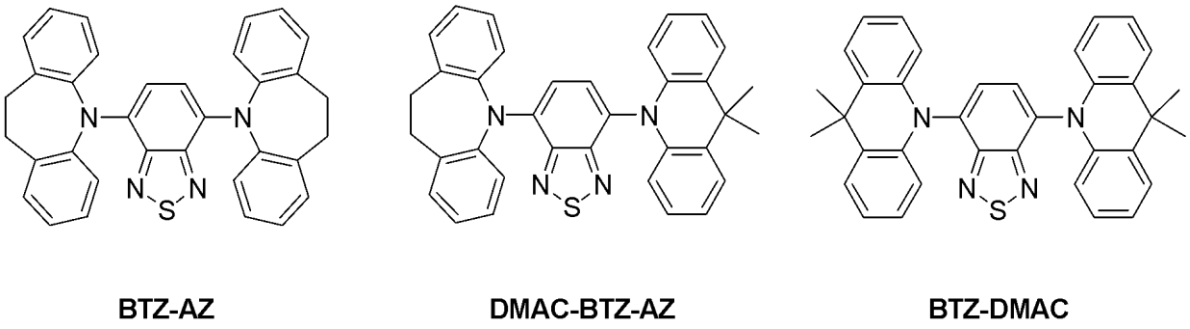

Figure 1. Structures of the donor-acceptor-donor systems.

[1] R. Dhali et al. Phys. Chem. Chem. Phys. 2021, 23, 378.
[2] J. Bauri et al. J Mater Sci 2021, 56, 18837.
[3] S. Qi et al. ACS Appl. Mater. Interfaces 2020, 12, 51293.
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-A P3-

Spectroscopic Study of the Behavior of Pyrocatechol Derivatives Regarding their Free Radical Scavenging Activity

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Free radicals are naturally occurring, highly reactive molecules possessing one or more unpaired electrons, capable of triggering damaging oxidative chain reactions within physiological cellular processes. This study investigates the quenching reaction between free radicals and pyrocatechol derivatives—serving as a fundamental model for di-phenolic analogues—to elucidate its underlying mechanism and kinetics through a multi-analytical approach using NMR, EPR, and UV-Vis Spectroscopies. Given the increasing interest from both the scientific community and the nutraceutical sector, understanding these interactions is vital for determining the effective radical-scavenging capacity of natural functional compounds [1].

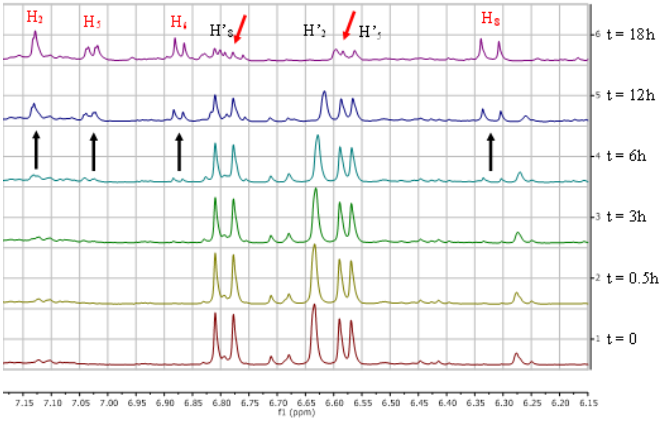

Figure 1. [1]H NMR time course following the completion of the pyrocatechol derivative-radical titration (6.15–7.15 ppm range). The disappearance of the oxidized species peaks (red arrows) and the reappearance of the pyrocatechol derivative peaks (black arrows) can be observed.

Our results demonstrate that the reaction is strictly dependent on the stoichiometric ratio of the reagents. The formation of transient radical species was observed through EPR measurements. Under conditions of radical excess, the reaction proceeds according to the widely accepted 2:1 (radical: derivative) stoichiometry. However, an excess of the pyrocatechol derivative triggers a reaction reversal, leading to the reformation of the starting compound from its oxidized form. Notably, in this scenario, the quenching efficiency increases significantly, with a single molecule of the derivative neutralizing more than two radical molecules. This suggests that the retro-transformation of the oxidized species is active throughout the process, effectively replenishing the antioxidant reagent (Figure 1). The identification of a non-stable equilibrium—characterized by a continuous exchange between oxidized and reduced forms—suggests a potentially autocatalytic reaction mechanism. These findings indicate that a simple direct titration is insufficient to fully characterize antioxidant capacity, requiring a more comprehensive investigation of reaction modes and operating conditions to accurately assess chemical reactivity.

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-A P4-

Self-Assembled Cobalt Nanochains for Magneto-Responsive Materials

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Magnetic nanochains (NCs) composed of strongly interacting single-domain nanoparticles offer unique opportunities for tailoring magnetic anisotropy and remanent magnetization (M_R) in nanoscale magnetic systems. In this study, we have investigated the controlled formation and magnetic behavior of cobalt nanochains assembled in the gas phase during the directed self-assembly of spark-ablated particles [1,2]. By tuning the external magnetic field distribution, chain alignment during deposition is modulated, promoting the transition from disordered aggregates to well-defined 1D architectures. We show that the morphology of these assemblies strongly dictates their magnetic response. Random nanoparticle clusters exhibit broad coercivity (H_C) distributions and weak anisotropy, whereas aligned NCs display pronounced uniaxial magnetic anisotropy and a ~100% increase in M_R due to enhanced dipolar coupling along the chain axis [1]. Post-assembly annealing leads to the formation of fused nanochains with significantly increased H_C (~+50%), reflecting the emergence of direct exchange interactions replacing dipolar-dominated reversal mechanisms. Magnetometry measurements, including angular-dependent remanence, and δm-plots, reveal the progressive evolution from magnetostatic to exchange-dominated behavior as chain order and interparticle connectivity increase. These findings highlight how nanoscale assembly governs overall magnetic interactions, enabling the design of highly anisotropic nanoarchitectures. As an application example, we show that these nanochains can be directly integrated into flexible polymers to produce magneto-responsive films (Figure 1) [2]. The ability to program morphology and magnetic properties on demand opens new pathways toward magnetic nanodevices.

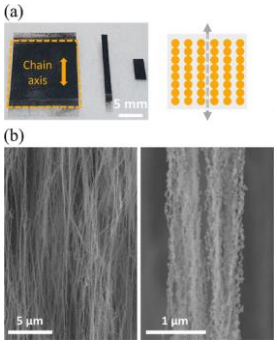

Figure 1. (a) Image of the magnetic soft film produced by directly integrating Co NCs onto polyolefin and a schematic depicting the chain orientation (axis) in the polymer layers. (b) SEM micrographs showing the formation of elongated structures composed of large bundles of NCs oriented along the in-plane magnetic field applied during the particle deposition, as schematically illustrated in (a).

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-A P5-

Extended Interfaces in Bi-Magnetic Nanoparticles: from Core–Shell to a Centre–Periphery Paradigm

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The magnetic properties of nanoparticles are governed not only by finite-size effects, but also by the internal spatial distribution of magnetically distinct regions (core, interface, and surface) whose relative contributions evolve strongly with particle architecture [1]. Such volumetric perspective reframes the interpretation of exchange coupling, spin canting, and dynamic freezing for the different possible magnetic nanocomposite systems. In this context, through a comparison of oxide bi-magnetic nanoparticles and metallic nanocomposites, the presentation will show that the conventional core–shell description is adequate for chemically sharp and spatially confined interfaces but breaks down when a magnetic interfacial region becomes volumetrically significant [2]. In the latter case a conceptual shift from a core–shell to a centre–periphery paradigm is not only justified but even required by the experimental results: according to such model, the extended interface can therefore be consistently described as a continuous gradient in magnetic structures and properties rather than a mere compositional discontinuity.

On this basis, the presentation reported here is not only to suggest a new paradigm for modeling systems of bi-magnetic nanocomposites systems with extended interfaces. In fact, is to shed light on how it is possible to reframe models (e.g. core-shell picture) not only by means of the indispensable and rigorous analysis of the experimental results but also working on the metaphorical frameworks and vocabulary adopted. It should be emphasized that such challenging focus of this research is developed through an interdisciplinary effort [3], bridging ‘hard’ sciences and the humanities, in order to refine ever more advanced and effective tools in the service of scientific inquiry and interdisciplinary dialogue.

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-A P6-

Ball Milling-Induced Structural and Magnetic Tuning in Hexaferrites

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The effect of ball-milling parameters on the structural, morphological, and magnetic properties of strontium hexaferrite (SFO) nanoparticles was systematically investigated. Among nanostructured materials, SFO, due to its low cost, excellent chemical stability, high coercivity, and high Curie temperature, has gained significant attention for practical applications such as permanent magnets [1]. SFO nanoparticles were synthesized via a sol-gel auto-combustion method [2] and subsequently subjected to different ball milling conditions by varying the milling time, ball-to-powder ratio (BPR), and milling speed to optimize the processing parameters. The Rietveld refinement of X-ray powder diffraction (XRPD) data showed a significant reduction in crystallite size from ~80 nm to ~20 nm with increasing milling time, indicating the effectiveness of the mechanical comminution process. Transmission electron microscopy (TEM) was employed to further determine the nanoparticles' size and morphology, supporting the structural analysis. Magnetic characterization performed using a vibrating sample magnetometer (VSM) revealed a continuous decrease in coercivity (H_c) from ~0.56 T to 0.21 T and reduced remanence value (M_r/ M_s^{2T}) from ~ 0.5 to 0.3, as milling time increased, which is attributed to particle size reduction and the associated modification of domain structure and magnetization reversal. These results demonstrate a clear correlation between particle morphology, crystal structure, and magnetic properties at the nanoscale, highlighting the strong impact of mechanical processing on functional magnetic behavior.

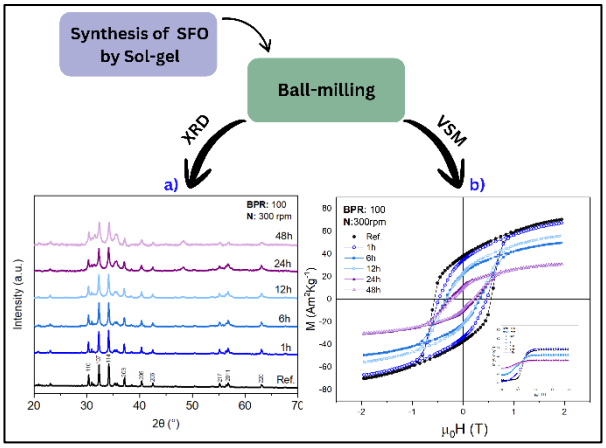

Figure 1. a) XRPD patterns; b) Magnetization (M) vs. applied field (H), for milled SFO samples with BPR:100, N:300 rpm.

[1] A. Davoodi et al. J. All. Compd. 2012, 512, 179.
[2] P. Maltoni et al. Sci. Rep. 2021, 11, 23307.

-A P7-

Enhancing Triplet Formation and Charge-Separated States Through Ultrafast Insights

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Enhancing triplet-state formation in organic chromophores is key to improving materials for TADF, long-lived charge separation, and photocatalysis. In this context, ultrafast spectroscopy provides crucial insight into the earliest excited-state events, revealing how photoexcitation is directed toward intersystem crossing, charge separation, or delayed emission. The four studies considered here highlight complementary molecular strategies (Figure 1) to achieve this goal. In phenothiazine-dibenzothiophene-S,S-dioxide donor-acceptor dyads, triplet formation and delayed fluorescence are governed by the balance between charge-separated and locally excited triplet states, showing that TADF is controlled mainly by state energetics and spin-vibronic coupling rather than by a simple heavy-atom effect [1]. In compact rhodamine–naphthalenediimide D-A-D systems, ultrafast charge separation followed by the formation of long-lived triplet charge-separated states demonstrates how molecular architecture and donor–acceptor coupling can extend excited-state lifetimes [2]. In pyrazole- and triazole-fused perylene bisimides, changing the redox state from neutral to dianionic switches the system from strong fluorescence to efficient intersystem crossing and long-lived triplet formation, underlining the importance of electronic structure and charge state [3]. Finally, perylenebisimide-TEMPO dyads show that attaching a stable radical directly enhances triplet population through spin dipolar and exchange interactions, providing a clear example of radical-enhanced ISC as a spin-engineering strategy [4].

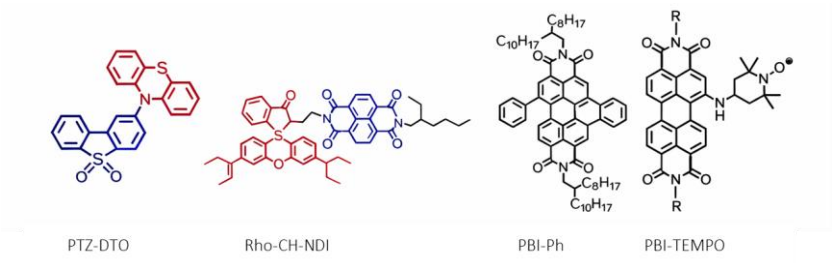

Figure 1. Molecular structures.

Together, these studies show that triplet enhancement can be achieved through multiple mechanisms, including D-A energetics, linker-controlled charge separation, redox-state tuning, and radical-induced spin interactions. Combined ultrafast and time-resolved spectroscopies reveal that efficient triplet design in organic systems requires simultaneous control of molecular geometry, electronic coupling, and spin dynamics. Mastering how triplets are populated and converted into function is therefore emerging as a general strategy for next-generation organic photochemistry.

[1] Y. Pei et al. Chem. Sci. 2025, 16, 19737.
[2] B. Tharmalingam et al. Phys. Chem. Chem. Phys. 2026, 28, 365.
[3] W. Feng et al. Chem. Eur. J. 2026, e70788.
[4] Z. Li et al. Pure Appl. Chem. 2026, 98, 115.

Session B

Theory, Modelling, and Data-Driven Physical Chemistry

-B O1-

Coarse Graining Photo-Isomerization Reactions: Thermodynamic Consistency and Implications for Molecular Ratchets

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We formulate thermodynamically consistent coarse-graining procedures for molecular systems undergoing thermally and photo-induced transitions [1]: starting from elementary vibronic transitions, we derive effective photo-isomerization reactions interconverting ground-state species. Crucially, the local detailed balance condition, that constrains reaction kinetics to thermodynamics, remains satisfied throughout the coarse-graining procedures. It applies to the effective photo-isomerization reactions just as it does to the elementary vibronic transitions. We then demonstrate that autonomous photo-driven molecular ratchets operate via the same fundamental mechanism as chemically driven ones. Because the local detailed balance remains satisfied, autonomous photo-driven molecular ratchets, like chemically driven ones, operate exclusively through an information ratchet mechanism. This reveals that their design and optimization should prioritize molecular properties governing the information ratchet mechanism, rather than those influencing energetic bias.

[1] F. Avanzini et al. J. Chem. Phys. 2025, 163, 134122.

-B O2-

Multiscale Molecular Dynamics for Probing Second-Timescale Protein Conformational Changes: The SHP2 Activation Case

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The SHP2 phosphatase acts as a central node in several pathways and is implicated in multiple cancers; blocking its activity can inhibit tumor progression [1]. SHP2 comprises a catalytic domain (PTP) and two SH2 domains, which are responsible for binding partners containing phosphotyrosine (pY) and for controlling its enzymatic activity. In its basal state, the N-SH2 domain occludes the PTP catalytic site, keeping SHP2 inactive; upon binding cognate proteins, a significant conformational rearrangement occurs, leading to enzyme activation. Many oncogenic mutations promote activation by destabilizing this autoinhibited conformation [2]. Despite the availability of structural data for both inactive and active forms, the activation mechanism of SHP2 is still not fully clarified [3]. Molecular simulations could help shed light on this process; however, the slow timescale of the transition (on the order of seconds) makes it difficult to study with conventional approaches. In this work, we report results obtained using enhanced sampling techniques (such as REMD and metadynamics), coarse-grained molecular dynamics simulations, and their integration, on both SHP2 alone and in the presence of peptides bound to its SH2 domains. These methods allowed us to characterize putative activation pathways.

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[2] G. Bocchinfuso et al. Proteins 2007, 66, 963.
[3] P. Calligari et al. Comput. Struct. Biotechnol. J. 2021, 19, 6125.

-B O3-

When Molecules Communicate: Entropy Production as the Thermodynamic Cost of Molecular Information Transfer

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Information transfer in molecular systems is traditionally described in terms of concentration variations of a chemical messenger propagating through a fluidic medium. In this work we propose a complementary thermodynamic perspective in which the act of communication is interpreted as an irreversible physical process characterized by entropy production. In such a framework, the transmission of a molecular symbol corresponds to a controlled perturbation of local equilibrium generated by the release of a messenger molecule from a transmitter (TX), its transport through a channel (CH), and its interaction with a receiver (RX). The transport of the messenger establishes a gradient of chemical potential that drives a diffusive flux. Within the formalism of nonequilibrium thermodynamics, each flux is associated with a thermodynamic force and generates local entropy production. As a consequence, the propagation of a molecular signal is intrinsically dissipative: information transfer cannot occur without entropy generation. In this view, the receiver does not simply detect the concentration of the messenger but experiences a transient irreversible evolution toward a new chemical state. The entropy produced during this transition therefore provides a physical signature of the reception event.
We show that the total entropy production associated with a molecular symbol can be expressed as the integral of the product between flux and thermodynamic force along the transmission pathway. This quantity represents the thermodynamic cost of information transfer and establishes a direct link between molecular communication and nonequilibrium transport theory. By solving the corresponding constrained optimization problem, we derive the optimal release profile of the messenger that minimizes entropy production while preserving the irreversibility required for signal detection.
This perspective opens a bridge between information theory and the thermodynamics of dissipative transport, suggesting that entropy production can serve as a fundamental observable for quantifying the physical cost and efficiency of molecular information transfer in complex fluid environments.

Acknowledgements. This work was supported by the European Union's Horizon Europe research and innovation programme under the EIC Pathfinder Open project ERMES – Information Transfer Between Medical Doctors and Implanted Medical Devices via Artificial Molecular Communication (Grant Agreement No. 101185661).

-B O4 -

The Perfect Couple: a Critical Analysis of CAM-B3LYP/SMD for Alcohol pKa Prediction

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Alcohols are ubiquitous compounds in both, biological systems and industrial applications. They play essential structural and functional roles in various contexts, such as in protein and carbohydrate chemistry as well as in industrial catalytic and reactor processes. Determination of their acid dissociation constant (pKa) is pivotal, as it directly affects compounds, solubility, bioavailability, membrane permeability, and other physicochemical characteristics which are fundamental for biological applications. However, the fact that their pKa is very close to that of water makes its predictability very difficult to achieve. Consequently, considerable efforts have been devoted to developing both, experimental and computational methodologies, for reliable pKa prediction [1]. Yet, achieving a consistent and accurate approach to compute the acid dissociation constant remains a long-standing challenge in computational chemistry [1]. Several studies have recently appeared in the literature aiming to find-out reliable and computationally efficient procedures, but these are often tailored to specific classes of compounds [1]. Recently, we proposed an "easy-to-use" approach for computing the pKa and pKb of different organic acids and bases. This method is based on atomic descriptors, and it aims to achieve a MAE below 0.5, without the need for post facto corrections. It combines a density functional theory (DFT) using a moderately demanding functional (CAM-B3LYP), the solvation model based on density (SMD), and a not diffuse basis set, 6-311G+(d,p) [2-4]. A rational attempt to clarify the reason beneath the remarkable reliability of CAM-B3LYP in combination with SMD will be presented, focusing on the computational pKa determination of alcohols as case study.

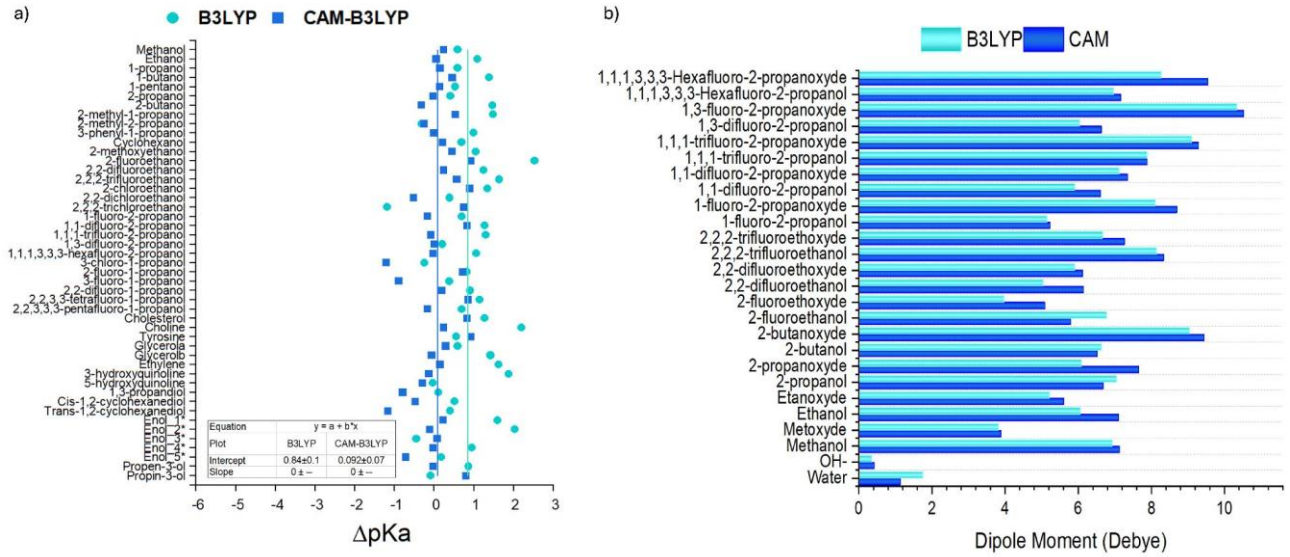

Figure 1. Panel a: DpKa graph of the values computed by B3LYP or CAM-B3LYP with respect to the average values. Panel b: dipole moment analysis of B3LYP and CAM-B3LYP values. Geometry was optimized keeping constant the basis set 6-311G+(d,p) and SMD as solvation model.

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[2] Pezzola et al. Molecules 2022, 27, 8590.
[3] Pezzola et al. Chem. Eur. J. 2024, 30, e202303167.
[4] Pezzola et al. J. Phys. Chem. A 2026, 130, 1607.

-B O5 -

Machine Learning and Data Fusion Strategies for the Investigation of Hofmeister Effects in Polysaccharide Systems Combining IR Spectroscopy and Thermal Analysis

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Specific ion (Hofmeister) effects strongly influence the physicochemical properties of macromolecular systems, affecting aggregation, conformation, and thermal behavior. However, their interpretation remains challenging due to the complexity of ion–macromolecule and solvent–macromolecule interactions [1]. This work presents a proof-of-concept study in which machine learning-based chemometric tools and data fusion strategies are applied to the classical physicochemical problem of interpreting complex results associated with Hofmeister effects [2]. Guar gum (GG) aqueous dispersions in the presence of kosmotropic and chaotropic cosolutes were investigated by combining ATR-FTIR spectroscopy and thermogravimetric analysis (TGA). Principal Component Analysis (PCA) applied to the individual datasets enables the unsupervised detection of ion-specific trends, highlighting the spectroscopic and thermal features that drive the differentiation according to the Hofmeister series. In particular, ATR-FTIR results reveal that GG structures the water network into distinct hydrogen-bonding populations, whose distribution is oppositely affected by kosmotropic and chaotropic ions. PCA on thermogravimetric profiles—especially through derivative analysis—identified changes in the dehydration behaviors arising from differences in water binding and release dynamics. The implementation of a mid-level data fusion approach based on the Common Dimensions (ComDim) algorithm results in a clearer sample differentiation according to the kosmotropic/chaotropic character of the cosolutes (Figure 1). Moreover, the analysis of saliences and loadings allows the identification of the relative contribution of each technique and of the key variables responsible for the observed clustering. Overall, this work demonstrates the potential of data-driven multiblock strategies for the investigation of ion-specific effects, offering a framework that can be extended to different macromolecular systems, cosolutes, and analytical techniques to advance the understanding of ion–macromolecule interactions in soft matter.

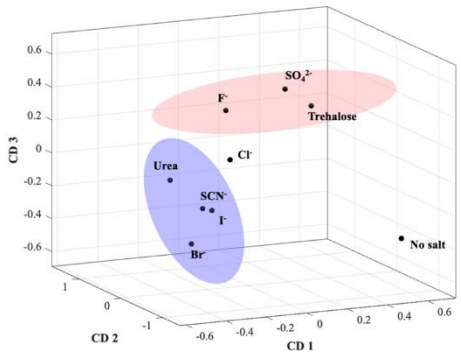

Figure 1. ComDim score plot obtained from the ATR-FTIR and TGA merged dataset.

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[2] A. Jakubowska et al. J. Chemom. 2019, 33, e3187.

-B O6-

Generating Molecules with Artificial Intelligence without Databases

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One of the central challenges in chemistry is the design of molecules with tailored properties, the so-called molecular inverse design (ID) problem. Addressing this challenge has profound implications across catalysis, drug discovery and, of course, energy harvesting.[1,2] Traditional data-driven machine learning approaches have shown promise in exploring chemical spaces (CSs), but remain fundamentally limited by the need for large, high-quality datasets and costly pre-training procedures.[3,4] In this talk, I will present a novel data-free framework for molecular ID (see Figure 1) that integrates deep reinforcement learning (RL) with quantum chemistry (QC) calculations, enabling the on-the-fly generation and evaluation of molecules without any reliance on pre-existing datasets.[5] As a proof of concept, we applied this approach to toy models targeting ground- and excited-state molecular properties. Our RL-QC engine efficiently explores large CSs using first-principles chemical rewards, converging rapidly to optimal candidates and solving the ID problem within known CSs. This promising strategy represents a conceptual shift toward quantum-driven AI for molecular discovery.

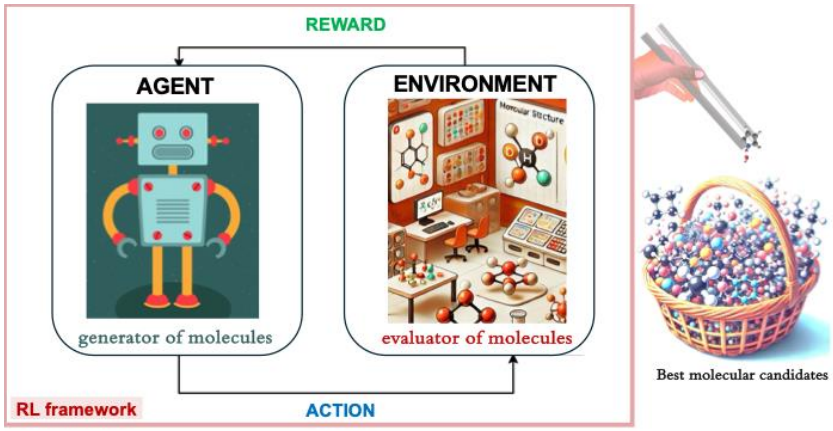

Figure 1. Reinforcement learning framework for molecular inverse design.

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-B O7-

Atomistic Insights into Hole Injection at Multi-Cation Perovskite/HTL Interfaces

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Lead halide perovskites (LHPs) are among the most promising materials for next-generation optoelectronic devices owing to their tunable band structure and long carrier diffusion lengths. Compositional engineering through the incorporation of multiple A-site cations—such as methylammonium (MA^+), formamidinium (FA^+), and cesium (Cs^+)—has proven effective in simultaneously improving device efficiency, thermal stability, and environmental robustness. Despite these advances, device performance is strongly influenced by interfacial processes, where the electronic structure alignment and charge-transfer kinetics at the perovskite/charge-transport-layer boundary govern both efficiency and operational stability.

In this work, density functional theory (DFT) calculations are employed to investigate the interfaces between selected hole transport layers (HTLs) and lead halide perovskite surfaces with di-cation [1] and triple-cation [2] compositions (Figure 1). The results indicate that FA^+ and Cs^+ enhance interfacial adhesion, while all investigated interfaces exhibit thermodynamically favorable charge transfer. Larger driving forces are observed for di-cation surfaces and PbX_2-terminated interfaces. Through the combined analysis of electronic coupling, projected density of states (p-DOS), and HTL HOMO contributions, the perovskite electronic states responsible for interfacial charge exchange are identified. The calculations predict ultrafast hole injection dynamics occurring on the femtosecond timescale. Interestingly, cesium atoms play a dual role: besides improving structural stability, it acts as an interfacial anchoring site that promotes efficient hole transport pathways. Its higher surface exposure in di-cation systems further accelerates charge-transfer dynamics. These findings provide atomistic insight into interfacial processes in modern LHP–HTL heterostructures and suggest strategies for optimizing device performance through compositional tuning, surface termination control, and interface engineering.

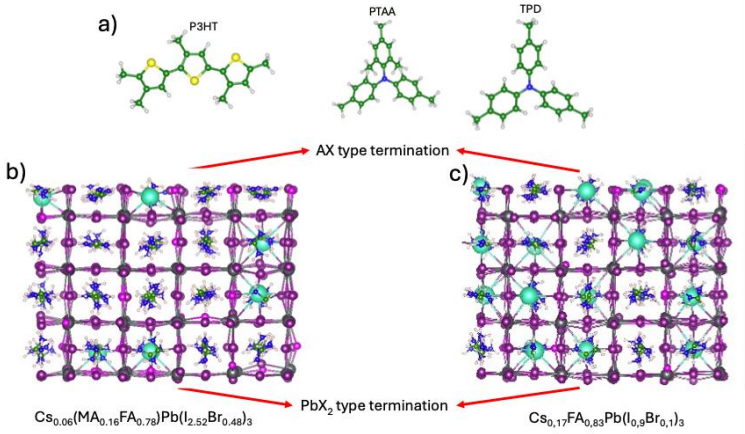

Figure. 1. Evaluated interfaces: a) hole transport materials b) tri-cationic, and c) di-cationic LHP slabs.

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-B O8-

From Electronic Structure to Nonradiative Pathways in INVEST Emitters: a Combined Electronic-Structure and Quantum-Dynamics Perspective

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In the last years, an increasing number of fully organic molecules capable of thermally activated delayed fluorescence (TADF) have been reported, often with very small or even inverted singlet-triplet (INVEST) energy gaps [1]. These molecules have the potential to fully harvest non-emissive triplet states, potentially overcoming the spin-statistical limitations of OLEDs. However, many molecular systems showing a negative ΔE_{ST} suffer from both a vanishing Spin-Orbit Coupling between the lowest singlet (S_1) and triplet (T_1) excited states and high energy differences with higher-lying singlet and triplet excited states, precluding their involvement in the spin conversion process [2].
In our works [3, 4] we proposed a new design strategy entailing the extension of the triangulene cores by connecting two INVEST triangulene units to form Uthrene- and Zethrene-like systems, doped with N and B atoms (Figure 1). A detailed inspection of the resulting molecular orbital distribution allowed rationalizing the electronic structure properties obtained employing wavefunction-based methods (NEVPT2, EOM-CCSD, SCS-CC2), showing how the Uthrene-like architecture can give origin to the energy proximity between the lowest singlet and triplet excited states, in some cases leading to their energy inversion. By using Fermi's Golden Rule and developing a computationally efficient quantum-dynamics protocol capable of treating quasi-full vibrational spaces, we evaluate the non-radiative rates for direct and indirect conversion pathways, including $T_1 \rightarrow S_1$, $T_1 \rightarrow S_2$, and $S_2 \rightarrow S_1$ processes. Feeding a kinetic model with such rate constants, we showed how the Extended INVEST (X–INVEST) design strategy can open new pathways to boost the spin conversion process and the population of the emissive S_1 excited state.

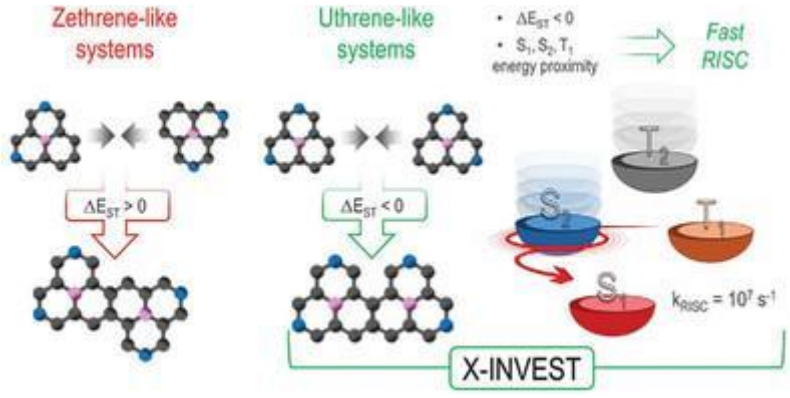

Figure 1. Schematic representation of the effects of extending the triangulene cores.

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-B O9-

First-Principles-Based Insights into Adsorption and Reactivity of Na^+ Salt and Room-Temperature Ionic Liquids at Sodium Metal Surface

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Recently, sodium metal batteries have attracted significant attention due to their higher theoretical capacities compared to conventional metal-ion systems. However, the use of sodium metal anodes with conventional organic electrolytes suffers from persistent challenges, including dendrite formation and unstable solid-electrolyte interphase (SEI) layers. Therefore, the choice of electrolyte plays a critical role in improving battery stability and performance. A promising alternative is represented by Room Temperature Ionic Liquid (RTIL), owing to their high thermal and electrochemical stability and favorable ionic conductivity. Here we present state-of-the-art density functional theory (DFT) calculations and ab initio molecular dynamics (AIMD) simulations to study early-stage SEI formation at the Na(110)/electrolyte interface. We investigate the interactions of RTILs containing N-methyl-N-propylpyrrolidinium (PYR_{13}^+) cation with bis(fluorosulfonyl)imide (FSI^-) and bis(trifluoromethanesulfonyl)imide ($TFSI^-$) anions ($PYR_{13}FSI$ and $PYR_{13}TFSI$), and the corresponding sodium salts NaFSI and NaTFSI. PYR_{13}^+ interacts weakly with Na(110) and remains structurally intact in both RTILs, while the anions display distinct interfacial behaviors depending on electrolyte environment. FSI^- both in RTIL and salt interacts strongly with the Na(110) surface and undergoes rapid spontaneous dissociation during structural relaxation at 0 K. AIMD simulation at 298 K shows that In $PYR_{13}FSI$, cleavage of S-F bonds yields $N(SO_2)_2$, whereas NaFSI follows a stepwise pathway involving S-F and N-S bond breaking, producing NSO_2 and SO_2 fragments. The detached F atoms exhibit high mobility and migrate into the Na(110) subsurface layers. In contrast, $TFSI^-$ in RTIL and salt is comparatively more stable, without any spontaneous dissociation at 0 K. At 298 K, $PYR_{13}TFSI$ shows delayed decomposition, whereas NaTFSI undergoes earlier fragmentation initiated by S-C bond cleavage and subsequent CF_3 defluorination. Both the anions show higher interfacial reactivity in salt environment than in RTIL. Overall, for both anions, NaF emerges as the dominant SEI product, known to contribute to SEI stabilization. These results highlight the crucial role of anion chemistry and electrolyte environment in governing SEI precursor formation on sodium metal.

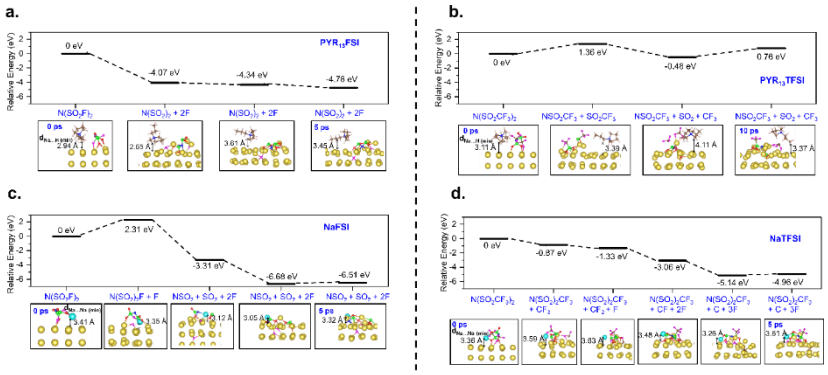

Figure 1. Anion decomposition pathways for (a) $PYR_{13}FSI$, (b) $PYR_{13}TFSI$, (c) NaFSI and (d) NaTFSI.

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-B O10-

Atomistic Modelling of Hydroxyapatite Surfaces: from Biomolecular Adsorption to Environmental Catalysis

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Hydroxyapatite (HA, $Ca_{10}(PO_4)_6(OH)_2$) is an exceptionally versatile material that has attracted considerable interest across multiple research domains. Owing to its intrinsic biocompatibility, tunable acid–base surface properties, and ion-exchange capability, HA has been widely investigated in biomedical applications, including biomaterials and drug delivery systems. In this context, its surfaces have been extensively studied for their interactions with biologically relevant species, ranging from water molecules to amino acids and large biomacromolecules such as collagen, providing fundamental insight into adsorption phenomena at the bio-inorganic interface [1,2]. These characteristics, together with the possibility of tailoring its composition through cation substitution, make hydroxyapatite a flexible platform for the design of functional materials.

More recently, HA has also emerged as a promising material for sustainable environmental applications. Its non-toxic nature, high adsorption capacity, chemical stability, and the possibility of being synthesized from natural or waste-derived resources within a circular economy framework make it particularly attractive for the mitigation of environmental pollutants. To this end, copper-modified HA models are considered to enhance catalytic activity while preserving the structural integrity of the material [3,4].

Building on our previous computational investigations of biomolecule-surface interactions, here we extend the study of hydroxyapatite surfaces to environmentally relevant catalytic systems. A periodic quantum-mechanical approach is employed to investigate the interaction between small reactive molecules (CO, NO, N_2O, NH_3…) and the most stable HA facets, namely (001), (010), and (101). Both pristine and Cu-substituted models are considered to evaluate the effect of cation substitution on the structural and electronic properties of the surfaces, while the influence of water is explicitly taken into account in comparison with available experimental observations. The analysis of structural, energetic, and vibrational features provides atomistic insight into the mechanisms governing molecule-surface interactions.

Beyond adsorption phenomena, the computational framework also enables the exploration of surface reactivity and elementary catalytic steps. In this perspective, the integration of machine-learning interatomic potentials and automated reaction exploration tools will allow the efficient screening of reactive pathways and the investigation of complex catalytic mechanisms at extended time and length scales [5]. Overall, the combined quantum-mechanical and machine-learning strategy provides a powerful platform for the rational design of hydroxyapatite-based catalysts and highlights the potential of this material as a sustainable platform for environmental catalysis.

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-B O11-

A New Method to Characterize the Porosity of Materials: Distribution of Nanoporous Volume, Specific Surfaces and Prediction of Gas Adsorption

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Nanoporous materials are essential for many technological applications and the characterization of their textural properties, like porous volume distribution and accessible surface area (ASA), is of paramount importance, also as a guiding tool to design new materials.
DFT fitting of experimental N_2 isotherms, nowadays the most used method for porous volume description, is based on pores of regular shapes, not fully suitable for amorphous materials like carbons. BET model, largely used to estimate ASA, is also based on a simplified model of surface, sometimes poorly performing, especially for microporous samples.

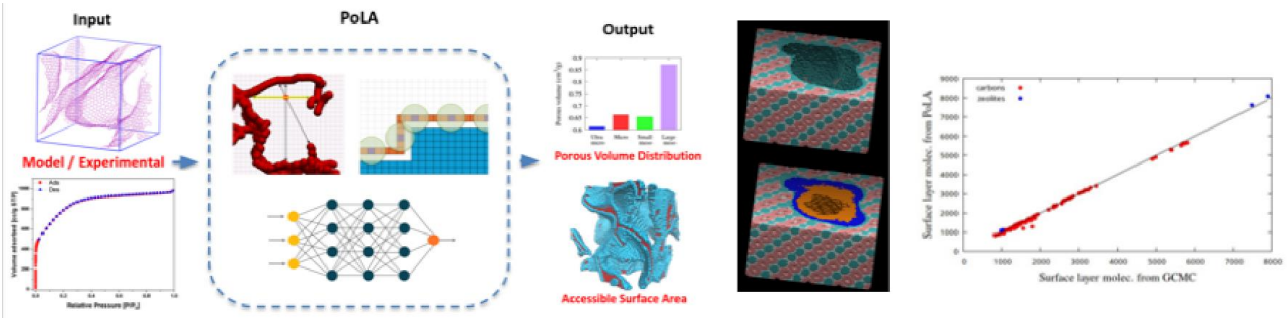

Figure 1. Left: a graphical representation of the algorithm applied to either an atomistic model or an experimental isotherm; center: microporous and mesoporous local volumes; right: ASA computed by PoLA vs. simulations.

Here we present a novel approach, called Porosity Local Analysis (PoLA), to provide an accurate and physically sound description of the porosity on atomistic models and real samples.
PoLA generates a reliable porous volume distribution (PVD) closely associated with host–guest interactions.and thus to the gas adsorption processes: we show that PoLA is able to predict the adsorption isotherms of several gases. Using a Machine Learning algorithm, specifically trained for PoLA results, we can apply the method also to real materials: starting from the N_2 adsorption isotherm, the method provides the PVD and also predicts accurately the H_2 isotherm.
The same approach can be used to define the ASA with great accuracy, in strict agreement with the results of accurate Monte Carlo simulations; also in this case, a Machine Learning algorithm allows the application to real materials as well as to atomistic models.

-B O12-

Computational Exploration of Derivatized Cyclodextrin-Based Drug Delivery Systems

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Cyclodextrins (CDs) are cyclic oligosaccharides composed of α-D-glucopyranose monomers linked by α-(1,4) glycosidic bonds, forming a truncated cone-shaped cavity capable of hosting a wide variety of guest molecules. Owing to their ability to form inclusion complexes with numerous substrates, CDs have attracted significant interest in drug delivery systems (DDS) [1], where both native and chemically derivatized forms are widely used to enhance the solubility, stability and bioavailability of pharmaceutical compounds. Among the most commonly employed derivatives are methylated and hydroxypropylated cyclodextrins, which serve as important functional excipients in pharmaceutical formulations [2-4].
However, derivatized CDs represent structurally heterogeneous systems characterized by a very large number of possible substitution patterns, which makes their computational modelling particularly challenging. To address this issue, we developed an automated multistep workflow for the generation and optimization of derivatized cyclodextrin structures starting from the native macrocycle. Substitution patterns corresponding to fixed degrees of functionalization were generated using the stk Python module[5], enabling the systematic construction of methylated and hydroxypropylated derivatives without introducing operator bias. In this framework, candidate structures are generated statistically and subsequently ranked according to their energetic stability.
In particular, hydroxypropyl-β-cyclodextrin (HPβCD) was systematically investigated by considering the most commonly encountered degrees of substitution, ranging from DS = 3 to DS = 11, corresponding to 3–11 hydroxypropyl groups distributed over the 21 available hydroxyl sites of the β-cyclodextrin scaffold. This approach allows the exploration of a representative portion of the substitutional landscape associated with commercially relevant materials.
The resulting structures undergo an initial geometry optimization at the GFN2-xTB [6] level to efficiently explore the conformational landscape, followed by re-optimization of the lowest-energy candidates using the composite r²SCAN-3c [7] method to obtain more accurate geometries. This automated strategy enables an efficient exploration of the large combinatorial space associated with derivatized CDs while producing representative host structures suitable for computational studies.
The generated library of native and derivatized cyclodextrins provides a versatile platform for investigating host–guest interactions with a wide range of molecules, including pharmaceutical compounds such as melatonin, caffeine, curcumin and vemurafenib, as well as small gaseous molecules (CO_2, CO, SO_2, H_2S, H_2 and CH_4). Beyond the characterization of structural conformations and energetic stability, these host structures will also be employed in equilibrium and non-equilibrium molecular dynamics simulations to investigate the kinetics of encapsulation and release, providing insights into the mechanisms governing controlled release processes in cyclodextrin-based delivery systems.

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-B P1-

First-Principles Study of Non-Fullerene Molecular Electron Transport Materials for Perovskite Solar Cells

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The rapid development of perovskite solar cells (PSCs) requires efficient and stable electron transport layers (ETLs). In these devices, the electron transport material plays a key role by extracting electrons from the perovskite absorber, transporting them to the electrode and blocking holes, thereby reducing charge recombination. In the promising inverted p–i–n architectures, ETLs often rely on transparent organic semiconductors, particularly fullerene derivatives. However, fullerene-based ETLs suffer from limited tunability of energy levels, morphological instability and costly synthesis, motivating the exploration of non-fullerene alternatives. Among molecular frameworks widely investigated in organic electronics, diketopyrrolopyrrole (DPP) and isoindigo (II) derivatives are particularly attractive owing to their strong electron-accepting character and rigid π-conjugated backbones. Although extensively studied in organic solar cells and field-effect transistors, their potential as ETLs in PSCs remains comparatively underexplored. Building on previous studies on these systems [1,2], we investigate a family of donor–acceptor–donor small molecules based on II and DPP cores. The molecular design follows a modular strategy in which the acceptor core is flanked by thiophene donor units and functionalized with electron-withdrawing terminal groups (DCV, CNBu, CNOx, ID, IDM and TB), enabling a systematic comparison of core and substituent effects. DFT and TD-DFT calculations on isolated molecules are employed to evaluate intrinsic descriptors relevant to ETL performance, including electron affinity, frontier orbital distribution, reorganization energy and energy-level alignment with reference perovskites. Our results reveal clear structure–property relationships governing charge-accepting ability and electron-transport-related descriptors. II-based systems tend to display deeper acceptor levels and greater structural adaptability upon charging, whereas DPP derivatives exhibit a more rigid response, lower reorganization energies on average and a stronger dependence of HOMO position and anion stabilization on the nature of the terminal groups. Among the substituents considered, DCV- and IDM-functionalized molecules emerge as the most promising candidates. Ongoing work is extending the analysis to thienoisoindigo derivatives and exploring solvent effects and alternative levels of theory to further refine the emerging structure–property relationships in non-fullerene ETMs.

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-B P2-

Computational Investigation of Organic Dyes in Deep Eutectic Solvents for Sustainable Energy Applications

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In recent years, there has been an increasing demand for sustainable and efficient alternatives to traditional energy sources. In this context, novel organic dyes have been designed to enhance the performance of high-efficiency devices, such as dye-sensitized solar cells (DSSCs) and photocatalytic systems for green hydrogen production [1-3]. More specifically, there is an increasing interest in dyes based on a D-π-A architecture, where an electron-rich donor group (D) is connected via a conjugated linker (π) to an electron-acceptor group (A), which is directly anchored to the semiconductor surface.
In this framework, this work focuses on recently proposed carbazole-based dyes (CBZ) functionalized with ethylene glycol and glycerol moieties (respectively denoted as CBZ-EG and CBZ-Gly) and solvated in their corresponding deep eutectic solvents (DESs) [1]. These systems represent a promising solution for DSSCs due to the specific interactions between the organic dye and the DES components, which significantly enhance device efficiency. In addition, DESs are biodegradable and highly eco-sustainable, thereby reducing the environmental impact associated with device fabrication.
Here, we have developed and applied a novel hybrid computational protocol based on the combination of molecular dynamics simulations and *ab initio* calculations to explore the conformational ensemble of these organic dyes and investigating how the interactions between the DES solvents and the organic dyes can modulate their electronic properties and their absorption maxima. We will demonstrate that our computational protocol has strong predictive value and broad applicability, thus enabling the future screening of promising organic molecules for applications in DSSCs and hydrogen production devices.

Acknowledgements: The authors thank the Ministero dell'Ambiente e della Sicurezza Energetica (SOLE-H2, Project RSH2A_000004 - CUP: F57G25000080006, funded by European Union - NextGenerationEU, Piano Nazionale di Ripresa e Resilienza (PNRR) Missione 2 Componente 2 Investimento 3.5 - D.D. 279 05/08/2025).

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-B P3-

First-principles Insights on Entropy-driven Mechanism in P2-Type Layered Oxides for Na-ion Battery Cathodes

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P2-type Na_xTMO_2 layered oxides (x < 1, TM = transition metal) are highly promising cathodes for Na-ion batteries due to their open Na+ diffusion pathways and favorable electrochemical kinetics [1]. However, their practical deployment is hindered by phase transitions and TM migration during cycling, leading to capacity fading and voltage hysteresis [2]. Introducing configurational entropy offers a powerful route to enhance both structural stability and electrochemical performance, yet the mechanisms underlying these entropy-driven effects remain poorly understood [3].

By comparing three P2-Na_xTMO_2 materials with increasing compositional complexity, *i.e.*, $Na_{0.68}Mn_{0.68}Ni_{0.32}O_2$ (low-entropy oxide, LEO), $Na_{0.68}Mn_{0.44}Ni_{0.19}Co_{0.25}Ti_{0.09}Mg_{0.03}O_2$ (medium-entropy oxide, MEO), and $Na_{0.68}Mn_{0.44}Ni_{0.19}Co_{0.19}Ti_{0.09}Mg_{0.03}Al_{0.05}Fe_{0.01}O_2$ (high-entropy oxide, HEO), we elucidate the role of entropy in modulating the structural and electronic response upon charge. Higher configurational entropy is shown to delocalize the redox process across multiple electroactive species with charge compensation burden, thus leading to improved electrochemical stability, as revealed by hybrid-DFT calculations and CV profiles. Stable cycling and less favorable TM/Na_{vac} antisite defects formation suggest that TM migration and dissolution in the electrolyte can be effectively discouraged, enabling superior reversible capacity. When cycled with a room-temperature ionic-liquid (RTIL) based electrolyte, the high-entropy cathode features enhanced structural retention, confirmed by ex situ XRD, owing to the mitigated TM octahedral distortions and suppressed layer gliding dissected from first principles.

These findings establish configurational entropy as a key design parameter for the development of durable, high-performance layered cathodes for next-generation Na-ion batteries.

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Session C

Soft Matter, Interfaces, and Complex Systems

-C O1-

Exact Stoichiometry Far-Off Neutrality Catanionic Nanotubes: Unconventional Self-Assembly of Oppositely Charged Surfactants

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Electrostatic energy plays a pivotal role in the minimization of free energy of self-assembling oppositely charged ions. This is a fundamental principle that guides the formation of aggregates and separation of phases characterized by a stoichiometric balance between the opposite charges [1,2]. However, this study unveils the self-assembly of catanionic nanotubes from a mixture of oppositely charged surfactants in aqueous buffer, comprising an anionic bile salt derivative and the cationic cetyltrimethylammonium bromide (CTAB) at an exact strongly unbalanced charge ratio of 9 anions to 1 cation. This anomalous aggregation leads to the formation of highly stable and ordered supramolecular nanotubes with a uniform cross-section of about 20 nm. The key to this behavior lies in the unique, rigid and facial amphiphilic structure of the bile salt derivative, allocating hydrogen bond donors/acceptors and an aromatic residue, which promotes geometrically constrained derivative-derivative interactions [3,4]. This facilitates the assembly of the anionic derivative into parallel, helically wrapped, negatively charged ribbons with interspersed CTAB cations acting to promote their adhesion. Supramolecular nanotubes are highly valued in nanotechnology for applications like catalysis and tissue engineering due to their rigidity, intrinsic directionality, and capability for dual compartmentalization (inner cavity and outer surface). The catanionic ones reported here are ordered architectures that allow for a high charge and a minimal interference from free monomers, which are essential for optimizing functions such as material loading. A loading ability was here demonstrated by the nanotube interaction with positively charged carbon dots and gold nanorods.

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-C O2-

Macro- and Nanoscale Electrostatics Govern the Static and Dynamic Behaviour of Charged Aqueous Interfaces

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Understanding how electrostatic interactions govern the structure and properties of aqueous interfaces is critically important across many areas, including emulsion and foam stabilization, catalysis, materials science, and biochemistry. Nevertheless, the specific roles of ionic strength and charged species remain only partially understood. In this work, we combine macroscopic and nanoscale structural and electrostatic analyses to clarify how ionic strength and cation valence influence both the organization and electrostatic response of negatively charged silica nanoparticles at the water surface.

Our results reveal a self-regulating mechanism in which the steady-state distance between nanoparticles is determined by a characteristic mesoscopic electrostatic potential together with a constant single-particle repulsive energy, regardless of the ionic species or ionic strength. Variations in electrolyte composition primarily affect the nanoparticle surface excess, which adjusts in order to counterbalance changes in the interfacial dipolar strength.

Moreover, the response of the monolayer to mechanical deformation shows the emergence of short-range inter-particle attractions that depend on composition and become stronger as either the ionic strength or the cation charge increases. These attractive interactions also control how the monolayer relaxes following compression. When strong attractions are present, relaxation occurs through the formation of two-dimensional nanoparticle clusters; conversely, when the particles remain mutually repulsive, relaxation results in isolated nanoparticles persisting at the interface.

We demonstrate that these two distinct relaxation pathways strongly affect the self-healing behavior of the monolayer after mechanical compression. Altogether, these findings provide additional strategies for designing aqueous interfaces with tunable structure, properties, and dynamic responses to external stimuli.

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-C O3-

Soluplus® Micelles Characterization and Application in Drug Delivery

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In the context of studying encapsulation systems using biocompatible polymers, the behaviour of Soluplus®, an amphiphilic block copolymer, has been explored. In aqueous solution, it undergoes self-assembly to form micelles, enabling the solubilization of molecules across a wide range of hydrophobicity. This is facilitated by the presence of vinyl caprolactam (a relatively hydrophilic monomer) in Soluplus's graft chain, which also enhances its interaction with more hydrophilic molecules.

To better understand the micellar behaviour of this polymer, Soluplus aqueous solutions at a wide range of polymer concentrations (0.01 g/mL – 0.3 g/mL) were analysed using diffusion NMR (dNMR), small-angle X-ray scattering (SAXS), static (SLS) and dynamic light scattering (DLS), and viscosity measurements. These techniques were complemented by surface tension measurements to determine the polymer's critical micellar concentration (CMC). dNMR, SAXS, DLS, and SLS indicate that, at all tested concentrations, two forms of Soluplus micelles were detected, with hydrodynamic radii of 3 nm and 26 nm [1].

The large micelles are spherical in shape with a core-shell structure while the small objects are less ordered but, a room temperature, accounts for 60–70 %wt of the total. SLS at variable temperature (T) demonstrate that the increase in T shifts the equilibrium towards the large spherical micelles. Interestingly, the formation of large particles occurs three orders of magnitude above the CMC determined from surface tension measurements. Instead of the traditional cooperative micellization process, we propose a thermally activated isodesmic self-assembly of the small aggregates into core-shell micelles.

As next step, the aim is to investigate the application of these micelles as a drug delivery system. Preliminary results on the use of Soluplus® micelles to encapsulate the anti-cancer drug doxorubicin will be also presented.

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-C O4-

Bio-Based Polyglycerol Esters for LLPS-Driven Soft Microencapsulation

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The replacement of petroleum-derived surfactants with bio-based alternatives is a key challenge for sustainable colloidal systems. In this study, polyglycerol esters (PGEs) were investigated as nonionic surfactants for the formation of matrix-type soft microcapsules through liquid-liquid phase separation (LLPS) [1].
Unlike conventional polymer-based core-shell capsules, these soft microcapsules form droplets in which the active ingredient is embedded within a viscous matrix, stabilized by a hydrated surfactant interfacial film. This approach enables the encapsulation of perfume raw materials (PRMs) in aqueous formulations relevant to household or personal care products, while avoiding microplastic-forming technologies [2].
A series of mono- and diesters of polyglycerol bearing C8–C18 fatty acid chains were screened as alternatives to ethoxylated alcohol surfactants. Surfactant selection was guided by physicochemical characterization including force tensiometry for CMC determination, Differential Scanning Calorimetry to probe headgroups-water interactions, Nuclear Magnetic Resonance for LogP estimation, and Size Exclusion Chromatography for molar mass distribution.
Soft microcapsules were obtained and characterized by macroscopic evaluations of stability and homogeneity, optical microscopy, and confocal Raman microscopy, revealing matrix-like spheres with active homogeneously distributed within the matrix (Figure 1). Long alkyl chain decaglycerol diesters produced the most stable dispersions with narrow size distributions. Dilution experiments confirmed the persistence of droplet structures and retention of active ingredients.
These results demonstrate that PGEs can promote the formation of LLPS-driven soft microcapsules, stabilized by steric and hydration effects at the interface [1]. The work highlights the importance of interfacial molecular architecture and surfactant selection for designing sustainable encapsulation systems as alternatives to conventional approaches [3].

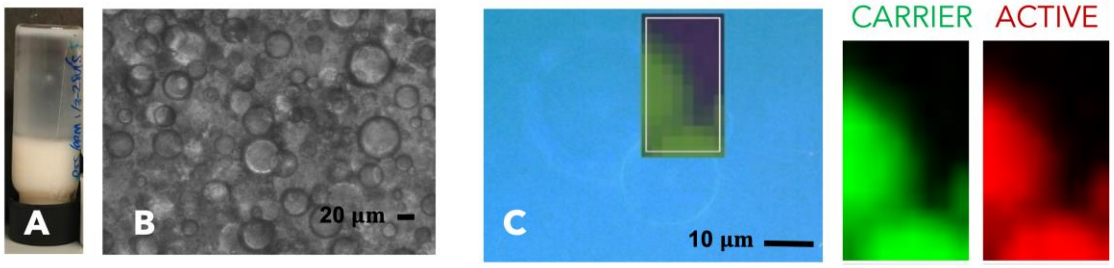

Figure 1. Macroscopic (A) and microscopic (B) observations, and confocal Raman mapping (C) of microcapsules stabilized with PGEs.

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-C O5-

Magnitude of Macromolecular Crowding Caused by Dextran and Ficoll

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The polysaccharides Dextran and Ficoll are commonly used as crowding agents to mimic the cellular cytoplasm [1]. They usually increase the conformational stability of the native state of globular proteins, and this effect has been rationalized by the excluded volume idea: the reduction of the volume available to host the protein molecule shifts the equilibrium towards the native state [1,2]. However, the experimentally measured increase in the denaturation temperature is lower than that calculated by means of theoretical models [3,4]. The present study would like to show that, applying a classic scaled particle theory approach that considers the density of the aqueous solutions, it is possible to provide reliable estimates of their stabilizing effect [5]. Density is a fundamental ingredient because it reflects the actual interactions among the solution molecules and allows the calculation of the number density and the volume packing density of the aqueous solution, two factors that play a major role in defining the magnitude of the solvent-excluded volume effect [6]. Application of the model to aqueous solutions of glucose, sucrose, Dextran-70 and Ficoll-70 demonstrates that the stabilization effect provided by the two polysaccharides is similar to that provided by glucose and sucrose (i.e., the two monomers), and this happens because of the low number density of the polymer solutions.

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-C O6-

The Empirical HLD-NAC Model of Microemulsion Can Be Rationalized on the Basis of Random Field Description of Oil/Water Domains

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The HLD-NAC (Hydrophilic-Lipophilic Difference – Net Average Curvature) equation of state is a powerful semi-empirical framework used to predict the phase behavior, solubilization, and interfacial properties of surfactant-oil-water (SOW) systems. It is based on the HLD equation state [1], coupled with a complementary curvature scaling model, the net-average curvature (NAC) theory [2]. The HLD-NAC is founded on the assumptions that the HLD is a normalized curvature of a hypothetical microemulsion (μE) described in terms of two fictious coexisting phases, one made of water speres dispersed in oil and one where oil spheres are dispersed in a water. The sizes of these two fictious droplets are combined into two quantities: the net-curvature H_n and the average-curvature H_a. Of course, such a description is very far from the real microstructure and a sound treatment about the equivalence of a true microemulsion and the model underlying the NAC is missing to date. μE have been also described in terms of random surfaces separating domains of oil and water whose ratio must fulfill the experimental volumes. This description can be profitably translated in terms of Gaussian random fields for which equation for the (surface-averaged) mean and Gaussian curvatures (<H> & <K>, respectively) have been obtained [3]. This model can be also used to analyze the μE SANS obtaining experimentally <H> and <K> (see fig. 1A and 1B below). The excellent agreement between model and experimental data indicates that the equations that relate <H> and <K> to the composition give a realistic description of the μE structure. Rearranging these equations, we demonstrated that the (area-averaged) mean curvature of the surfactant film has the same form of the net-curvature of the NAC model. We were also able to demonstrate that the empirical parameter HLD is the preferred mean curvature, scaled by the film thickness (l_s<H>$_{pref}$). By leveraging the latter relation, it is possible to predict the μE composition from the HLD (see Fig. 1C for two examples. The possibility to evaluate the preferred mean curvature and compare it with the HLD equation of state opens the way to further in-depth analysis about the link between the film curvature and the parameters entering the HLD-NAC (viz. chemical structure of oil and surfactant, temperature and the ionic strength).

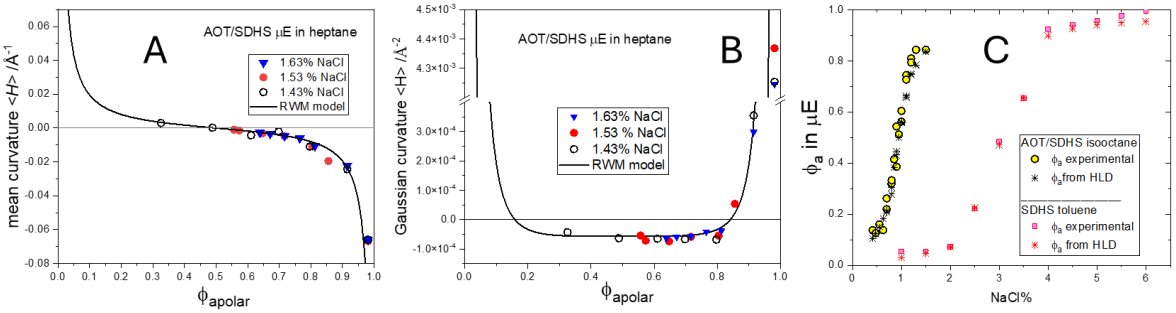

Figure 1 A) mean curvature; B) Gaussian curvature. line = model, points= SANS results. C) composition

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-C O7-

Complex Coacervation Between Sodium Decanoate and Cationic Inulin: Structural and Deposition Studies of Bio-Based Polymer and Surfactant Mixtures

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Oppositely charged polymer-surfactant systems form coacervate complexes near charge neutrality, with applications in deposition or encapsulation triggered by dilution. A transition towards sustainable and edible ingredients is occurring, though these often show complex properties: fatty acid salts have complicated phase behavior (pH-, counterion-, temperature-dependence), and bio-based polymers have less controlled composition, giving wider molecular weight distributions and higher impurity levels. We studied mixtures of sodium decanoate (NaC10) and hydroxypropyl trimonium inulin, a fructan with varying degree of cationic substitution ("Quatin" from Cosun Beet Company), and found that coacervate formation occurs when the surfactant concentration approaches the cmc (3-1 wt%), evidenced by instantaneous turbidity and separation of a denser liquid phase (Figure 1). Bulk DLS and SAXS were used to estimate size and internal structure of aggregates at different compositions. At high surfactant concentration Quatin appears partially embedded in the micelles' shell; coacervate samples showed enhanced contributions from clustered micelles within concentrated droplets; below a threshold concentration only oligosaccharide scattering is observed. In-situ dilution experiments with ellipsometry and neutron reflectometry detected deposition dependence on mixing protocols [1], while synchrotron SAXS in a microfluidic chip revealed details on early mixing events.

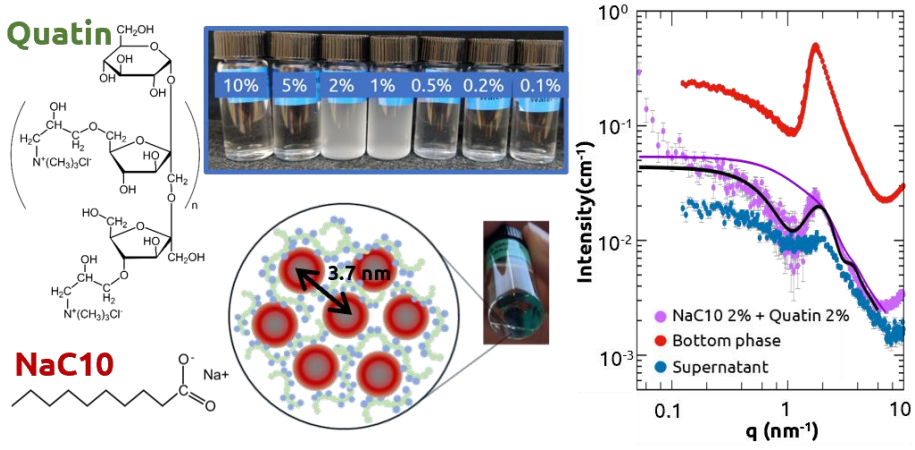

Figure 1. Molecular structures of Quatin and NaC10. Visual appearance of clear and turbid samples. SAXS patterns of a coacervate sample (NaC10 2wt%+Quatin 2 wt%) and the supernatant and bottom phases resulting after sedimentation. The simple sum of a core-shell sphere and gaussian chain fitting the two pure components (purple line) is shown, and a modified model (thick black line) with better agreement.

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-C O8-

Microfluidic Production of Rhamnolipid Coacervates: Linking Droplet Formation to Internal Organization

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Rhamnolipids are microbial glycolipid biosurfactants composed of one or two rhamnose units linked to β-hydroxy fatty acid chains. Commercial samples exhibit significant chemodiversity, consisting of mixtures of mono- and dirhamnolipids with variable chain length and unsaturation [1,2]. Their amphiphilic architecture promotes spontaneous self-assembly in aqueous media leading to supramolecular structures such as micelles and anisotropic aggregates whose properties depend on concentration, pH, and ionic strength [1,2].
Under specific solution conditions, surfactant solutions may undergo liquid–liquid phase separation (LLPS), generating dense liquid phases known as coacervates, where solute-rich droplets coexist with a dilute continuous phase [3,4]. In surfactant systems, coacervation can be triggered by variations in ionic strength, as salt addition screens electrostatic repulsion between charged headgroups and enhances intermolecular association.
In this work, rhamnolipid-based coacervate droplets were generated under high ionic strength conditions using microfluidics. Experiments were performed with a Dolomite flow-focusing junction chip, where the rhamnolipid solution flowed through the central channel while saline solutions were injected from two lateral channels. Hydrodynamic shear at the junction breaks the central stream into discrete droplets, enabling precise control of droplet formation. The microfluidic setup produced monodisperse coacervate droplets in the micrometric range with controlled morphology and reproducible size distribution. The systems were investigated using optical and confocal microscopy to observe droplet morphology and dynamics, while electron paramagnetic resonance (EPR) provided information on internal organization. ζ-potential and rheology measurements further characterized interfacial properties and interparticle interactions, enabling the establishment of structure–property relationships.

Acknowledgments. The authors acknowledge financial support by the Italian MUR, Project Title: Phenolic polymers at biointerfaces (PhenoVectors): selfassembled functional nanovectors with controlled colloidal properties and enhanced antioxidant activity (Project number 202299B4SC) – CUP E53C24002170006 - Grant Assignment Decree No. 18508 adopted on 18/09/2024.

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-C O9-

Physicochemical Characterization of PVA-Based Twin Chain Polymeric Networks Loaded with a Citric Acid Solution

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Citric acid is a well-known biomolecule widely employed in a broad range of industrial applications due to its low production cost, easy availability, non-toxicity, biocompatibility, versatility, and the safety of its degradation products. Its use spans several fields, including the cosmetic, pharmaceutical, food, and agricultural industries. Its functions range from antioxidant and pH regulator to antibacterial and chelating agent, as well as cross-linker and plasticizer. In the field of cultural heritage conservation, citric acid is primarily used as a chelating agent to remove corrosion patinas from metal and stone, due to its ability to complex metal ions such as Fe^{3+} and Cu^{2+} and remove them from the substrate. In most applications, it would be advantageous to confine citric acid within a gel matrix to gain controlled release, increased contact on the substrate, and feasible application even on vertical surfaces. However, only a limited number of studies have investigated the behaviour of this molecule when confined within gels. Our aim is to thoroughly investigate the physicochemical behaviour of citric acid confined in a PVA-based "twin-chain" polymeric network, currently the most effective class of hydrogels in the cleaning of cultural heritage materials. To this aim, three types of PVA-based cryogels, functionalized with green sebacic, succinic, and adipic acids, were employed, studied and tested. We evaluated how the presence of citric acid modifies the characteristics of the gels at the nanoscale, using Small-Angle X-ray Scattering (SAXS), and the mechanical properties, through rheological measurements. In addition, diffusometry and relaxometry studies were carried out by means of ^{1}H Nuclear Magnetic Resonance (^{1}H-NMR), investigating the systems at five different temperatures (25 °C, 27.5 °C, 35 °C, 45 °C, and 55 °C). This allowed exploration of how confinement within the gel modifies the diffusion of citric acid and affects the motility and flexibility of the polymeric chains. Application of the gels was carried out on corroded bronze mock-ups, to mimic the degradative pitting typical of bronze disease, i.e. one of the most complex degradative processes affecting metal artifacts. The cleaning effectiveness of the resulting materials was assessed through a comparative photographic evaluation of the treated areas, using Scanning Electron Microscopy – Energy dispersion X-ray spectroscopy (SEM-EDX) and 2D FTIR Imaging to monitor the presence of residual chlorides. Overall, this work does not only aim at proposing new materials and tools to treat complex degradative pathways typical of historic artifacts but also shows how the complex interplay of gel's features, studied via a robust characterization protocol, should be tailored to boost the gel's performances. In principle, this approach could be transferred to different types of materials used and developed for multiple transversal sectors where surface interactions play a central role, resulting, we believe, in strong scientific and technologic advancements.

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-C O10-

Ion-Programmed Biopolymer Organohydrogels for Multiresponsive Soft Electronics

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Soft electronic devices require materials that combine mechanical compliance with finely controlled ionic transport [1-3]. Alginate-gelatin organohydrogels naturally achieve this balance: alginate provides carboxylate coordination sites that define the network topology, while gelatin imparts elasticity, flexibility, and thermoresponsive behavior [4]. Their properties are therefore governed not only by composition, but also by the chemistry of the ions responsible for alginate crosslinking [5,6].

Using ions spanning the alginate affinity scale (Mn^{2+}, Cu^{2+}, Fe^{3+}, Zr^{4+}) these hybrid networks can be programmed to exhibit multiresponsive behavior, enabling the simultaneous detection of strain, temperature, humidity, and visible light. The achieved sensitivities—gauge factors above 1.6, thermal sensitivities close to 0.2 K^{-1}, and a photoresponsivity of 9.2 µA W^{-1}—originate from ion-specific reorganization of the polysaccharide framework, which modulates polymer mobility and nanoscale packing within the gelatin-rich matrix [5].

This molecular design strategy extends naturally to gel polymer electrolytes (GPEs), where ionic coordination governs transport pathways and electrochemical performance. Strong crosslinkers such as Cu^{2+} produce compact and rigid architectures, whereas weaker Mn^{2+} interactions generate more permeable networks that respond strongly to Li^{+} doping, softening the matrix and enhancing ionic mobility. Small-Angle X-ray Scattering (SAXS) quantifies these effects by revealing systematic variations in correlation length, establishing a robust structure-function relationship that explains capacitances approaching 600 mF cm^{-2} together with stable cycling behavior [6].

Overall, this work highlights ionic coordination as a versatile design principle for controlling structural hierarchy, transport phenomena, and multifunctional responses in soft biopolymer systems. By treating ions as programmable structural regulators rather than passive additives, alginate-gelatin organohydrogels emerge as a powerful and sustainable platform for next-generation soft electronic devices.

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-C O11-

From Nature to Nanoscience: Peptide Building Blocks Driving Photoinduced Electron Transfer

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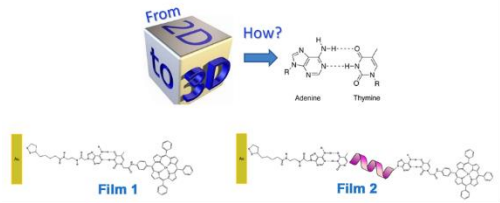
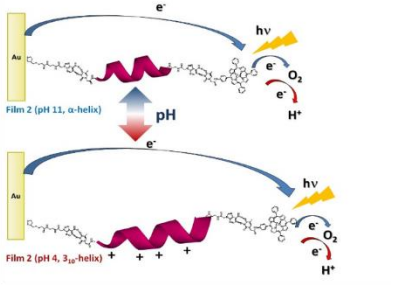
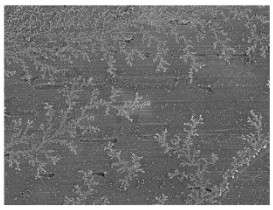
The controlled organization of molecules on surfaces is a crucial step toward the development of efficient photoelectric conversion devices. Previous studies on dye-sensitized solar cells have demonstrated that precise control over molecular aggregation and electron-transfer directionality at interfaces is essential to enhance photoconversion efficiency. In nature, photosynthetic systems achieve this control through highly ordered assemblies of chromophores templated by proteins, which ensure optimal spacing, orientation, and charge separation.

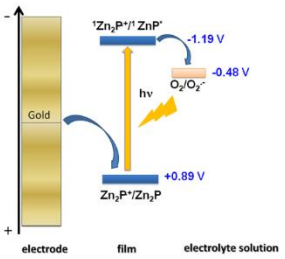
Inspired by these biological strategies, bioinspired approaches based on proteins and peptides have been explored for artificial photoactive devices. While photosynthetic proteins show promising performance, their limited stability under operational conditions restricts practical applications. Peptides offer a valuable alternative, retaining key protein functionalities while providing higher stability and self-organization capabilities.

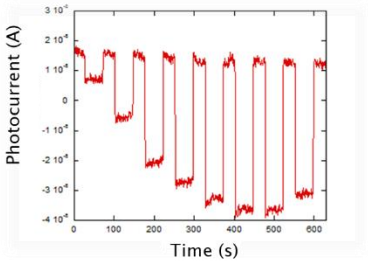
In this context, we have developed supramolecular and bioinspired design strategies to enable the formation of ordered, stable architectures on surfaces, capable of directing electron flow and generating photocurrent efficiently, offering a versatile route toward sustainable, high-performance photoactive materials. Can this approach provide a paradigm shift in the design of stable and efficient photoactive interfaces?











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-C O12-

Repurposing Bacterial Photosynthesis

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For decades, the intricate mechanisms by which bacteria convert sunlight into energy have been meticulously mapped, bringing the field of bacterial photosynthesis to a state of scientific maturity. Today, this deep understanding is fueling a strategic shift: rather than simply investigating and studying these systems, researchers are now repurposing photosynthetic components as functional soft materials for non-biological engineering.
What began as theoretical exploration is now rapidly manifesting as concrete solutions within materials science. The presentation will highlight a curated selection of these applications, showcasing how photosynthetic machinery can drive next-generation technologies. By critically evaluating both the functional advantages and the practical constraints of these systems, this analysis offers a realistic roadmap for integrating bacterial components into the emerging technological landscape.

Acknowledgements. Project APACE **-** Towards a bio-mimetic sunlight pumped laser based on photosynthetic antenna complexes (Project n. 101161312) funded by Horizon-European Innovation Council is acknowledged.

-C O13-

A Physicochemical Approach to Surfactant-Mediated Deposition of Volatile Compounds from Detergent Formulations onto Fabrics

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The development of innovative surfactant formulations strictly depends on advancements in colloid and interface science [1]. In detergent formulations, surfactants and functional additives form a dynamic colloidal system in which micelles, mixed aggregates, and transient interfacial structures compete to solubilize fragrances, which are the main factor driving customer preference among laundry care products. These interactions ultimately control the concentration of free fragrance in solution and its subsequent transfer to textile fibers. Some laundry detergents use encapsulated fragrances to improve deposition and release efficiency and prevent degradation. Microcapsules, however, are under great scrutiny due to environmental concerns: they are classified as primary microplastics, and thus their use has been greatly limited through the European Commission Regulation (EU) [2]. Moreover, special rheological properties are required to obtain suspension of microcapsules over time. For these reasons, there is renewed interest in understanding how naked aroma chemicals interact with textile substrates in multicomponent aqueous environments. In this study, we employed UV-Visible spectroscopy to determine the adsorption kinetics and thermodynamics of volatile odorous compounds (e.g. eugenol, ethyl cinnamate) on different fabrics in complex acqueous media. Model detergent formulations containing commercially available linear alkylbenzene sulfonate and/or alcohol ethoxylate were characterized and tested in standardized washing simulations. UV-Visible spectroscopy was used to quantify the amount of model fragrance in the water phase at small time intervals, quantitatively revealing a decrease in concentration due to adsorption on the textile material. The results were consistent with the chemical nature of the surfactants and fabrics, as well as with the existing literature [3,4,5]. This study highlights the importance of physicochemical knowledge of supramolecular interactions as a foundation for the rational design of detergent formulations.

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-C O14-

Controlling Fibroin Self-Assembly in Sustainable Consolidants for Fragile Silk Artifacts

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Silk artifacts possess remarkable cultural and artistic value but are highly susceptible to degradation processes that modify the secondary structure of fibroin, the main structural protein of silk, leading to a gradual loss of mechanical integrity. Effective and compatible consolidants for historical silk artifacts are still lacking, highlighting the need for improved and reliable materials to safeguard and transmit this heritage. To address this challenge, we developed consolidation formulations based on self-regenerated silk fibroin (SRSF) obtained from waste silk, combining conservation requirements with sustainable material sourcing. In particular, hybrid formulations composed of SRSF and cellulose nanocrystals (SRSF–CNC) demonstrated improved consolidation efficiency when applied to artificially aged silk fibers [1][2]. However, while the incorporation of CNCs enhances mechanical reinforcement, it also accelerates fibroin self-assembly, resulting in reduced formulation stability and a shorter shelf life. To overcome this limitation, we designed sustainable SRSF and SRSF–CNC formulations incorporating bio-derived additives, namely L-arginine and sericin, with the aim of regulating fibroin self-assembly and improving dispersion stability. Their self-assembly behavior and their effectiveness as consolidants for aged silk fibers in the presence of these additives were examined using complementary physicochemical characterization techniques. In addition, application tests on historical textiles were performed in collaboration with the Metropolitan Museum of Art (MET, New York). The results indicate that both L-arginine and sericin effectively modulate fibroin self-assembly without compromising consolidation performance, while maintaining the visual appearance of silk artifacts. Overall, this work proposes a sustainable and versatile strategy for silk consolidation based on colloids and soft-matter systems, contributing to the development of innovative conservation materials within a circular economy framework and offering new perspectives for the long-term preservation of historical textile collections.

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-C 015-

Influence of Surfactants on Industrial Cheese Sauces

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Ready-to-eat cheese sauces are complex colloidal systems, and their stability is crucial both for the producer, as it define the shelf life of the product, and for the consumer, since it greatly affects their taste and their usability in recipes. In this work, the kinetic stability of two different cheese-based sauces for pasta (based on *four Cheeses* and *carbonara* recipes) was investigated by means of rheological analyses and dynamic light scattering (on the colloidal fraction of diluted samples), both in the absence and in the presence of food grade FDA-approved surfactants (Tween 80 and Span 80). The amphiphiles were added to the original products that showed phase separation, to try and recover their original stability.
DLS analyses showed that the addition of surfactants led to a decrease in the polydispersity index (PI) of the systems, thus improving the uniformity of colloidal particle size in both sauces. Regarding viscoelastic parameters, the two sauces exhibited opposite behaviors: in the *four cheeses* sauce, both viscosity and viscoelastic moduli (G′ and G″) decreased, whereas in the *carbonara* sauce these parameters increased. This suggests that surfactants improved the structure and stability of both systems, but through different mechanisms depending on the composition and initial structure of the two sauces, as well as on the specific structure of the surfactant.
This work represents a preliminary approach to the study of the physicochemical properties and stability of these cheese-based sauces, also in the presence of food-grade emulsifiers. The results provided a foundation for further investigations aimed at improving the understanding of the stability of these complex colloidal systems.

-C 016-

Interfacial and Emulsifying Properties of Potato Protein Hydrolysates Obtained by Enzymatic Processing

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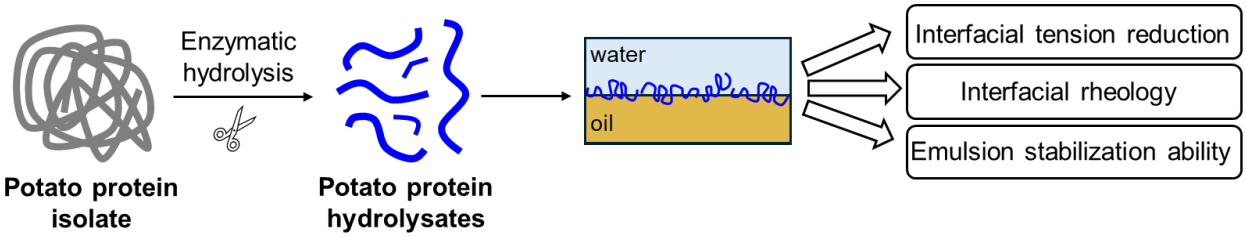
Plant-based proteins are receiving growing attention as sustainable stabilizers for foams and emulsions due to their biodegradability and low cost. Moreover, their use as bio-based surfactants represents an effective approach for the valorization of plant-derived protein by-products [1]. In this context, potatoes emerge as a particularly promising resource [2]. During potato starch production, large volumes of potato fruit juice are generated as a by-product. This stream contains high concentrations of amino acids and proteins, which can be recovered by means of acidic precipitation and thermal coagulation. However, the resulting potato protein isolates typically possess limited foaming and emulsifying properties, primarily due to its relatively high molecular weight and poor solubility in both aqueous and oil phases.
Enzymatic hydrolysis represents an effective strategy to improve the techno-functional properties of potato proteins, enabling the development of novel plant-based surfactants [3,4]. In this study, a potato protein isolate was enzymatically hydrolyzed using different proteolytic enzymes (Alcalase® 2.4L FG, Flavourzyme® 1000, Neutrase®, Protamex®, and Papain). The emulsifying properties of the obtained potato protein hydrolysates were evaluated for their potential use as bio-based surfactants.
The study first focused on the characterization of the peanut oil/water interface using both static and dynamic interfacial tension measurements, along with interfacial shear rheology analyses. Moreover, the stability of protein-stabilized interfacial films was assessed using the thin film balance technique. Circular dichroism spectroscopy was employed to study the different surface activities of the prepared hydrolysates. Finally, oil-in-water emulsions were prepared, and formulation parameters were optimized by means of chemometric analysis (Figure 1).



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-C O17-

Physicochemical Characterization of High-Performance Chitosan Based Adhesives: a Sustainable Approach to Enhances Interfacial Adhesion

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The transition toward sustainable materials science requires the development of bio-based adhesives capable of competing with petroleum-derived synthetic glues [1]. This study reports the design and physicochemical characterization of a high-performance chitosan-based adhesive system, specifically engineered to overcome the intrinsic limitations of polysaccharide materials, such as poor water resistance [2]. To enhance adhesive performance, a sustainable enzymatic strategy was employed using laccase from *Trametes versicolor* to catalyze the oxidative polymerization of catechol-based phenolic compounds. Compared to conventional chemical oxidation, this approach provides a greener and more controllable pathway for the in situ functionalization of the biopolymeric matrix. The structural, thermal, and mechanical properties of the resulting formulations were investigated through a comprehensive multi-technique approach, including FT-IR, UV–Vis, and EPR spectroscopies, dynamic light scattering (DLS), thermogravimetric analysis (TGA) and tensile testing. A pronounced synergistic effect among the components resulted in a significant enhancement of both cohesive strength and interfacial adhesion. Mechanical tests conducted on glass, cardboard, and textile substrates demonstrated high bonding performance. Notably, the optimized system exhibited excellent water resistance, maintaining structural integrity under water continuous immersion. Furthermore, TGA and flammability tests revealed intrinsic flame-retardant behavior [3]. Comparison with commercial glue highlights the potential of this bio-inspired adhesive as a robust and eco-friendly alternative for industrial applications, particularly in packaging and textiles, offering an effective balance between biocompatibility and mechanical reliability.

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-C P1-

Sustainable Bio-Based Emulsifiers from Wine Lees Valorization

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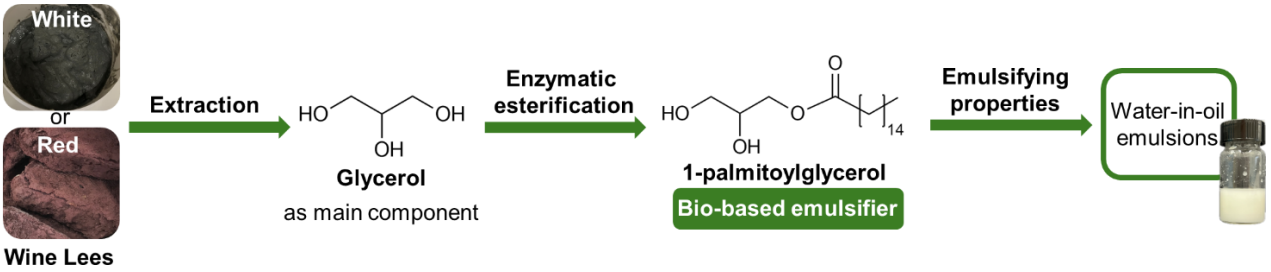
Wine lees are solid residues formed at the bottom of fermentation vessels during wine production. Although their composition varies depending on grape variety, geographical origin and environmental conditions, wine lees mainly consist of yeast cells, tartaric and phenolic acids, proteins, sugars and residual metabolites [1,2]. This by-product of the agri-food industry represents a valuable source of glycerol, which can be recovered and valorized as a renewable feedstock for the synthesis of monoacylglycerols (MAGs). MAGs are non-ionic surfactants widely used in the pharmaceutical, cosmetic and food industries. Conventional chemical synthesis of MAGs requires acidic or basic catalysts and high temperatures, resulting in a mixture of glycerides that must be separated via high-vacuum distillation, which raises production costs. In contrast, enzymatic approaches represent a sustainable and promising alternative, offering enhanced selectivity, simpler processing, and lower energy consumption during downstream operations [3].
In this study, red and white wine lees were used as raw materials to produce bio-based emulsifiers (Figure 1). Glycerol was recovered from both types of wine lees using different extraction techniques, including standard solid–liquid and Soxhlet extractions. To improve the extraction efficiency, both one-pot and sequential extraction approaches were investigated using solvents of increasing polarity (*n*-hexane, ethyl acetate, acetone, ethanol, and water) [4]. The main classes of compounds present in the extracts were characterized by spectrophotometric assays (Folin–Ciocalteu, Anthrone, and Bradford methods), whereas glycerol content was quantified by NMR spectroscopy.
Extracts enriched in glycerol were subsequently subjected to solvent-free enzymatic esterification using Novozym® 435 as the biocatalyst and palmitic acid as the acyl donor, yielding 1-palmitoylglycerol. The surface-active properties of the synthesized MAGs were studied by measuring their ability to reduce interfacial tension and to stabilize water-in-peanut oil (W/O) emulsions over time.



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-C P2-

Formulation Optimization of Highly Stable and Responsive Pickering Emulsions

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Recent advantages in soft matter technologies are awaking interest in Pickering emulsions as an attractive alternative to conventional surfactant-stabilized emulsions, attempting to overcome the environmental and health issues associated with surfactants [1]. Even if Pickering emulsions generally display high stability, optimizing the formulation and eventually scaling up the process requires careful tailoring of numerous parameters: oil/water composition, phase volume ratio, pH, oil phase viscosity, emulsification technique, and nature and surface modification of emulsifier particles. However, this complexity is also an asset to tailoring the physicochemical properties of the system. The wide range of newly considered emulsifiers, such as oxide semiconductors [2], carbonaceous particles [3] and naturally derived nanoparticles [4], open the door to the application of Pickering emulsions in various fields (such as medicine, beauty industry, food formulation, sensing) owing to the assorted chemistry of the different particles. Moreover, the responsiveness of selected particle emulsifiers to stimuli (i.e. change of pH or light irradiation) can be exploited to destabilize the emulsion and release an active species previously loaded inside the dispersed phase [5].
Our research group previously focused on the development of ZnO-stabilized Pickering emulsions obtained by *in situ* functionalization, which is a highly stable system suitable for the triggered release of active ingredients using stimuli such as UV lamp irradiation, acids addition or CO_2 bubbling [5]. Here we report on extending this one-step emulsion preparation procedure to other emulsifier materials and on the scaling up of the process. A systematic investigation was performed on parameters such as the quantity and type of powder (TiO_2, Al_2O_3 and carbonaceous materials), phase ratio (from 1:9 to 1:9 oil:water ratio), emulsification technique (sonication, rotor stator homogenization) and final pH (from 5 to 9). Due to the high number of variables involved, a chemometric tool, Design of Experiment, was employed to obtain a time-efficient tuning of the emulsification conditions. Emulsions were characterized by their droplet size, actual phase volume, emulsion stability index and encapsulation efficiency. These results were complemented by an in-depth characterization of the structural, morphological and surface properties of the tested emulsifier materials. Results show that both O/W and W/O emulsions with a broad range of phase volumes could be obtained by a suitable choice of emulsification technique. The emulsification strategy also plays a key role on the average droplet size, with a notable effect of emulsion pH on the actual disperse phase amount and size distribution, which are strongly related to the droplet surface charge. Our work offers fundamental insights into the interplay between materials chemistry and emulsification procedure in developing highly stable and stimuli-responsive Pickering emulsions.

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-C P3-

Chemical PVA, and PVA-Collagen Hydrogels

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Hydrogels are cross-linked hydrophilic polymer networks capable of absorbing large amounts of water. Because of this property, they play a vital role in biomedical applications such as wound healing, bone regeneration, tissue engineering, targeted drug delivery, and 3D printing [1]. Poly(vinyl alcohol) (PVA) is a synthetic, water-soluble, biocompatible polymer that exhibits excellent mechanical properties. Due to its high biocompatibility, it has garnered significant interest in biomedical fields like contact lenses, artificial joints, and wound dressings [2]. However, owing to the highly hydrophilic nature of PVA, the adsorption of essential cell-adhesion proteins is limited, thereby inhibiting cell attachment [3]. Nonetheless, functionalizing PVA hydrogel with fibronectin—a key component of the extracellular matrix (ECM)—significantly enhances cell adhesion and migration [4]. Motivated by this, to address the inherent bioadhesive feature of PVA, we investigated chemical PVA hydrogels combined with collagen, the main protein of the ECM involved in biological processes critical for wound healing, especially regarding cell adhesion and migration. [5].
In this study, PVA hydrogels were formed without external crosslinkers such as glutaraldehyde, which can reduce biocompatibility. The PVA backbone contains several 1,2-glycol units (vicinal diols) along with 1,3-glycolic units. The 1,2-glycol units can be separated using sodium periodate. As a result, macromers of PVA, called telechelic PVA (tel-PVA), are produced, bearing aldehyde groups at both ends of the chain. This method allows tel-PVA to act as a crosslinker, where PVA chains are linked through condensation reactions between aldehyde end groups and hydroxyl groups, forming a chemically homogeneous PVA network [6].
In this work, we have studied the synthesis and characterization of the chemical PVA hydrogels, which are cross-linked by tel-PVA, and we incorporated collagen into the network.
We discuss the effects of collagen on the structural and mechanical features of the system, as well as its biological influence.

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-C P4-

Tuning Bicontinuous Sulfosuccinate Microemulsions Structure through Salinity

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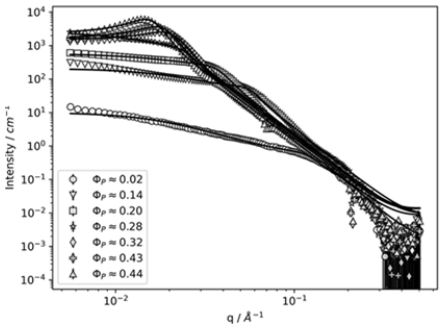
Microemulsions (μEs) are thermodynamically stable, transparent, isotropic single-phase mixtures of immiscible liquids stabilized by surfactants [1]. The rational formulation of μEs with a desired morphology and curvature is complex, as the final structure depends on surfactant and oil composition, as well as ionic strength and temperature. Major advances in predicting microemulsion formulation have been achieved through the Hydrophilic–Lipophilic Difference (HLD) model, which rationalizes phase behavior by balancing surfactant affinity for oil and water as a function of variables such as ionic strength, oil nature, and temperature [2]. In its modern interpretation, HLD is directly linked to the curvature of the surfactant interfacial film, with bicontinuous μEs characterized by HLD ≈ 0, In which the volume fractions of water and oil are comparable.

By employing a surfactant blend composed of sodium bis(2-ethylhexyl) sulfosuccinate (AOT) and its more hydrophilic analogue, sodium dihexyl sulfosuccinate (SDHS), at a fixed mass ratio (SDHS/AOT = 1), bicontinuous microemulsions can be obtained in heptane over a relatively broad salinity range. Moreover, these systems can be formulated under conditions of aqueous phase deficit. Thus, enabling the investigation of slightly unbalanced microemulsion structures across different salinities.

The water and heptane contents of the microemulsions were quantified using two independent methods, graduated-cylinder measurements and NMR integration. They also reveal the same trend: small brine additions expel oil, whereas larger additions allow the bicontinuous phase to reabsorb it. Diffusion NMR (DOSY) experiments further supported the change in connectivity, showing convergence of diffusion coefficients for both aqueous and oil species near the triphasic system. Samples were studied with small-angle neutron scattering (SANS) technique. The measurements revealed different scattering features among the samples (Fig.1).



For the study of bicontinuous systems in bulk contrast, we have implemented a numerical code based on the Clipped Random Wave (CRW) model [3], yielding physically meaningful values of mean and Gaussian curvatures. This model allowed us to describe all samples within a single framework, even across different morphologies. We observed how the mean, Gaussian curvatures evolves systematically with oil and water and salinity refining the understanding of interfacial curvature in AOT/SDHS systems.

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-C P5-

Deciphering and Controlling Biofilm Formation in Functionalized Porous Matrices

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Bacteria motility is a key factor in understanding bacteria activity and the interaction with their surroundings. Confinement within porous matrices, concentration, and flow are some of the most critical parameters affecting bacteria motility [1]. Dense bacterial colonies can give rise to specific multicellular aggregates such as biofilms. These structures limit movements but provide greater protection against harmful agents, resulting in the most common form that can be found in infection scenarios [2]. We recently investigated the motility of *B. subtilis,* a model microorganism non-pathogenic and simple to manage, under different degrees of confinement induced by PEGDA porous hydrogels [3]. The bacterial motility, along with the pore morphology, was characterized by Laser Scanning Confocal Microscopy (Fig. 1) and particle tracking. The dynamical behavior of the bacteria at short times was estimated through mean squared displacements (MSDs) revealing that the run-and-tumble dynamics of unconfined *B. subtilis* progressively turns into sub-diffusive motion with increasing confinement. Analyzing single-trajectories, we showed that the average dynamical behavior is the result of complex displacements, in which active, diffusive and sub-diffusive segments coexist. These findings were interpreted using a recently proposed hopping and trapping model. Moreover, we found that the introduction of negative charges in the polymer network of the hydrogel, through the addition of acrylic acid, determines globally a reduction of the available pore volume for the bacteria displacement. All the results collected so far, obtained in a 2D section of the hydrogels, are not however sufficient to fully understand biofilm formation on complex surfaces of 3D porous materials. We therefore recently extended these studies to investigate motility in 3D under similar confinement conditions, and in comparison with the bulk phase. These studies are the starting point for a comprehensive characterization of confined bacterial motility in 3D, that will later consider more complex interactions (gel functionalization) as well as variations of the size and shape of the pore architecture.

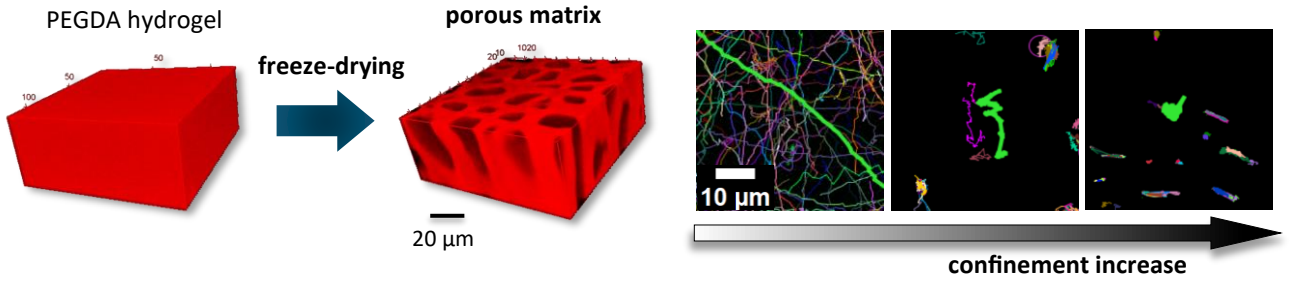

Figure 1. (a) 3D stacks of PEGDA heterogeneous porous matrices acquired via LSCM; (b) Particle Tracking of B. Subtilis *cells at increasing confinement level into porous substrates.*

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Session D

Physical Chemistry
for Health and Life Sciences

-D O1-

Modulating Disease-Related Biocondensates with Small Bioactive Peptides

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Eukaryotic cells contain both membrane-bound organelles and membraneless compartments. The latter arise from the demixing of biomacromolecules through liquid–liquid phase separation (LLPS), leading to the formation of biocondensates (BCs) or droplets [1]. BCs are liquid-like assemblies that allow cells to regulate biochemical reactions in space and time, providing a dynamic mechanism for intracellular organization. Increasing evidence shows that BCs are involved in the onset and progression of several diseases, including neurodegenerative disorders, viral infections, and different types of cancer [1,2]. Because of their role in disease-related processes, BCs are attracting growing attention as potential therapeutic targets. Molecules that can act as modulators of biocondensate properties are bioactive peptides, including antimicrobial peptides (AMPs). AMPs are short, cationic peptides with activity against bacteria, viruses, and even cancer cells [3]. They can interact with pathogen membranes or translocate across them and target intracellular components such as proteins and nucleic acids. In this presentation, it will be shown how peptides can be exploited to target biomolecular condensates involved in viral infections and neurodegenerative diseases, through two representative examples (Figure 1). In the first case, it will be demonstrated how the peptide LL - III inhibits the fibrillation of α-synuclein, a process associated with Parkinson's disease that involves the formation of biocondensates [4]. In the second example, it will be shown how three peptides affect the morphological properties of condensates formed by the SARS-CoV-2 nucleocapsid protein involved in the viral infection process, leading to distinct alterations depending on their sequences and physicochemical properties [5]. Overall, these results suggest that antimicrobial peptides can modulate the physical properties of disease-related biomolecular condensates. This approach could pave the way for the development of a new class of peptide-based agents targeting biomolecular condensates, extending the potential applications of bioactive peptides beyond their traditional antimicrobial roles.

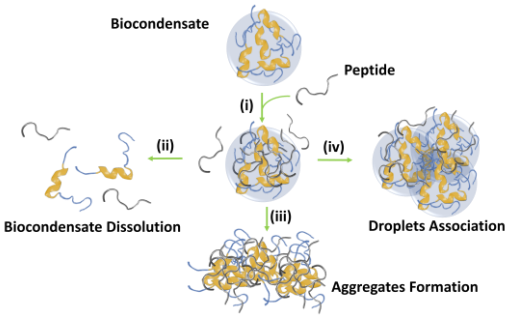

Figure1. Possible effects of antimicrobial peptides on biomolecular condensates: (i) peptides can partition into the droplets, altering their internal dynamics; (ii) peptides can induce droplet dissolution; (iii) droplet dissolution followed by irreversible aggregation of macromolecules; and (iv) reversible droplet association. The prevailing effect depends on the physicochemical properties of both the peptide and the condensates.

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-D O2-

Membrane Interactions of Antimicrobial Peptides: a Kinetic Perspective

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Antimicrobial peptides (AMPs) are promising agents against drug-resistant microbes due to their ability to kill bacteria by disrupting their cellular membranes. Our previous studies enabled the characterization of AMP interaction with both real cells and model systems [1,2], demonstrating several insights in AMP mechanism of action. We closed the gap between biophysical investigations on model membranes and microbiological assays by applying experimental conditions that allow quantitative analysis on the interaction between AMPs and living cells. Our results revealed that millions of peptide molecules must attach to a single cell to induce its death, much more than what would be required to merely cover the cell membrane [1,3]. To gain further insight into the sequence of events involved in bacterial killing, we carried out kinetic studies on peptide–bacteria interactions using a dansyl-labeled variant of the AMP PMAP-23. By combining stopped-flow measurements with fluorescence-based kinetic analyses, we examined these interactions over a wide range of timescales, from milliseconds to minutes. Our findings indicate that the peptide associates with bacterial membranes in under a second, perturbs them leading to bacterial killing prior to inner membrane perturbation, and ultimately accumulates within the cells (Figure 1). In addition, confocal microscopy further reveals that, at bactericidal concentrations, DNS-PMAP-23 mainly localizes at the membrane but partially enters the cytoplasm. Quantitative analyses of peptide–DNA interactions suggest that the peptide targets multiple intracellular components in addition to nucleic acids. Overall, these results show that kinetic approaches can offer a deeper understanding of the steps leading to bacterial death induced by AMPs.

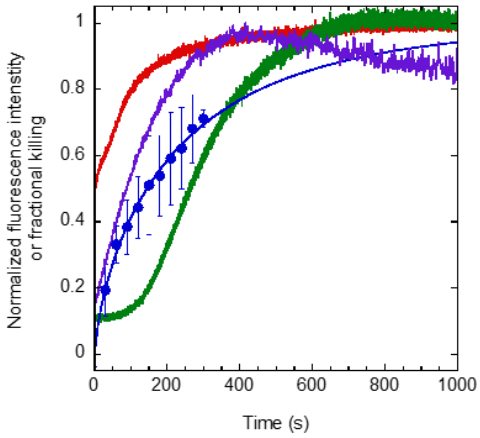

Figure1. Comparison of AMP/bacteria interaction kinetics: interaction of DNS-PMAP23 with E.coli monitoring dansyl fluorescence (red); E.coli killing kinetics (blue) and bacterial inner membrane perturbation induced by DNS-PMAP23 monitoring propidium iodide fluorescence (green E.coli and purple S.epidermidis).

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-D O3-

Aerosol-Assisted Atmospheric Pressure Plasma Jet Deposition of Antimicrobic Zinc- Based Nanocomposite Thin Film

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Agricultural crops can be affected by a wide range of phytopathogens. Among bacterial diseases, a significant one is caused by *Erwinia carotovora*, a Gram-negative pectolytic pathogen responsible for soft rot in several horticultural crops. Equally critical are fungal pathogens that infect wheat, particularly *Fusarium* species [1], resulting in drastic reductions in grain yield and quality. In this framework, zinc oxide nanoparticles (ZnO NPs) have been extensively studied for their antibacterial properties and for the treatment of major fungal diseases caused by *Fusarium* species. ZnO NPs can be combined with innovative technologies such as atmospheric pressure plasma (APP) processes, providing sustainable alternatives for crop protection [2].
In this study, aerosol-assisted atmospheric pressure plasma jet (AA-APPJ) deposition is proposed for the preparation of polyethylene-glycol-like (PEG-like) nanocomposite coatings embedding ZnO NPs or zinc acetate (ZAD) on both polyethylene (PE) model substrates and wheat seeds. The aim was to develop multifunctional antimicrobial coatings capable of protecting crops from bacterial and fungal phytopathogens while reducing the reliance on conventional chemical treatments.
The antibacterial activity of the Zn-containing coatings against *Erwinia carotovora* demonstrated a marked antimicrobial effect, which increased with the zinc content within the coatings. PEG-ZnO NPs nanocomposites showed higher antibacterial efficiency than PEG-ZAD at comparable concentrations, highlighting the importance of the zinc chemical form in determining antimicrobial effectiveness. Furthermore, the coatings were deposited onto wheat seeds and evaluated against *Fusarium graminearum*, *Fusarium culmorum*, and *Fusarium moniliforme*. The treatments exhibited a protective antifungal effect, reducing infection symptoms while maintaining high germination rates and slightly promoting early seedling growth.
These results demonstrate that plasma-deposited zinc-based nanocomposite coatings represent a promising and sustainable alternative to conventional seed dressing treatments. The proposed approach may serve as a starting point for broader agricultural applications, including antimicrobial seed coatings and active mulching technologies aimed at improving crop protection and agricultural sustainability.

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-D O4-

Magnetic Response of Giant Unilamellar Vesicles Embedding Functionalized Magnetite Nanoparticles

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The integration of nanomaterials within biomimetic compartments offers a versatile platform for remote actuation and responsive soft matter systems [1,2]. In this work, we investigate the encapsulation of functionalized Fe_3O_4 magnetic nanoparticles (NPs), with average particle size of 7 nm, within Giant Unilamellar Vesicles (GUVs) and evaluate the interplay between nanoparticle loading, spatial distribution, and magnetic response. Hydrophilic NPs coated with dihydrocaffeic acid (DHCA) were encapsulated in the inner aqueous phase of GUVs (5–50 µm diameter, POPC:cholesterol 2:1, Figure 1-left side), while hydrophobic oleic acid (OA)-coated NPs were incorporated into the lipid phase during vesicle formation. A clear threshold behavior was observed: GUVs containing ≥0.2 wt% DHCA-coated NPs in the aqueous core exhibited directional motion under an external magnetic field, whereas lower concentrations resulted in negligible response. Similarly, membrane-loaded systems required high NP volume fractions to achieve magnetically induced motion. Magnetic characterization of GUV-embedded hydrophilic NPs was performed using Quantum Design PPMS magnetometer, equipped with a VSM head. The analysis of the temperature dependent data revealed a systematic decrease in the temperature at which the zero-field cooled (ZFC) curve reaches its maximum (i.e., T_{MAX}, proportional to the blocking temperature) from ~130 K to ~85 K with decreasing NP loading (Figure 1-right side). This trend suggests a progressive reduction of dipolar interparticle interactions, leading to a more weakly interacting system [3]. Changes in effective anisotropy may also contribute, reflecting the confined environment within the vesicular core.These results demonstrate that both NP loading and spatial confinement critically govern the magnetic responsiveness of GUV systems. The findings provide insight into the design of magnetically controllable soft compartments for applications in targeted delivery, microfluidics, and synthetic cell engineering.

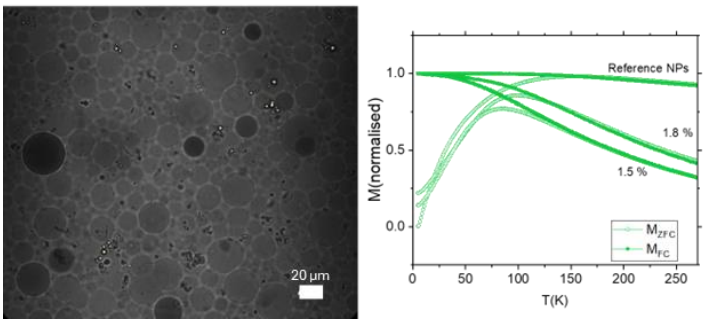

Figure1. Optical image of GUVs with embedded NPs and corresponding zero-field cooled – field cooled (ZFC-FC) magnetic curves for the reference hydrophilic NPs and GUVs with different loads.

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[3] D. Peddis et al. Langmuir 2025, 41, 11977.

-D O5-

Photothermal Effect of Gold Nanostructures on Amyloid Aggregates: Role of Shape and Size in the Optical Response

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The tendency of native proteins to form highly ordered protein aggregates, known as amyloid fibrils, can be influenced by specific conditions such as low pH, elevated temperature, and increased ionic strength. Amyloid fibrils no longer retain the functional properties of the native protein, often exhibiting high toxicity and cytotoxicity that can be related to neurodegenerative diseases [1]. To date, scientific research has been focused on the study of fibrillation mechanism and the research of promising molecules to inhibit amyloid formation [2]. Beyond their established role in different light-based applications, metal nanoparticles can be exploited for the disruption of preformed amyloid fibrils by plasmon-induced photothermal effect. Depending on the metal and the interface, relaxation of localized surface plasmon resonance can occur through non-radiative processes, resulting in significant heat release near the surface of the nanoparticles; the conversion of light into heat (photothermal effect) enables the activation of the photothermal modification of the materials located on the close proximity of the plasmonic structures. The present work explores the effects of sizes and morphologies of citrate-capped gold nanostructures on the interaction with lysozyme amyloid aggregates. The photothermal response (Figure 1) was investigated both theoretically, performed by COMSOL Multiphysics software, and experimentally for gold nanosphere with diameters of 23 nm and 45 nm, and for gold nanorods with aspect ratio of 2 (22 nm in diameter and 44 nm in length). The effect of the temperature enhancement was theoretically examined in media with different refractive index. Lysozyme fibrils were irradiated through a incoherent plasmonic excitation in the presence of spherical gold nanoparticles or gold nanorods. Changes in the structure and the spectroscopic properties of amyloid complexes were monitored by UV-Vis, fluorescence and ATR-IR spectroscopies, as well as TEM and AFM microscopy. The simulations results predict that larger spherical nanoparticles display the highest temperature increases, in perfect agreement with the experimental data. The photothermal properties of gold nanoparticles are size-tunable, and the variation of efficiency can be correlated to the absorption/extinction ratios calculated by Finite Element Method for different particle sizes and shapes. The combination of theoretical and experimental approach leads to more accurate modeling and optimization of gold nanostructures-based technologies for photothermal therapy.

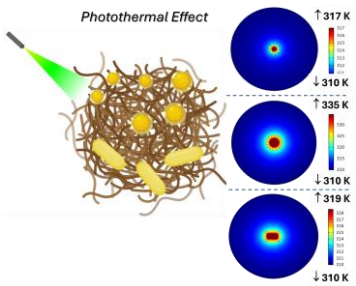

Figure1. Scheme of the photothermal effects investigated through simulation performed by COMSOL Multiphysics.

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-D O6-

Plasmonic Au NP-Derived Thin Films for Monitoring Cardiac Cells and Their Biomarkers

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Organ-on-Chip (OoC) platforms are powerful tools for disease modelling [1] and monitoring cellular behavior [2], particularly in the case of human iPSC-derived cardiomyocytes, which require long maturation times and stable sensing interfaces. Conventional microelectrode fabrication, based on photolithography and physical vapor deposition (PVD), is reliable but costly and time intensive [3]. This work presents an easier and more sustainable alternative relying on spray-coated gold nanoparticles (AuNPs) patterned through inkjet-printed water-soluble sacrificial masks.

AuNPs synthesized by laser ablation in solution (LASiS) were deposited by spray-coating to form nanostructured thin films [4], combining good electrical conductivity with strong Surface Enhanced Raman Scattering (SERS) activity (*Figure 1*). The approach enables large-area deposition with reduced material consumption, while micrometric electrode geometries are defined using a polysaccharide-based sacrificial mask fabricated by inkjet printing.

The resulting plasmonic platforms allowed the detection of adenine, ATP, and hypoxanthine at micromolar concentrations via SERS mapping, supported by multivariate chemometric analysis for accurate quantification in complex environments. In parallel, cardiomyocytes cultured directly on the patterned electrodes were monitored by electrochemical impedance spectroscopy (EIS), showing a characteristic impedance signature absent in control substrates.

Overall, this strategy provides a cost-effective, scalable, and multifunctional plasmonic platform that integrates electrophysiological monitoring with label-free metabolic sensing, offering a promising solution for advanced cardiac OoC applications.

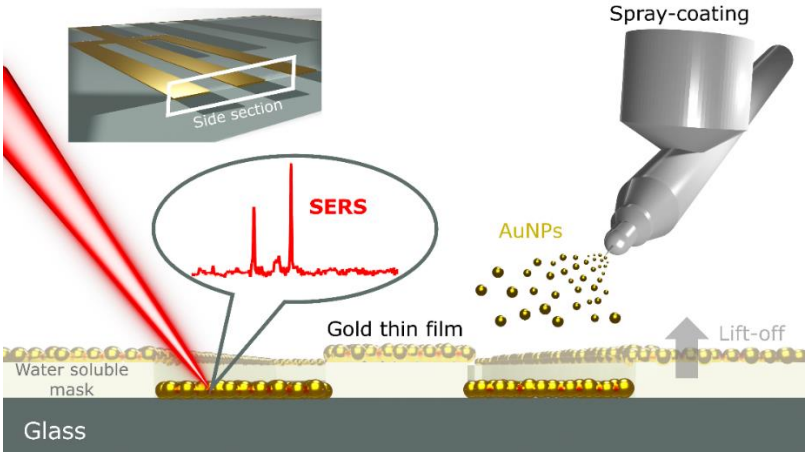

Figure1. Schematics of the plasmonic microelectrode and the required fabrication steps.

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-D O7-

Functionalized Petal-Like ZnO as a Promising Nanoplatform for Gene Delivery

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Nanostructured metal oxides have attracted tremendous attention in the field of biomedicine, thanks to their unique physicochemical properties. Their excellent optical, magnetic, electrical, and chemical properties make them highly valuable for a range of nanotechnology applications, offering promising opportunities in diagnostics, imaging, drug delivery, and regenerative medicine [1]. Among these nanomaterials, Zinc Oxide (ZnO) has emerged as a multifunctional material with high chemical stability, a high electrochemical coupling coefficient, broad radiation absorption, and high photostability [2]. In this frame, we report a versatile, direct, and rapid method for obtaining spherical ZnO nanoparticles composed of petal-like structures (P-ZnO NPs). To enhance their stability in aqueous environments and improve their biocompatibility, we developed three formulations by coating P-ZnO NPs with polycations, including polyethyleneimine (P-ZnO@PEI), chitosan (P-ZnO@CS), and protamine (P-ZnO@Prot). These tailored surface modifications were designed to create a robust nanoplatform for gene delivery applications by controlling the adsorption of a plasmid coding for a fluorescent protein reporter onto the polycation-coated P-ZnO surface. The plasmid-ZnO nanostructures were administered *in vitro*. We demonstrated that, in addition to excellent biocompatibility, the functionalized P-ZnO NPs efficiently penetrated cells due to their sharp-tipped surface architecture, thereby facilitating intracellular delivery and promoting the effective expression of the reporter plasmid. The results reported here indicate that the functionalized petal-like ZnO-based nanoplatforms can offer clear benefits in nanomedicine. Further clinical development of the designed nanosystem concept as a novel gene delivery system may benefit patients in the future.

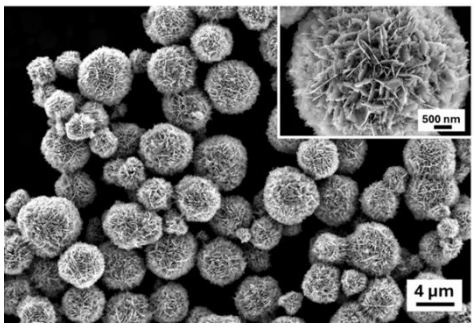

Figure1. SEM images of Petal-like ZnO.

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-D O8-

Liposomal Co-Encapsulation of Curcumin and Quercetin Enhances the Protective Effect on Endothelial Cells from TNF- α-Induced Inflammation, Oxidative Stress, and Apoptotic Damage

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Neurodegenerative and cardiovascular diseases share common features such as vascular dysfunction and chronic inflammation, which are exacerbated by aging [1]. Natural bioactive compounds have shown beneficial effects in these conditions, and liposomes can enhance their bioavailability and biological activity, promoting synergistic effects even at non-pharmacological doses. This approach may provide dual protection against early events in both atherosclerotic cardiovascular disease and blood–brain barrier-related central nervous system disorders.
PEGylated liposomes containing curcumin (VC), quercetin (VQ), and both antioxidants (VCQ) were prepared using the thin-film hydration method, followed by extrusion to obtain homogeneous unilamellar vesicles. The formulation was optimized to maximize encapsulation efficiency (EE%) and loading content (LC%). DLS and TEM analyses showed that all formulations consisted of monodisperse vesicles (PDI < 0.3), with an average diameter of approximately 100 nm and a regular spherical shape. The liposomes retained their characteristics after storage both in solution at 4 °C and after lyophilization for about one month. In addition, cargo release profiles over time and antioxidant activity (TEAC) values were determined. Biological assays showed that VC and VQ protect endothelial cells from TNF-α-induced cytotoxicity more effectively than free antioxidants. Moreover, the liposomal co-encapsulation of curcumin and quercetin enhances protection against TNF-α-induced endothelial damage. TNF-α induces strong inflammatory activation and oxidative stress in endothelial cells, increasing the expression of adhesion molecules (VCAM-1, ICAM-1), cytokines (MCP1, IL-6), lipid peroxidation, and ROS production. Pre-treatment with VC+VQ significantly reduced these effects; however, the co-encapsulated formulation VCQ proved more effective, further attenuating adhesion molecule expression, cytokine secretion, and oxidative stress, demonstrating superior anti-inflammatory and antioxidant activity compared to the free compounds. VCQ is more effective than the combination of VC and VQ in restoring mitochondrial respiration and cellular metabolic activity, indicating superior protection against inflammation-induced bioenergetic damage. Moreover, it is also more effective in reducing TNF-α-induced apoptotic cell death. Overall, these results suggest that VCQ could be a promising nanoplatform to enhance the therapeutic potential of curcumin and quercetin, offering a feasible strategy to counteract endothelial dysfunction and inflammation-related diseases.

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-D O9-

Advanced Yb^{3+}/Er^{3+}-TiO_2 Architectures: Mastering Upconversion for NIR-to-Visible Light Harvesting

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The use of appropriately designed nanomaterials enables the creation of highly selective systems capable of simultaneously performing diagnostic and therapeutic functions. Promising perspective relies on the use of engineered nanosystems for imaging and photodynamic therapy (PDT). Current photosensitizers for PDT present, as their main limitation, the need to use a visible light for activation, thus restricting their applications mainly to superficial tissues; the same limitation is showed by conventional organic fluorophores, which are excited by visible light which render the translation into clinic quite difficult. The possibility of exploiting the upconversion (UC) phenomenon in materials capable of emitting in the visible region following irradiation with near-infrared (NIR) light has attracted considerable interest in recent years, thanks to the greater penetration depth of NIR light [1]. Furthermore, by using a matrix such as TiO_2, surface chemical functionalization is not required, since titania itself acts as the photosensitizer, given that the UP could be tailored to reach TiO_2 efficiently.

In this contribution, the synthesis, via the sol–gel method, and characterization of upconverting nanomaterials based on lanthanide ions, inserted in TiO_2 matrix, is presented. The studied nanomaterials consist of TiO_2 nanoparticles co-doped with Er and Yb ions as the UC pairs. In order to extend the UP process up to the TiO_2, thus triggering the photorelease of ROS, TiO_2 was also doped with N-riche compound or with Ag to shift the TiO_2 band gap towards to the visible region [2]. Preliminary results (Figure 1) showed that the co-incorporation of Er/Yb couple within TiO_2 matrix with extended band gap was successful and that lanthanide ions were stably incorporated within the matrix.

The TiO_2-based samples were characterized to evaluate their structural features and possible differences attributable to the synthesis method through X-ray diffraction (XRD). Morphological and elemental analysis was performed using FE-SEM microscopy coupled to EDX microanalysis. Optical absorption and emission properties were investigated by DR-UV-Vis-NIR spectroscopy and fluorescence spectroscopy. The upconversion properties of these materials were tested by irradiating the samples with a 980 nm laser and collecting the corresponding fluorescence spectra.

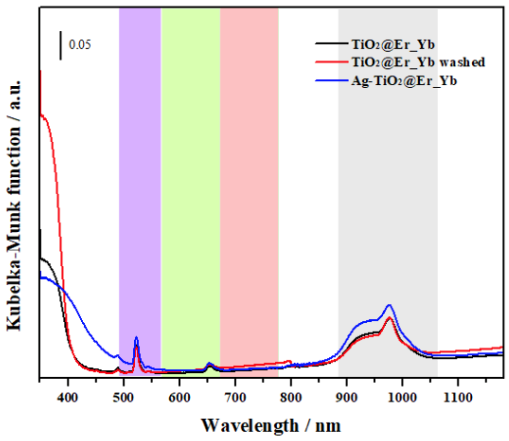

Figure1. DR-UV-Vis spectra of TiO_2 nanoparticles doped with Er and Yb and effect of Ag incorporation on the TiO_2 band gap.

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-D O10-

Tuning Physicochemical Properties of PEDOT: PSS/HNTs Nano Composites for Smart Bioactive Interfaces

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The development of advanced biointerfaces requires materials that combine high electrical and electrochemical performance with mechanical robustness and compatibility with hydrated biological environments. Conductive polymers are particularly attractive in this context, and poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) [1] stands out due to its mixed ionic–electronic conduction, processability, and stability in aqueous media. However, further control over its mechanical and interfacial properties is essential to enable reliable bioelectronic applications.

In this work, we report on PEDOT:PSS-based nanocomposite [2] thin films obtained by incorporating halloysite nanotubes (HNTs) [3], naturally occurring aluminosilicate nanotubes characterized by high aspect ratio, hollow morphology, and large interfacial area. The resulting films were systematically characterized by Atomic Force Microscopy for morphology and nanomechanics, local current–voltage spectroscopy for charge transport, Scanning Kelvin Probe and Capacitance Microscopy to probe surface potential and local electrostatic properties, shedding light on the p-type nature of the polymer and the mobility of charge carriers, cyclic voltammetry for electrochemical response, and ellipsometric spectroscopy for thickness and optoelectronic properties.

Despite the intrinsically insulating nature of halloysite, its controlled incorporation leads to a simultaneous enhancement of electrical conductivity and enhances holes transport, electrochemical capacitance, and mechanical stiffness of the PEDOT:PSS films. These effects are attributed to the formation of a hybrid percolative network in which the nanotubes promote polymer chain organization, improved charge transport pathways, and more efficient ion diffusion within the hydrated matrix. Notably, composites containing PEDOT:PSS-loaded HNTs exhibit the strongest improvements, highlighting the key role of interfacial confinement and volumetric charge exchange.

Preliminary biological validation was carried out by MTT assays, demonstrating not only preserved cytocompatibility but also an improvement in cell viability on PEDOT:PSS/HNT nanocomposites compared to pristine PEDOT:PSS films, identifying PEDOT:PSS/HNT nanocomposites as promising materials for stable and responsive biointerfaces. These results provide a materials-level strategy to tune the mechanical, electrochemical, and biological performance of conductive polymer films, paving the way toward their integration in bioelectronic devices, soft implantable electrodes, and controlled-release platforms.Lead-free piezoceramics,

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-D O11-

Development of Dielectric/Metal/Dielectric (DMD) Architectures for Optical Biosensing Applications

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Dielectric/Metal/Dielectric (D/M/D) architectures are multilayers of thin films with thickness in the nanoscale that have been widely exploited for applications in sensing and optoelectronics [1]. In particular, the D/M/D multilayers are characterized by high electrical conductivity comparable to regular conductive materials. In addition, D/M/D shows tunable spectral properties, such as spectral selectivity, controlled transparency in the UV-Vis-NIR range and flexibility [2]. Indeed, these systems can represent advanced sensing platforms based on the changes in the optical plasmonic signal from the metal component, upon the physisorption of the target analyte molecules. In this work, new architectures of chemically asymmetric Ag-based D/M/D are reported for the detection of model proteins of interest for human health. More specifically, the D/M/D multilayers were fabricated by thermal evaporation [3] to obtain an Ag layer a few nanometers thick sandwiched between a transparent indium tin oxide (ITO) electrode and a tungsten oxide (WO_x) top dielectric layer to obtain the structure ITO/Ag/WO_x. This multilayer and the deposition method are compatible with both glass and polymeric flexible substrate such as Polyethylene Terephthalate (PET). The top dielectric layer thicknesses were properly controlled within 0-40 nm to tune the optical features as well as the surface chemistry to modulate the plasmonic signal in the visible range and the adsorption processes. Indeed, this thickness engineering allows the signal modulation through multiple optical interference and plasmon sensitivity to the refractive index at the interface of the top layer. Protein adsorption from aqueous solution induces plasmonic spectral shifts due to combined thin-film interference and metal-layer plasmonic effects, reflecting refractive index changes near the surface (Figure 1). For instance, bovine serum albumin (BSA) was tested as a model protein analyte at the micromolar level. In addition to the detection and quantification of the protein analytes, the kinetics of the optical response may also provide insight into the mechanism of protein adsorption at the solid/liquid interface [4]. In conclusion, the reported asymmetric D/M/D multilayers represent a versatile plasmonic platform for sensing and physicochemical studies. The simple fabrication and compatibility with flexible substrates make these structures promising for compact, point-of-care sensing devices.

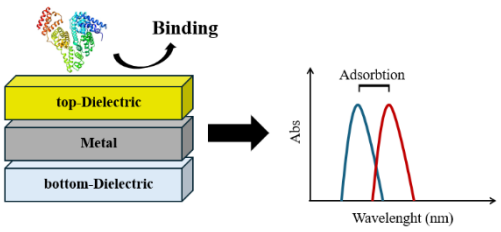

Figure1. Schematic of a D/M/D sensor and protein detection via UV–Vis–NIR absorption changes.

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-D O12-

Photomodulation of Vesicle Dynamics Using Fluorescent Photoswitchable Amphiphiles

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Stimuli-responsive biomimetic compartments are promising platforms for controlling membrane biophysical properties in response to external physical (e.g., light) or chemical (e.g., pH) inputs. These systems are relevant both for investigating fundamental properties of living matter and for developing innovative biomedical and therapeutic technologies.
In this context, a photoswitchable amphiphilic molecule was incorporated into giant unilamellar vesicles (GUVs) to achieve light-controlled modulation of membrane behavior. The vesicles are composed of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) doped with an azobenzene-derived amphiphile designed and synthesized in-house. Upon UV-A and blue light irradiation, the molecules undergo reversible E/Z photoisomerization, altering its geometry and the occupied volume. These conformational changes modify the bilayer order and dynamics modulating membrane permeability and morphology though controllable transient pore formation and cargo release (Figure 1). The extent and spatiotemporal regulation of these effects can be tuned by adjusting amphiphile concentration and irradiation intensity [1]. To directly visualize membrane incorporation, a fluorescently labeled derivative of the photoresponsive amphiphile was developed enabling a more accurate correlation between membrane localization and functional effects [2]. Furthermore, the system was efficiently miniaturized in nanoscale liposomes (~100 nm) to explore potential smart drug-delivery applications [2]. More recently, we demonstrated the biological relevance of this approach by interfacing light-responsive GUVs with human cells [3]. Model signaling molecules were encapsulated within the vesicle aqueous core and rapidly released upon light stimulation, triggering calcium oscillations in nearby HeLa cells. Importantly, in the absence of irradiation, the vesicles remain functionally inert, exhibiting a stealth-like behavior. Overall, this platform establishes a versatile framework for the development of adaptive drug-delivery systems capable of controlled communication with living cells, with potential applications in targeted therapies.

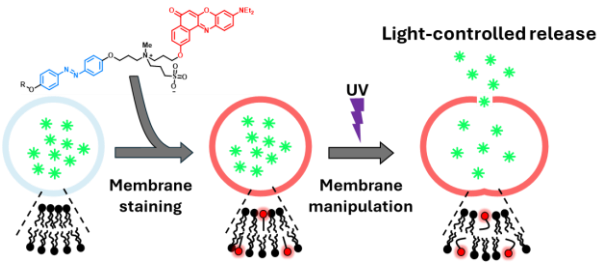

Figure1. Lipid vesicle functionalized with fluorescent photoswitchable molecule enable light-controlled cargo release. Reproduced from [2].

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-D O13-

pH-Responsive Dendritic Large-Pore Mesoporous Silica Nanoplatforms for 5- Fluorouracil Delivery in Colorectal Cancer

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Harnessing nanotechnology for cancer therapy stands as a formidable challenge for scientists. Within the realm of nanomedicine, mesoporous silica nanostructures (MSNs) have garnered considerable attention due to their distinctive physical-chemical characteristics, as large surface area and pore volume, biocompatibility, facile surface functionalization, and high therapeutic loading capability [1]. Tuning MSNs pore size is crucial for accommodating large amounts of guest compounds or macromolecules. Here, core@shell nanostructures (SiO_2@MSNs), consisting of non-porous silica core and dendritic mesoporous silica shell were designed, synthesized and loaded with a chemotherapeutic agent, namely 5-fluouracil (5-FU), for the targeting and treatment of colorectal cancer (CRC). Furthermore, the surface of these nanostructures was functionalized with polyacrylic acid (PAA), selected for its pH sensitivity, and with Frizzled-10 (FZD10) antibody [2], for creating a tumor-targeted delivery system based on pH-based stimuli. Luminescent carbon dots were also incorporated into the solid core to achieve optical traceable nanostructures. SiO_2@MSNs were obtained by means of a biphasic soft-templating strategy, by using cetyltrimethylammonium bromide (CTAB), as cationic surfactant and tetraethyl orthosilicate (TEOS) as silica precursor in alkaline conditions. Physical-chemical characterization, drug loading and release assay were performed. SiO_2@MSNs with dahlia-like morphology showed an average size of about 100 nm, a good colloidal stability in aqueous media, large pore size (4–20 nm) and a significant drug loading. Drug release studies demonstrated a pH-responsive behavior with higher 5-FU release at pH > 5 (colon conditions) due to PAA expansion and pore opening, and lower release at pH < 5 (gastric conditions). To assess the biological properties, different *in vitro* studies of cytotoxicity, cell proliferation and uptake were conducted on normal and cancerous human colorectal adenocarcinoma cells, resulting in a higher biocompatibility and enhanced targeting ability toward CRC cell lines. An *in vivo* pilot study was also conducted using the AOM/DSS mouse model, demonstrating that targeted 5-FU-loaded SiO_2@MSNs, administered at tenfold lower doses than standard chemotherapy, substantially reduced tumor burden, particularly large polyps, while preserving colon tissue integrity. These findings highlight the potential of SiO_2@MSNs as pH-responsive nanocarriers for targeted CRC therapy.

Acknowledgments. This work was supported by Bilateral Project CNR-RFBR Russia Joint research project (2021-2023); NHYLODEA (PRIN 2022 PNRR, code P2022RLFZB CUP H53D23007980001); PNRR(MCNT2-2023-12377885): "Handling of mesenchymal-like circulating pancreatic cancer cells as an innovative approach to restrain disease progression"

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-D O14-

Decoding Molecular Information via Mass Transport–Electron Transfer Coupling

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In living systems, molecular communication (MC) elucidates how information is encoded and propagated through the controlled release, transport, and selective recognition of chemical species—a principle that has inspired artificial MC networks and the broader vision of the Internet of Bio-NanoThings (IoBNT), in which nanoscale biological or bio-inspired units act as nodes capable of exchanging molecular messages via physicochemical processes such as diffusion, enzymatic turnover, membrane transport, and redox conversion. Within this framework, the design of molecular receivers remains a central challenge, as a receiver must not merely register concentration changes but decode the informational content embedded in the chemical state of the medium. Here we introduce an electrochemical receiver that addresses this challenge by directly coupling mass transport with interfacial electron-transfer kinetics. Perturbations in the chemical environment—whether concentration pulses, redox transitions, or the formation of reactive intermediates—modulate the electrochemical potential of the solution, while an electrode placed at the boundary acts as a well-defined electron reservoir that converts these perturbations into reproducible current signatures encoding the transmitted message. This strategy provides a physically grounded mechanism linking molecular events to electronically readable outputs. Our experimental results show that electrochemical interfaces can reliably detect, decode, and quantify molecular information. Despite its simplicity, the platform performs the essential tasks required for IoBNT systems—detecting, translating, and modulating chemical signals—and lays the groundwork for future hybrid communication technologies that integrate molecular processes with conventional electronics.

Acknowledgments. This work was supported by the European Union's Horizon Europe research and innovation program under the EIC Pathfinder Open project ERMES – Information Transfer Between Medical Doctors and Implanted Medical Devices via Artificial Molecular Communication (Grant Agreement No. 101185661).

-D P1-

Light-Triggered Communication Between Synthetic and Living Cells via Photoswitchable Membranes

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This study explores a hybrid system for communication between synthetic and biological cells, using giant unilamellar vesicles (GUVs)[1] as biomimetic platforms for controlled signaling molecule release. GUVs were engineered by functionalizing the lipid membrane with an azobenzene-based photoswitchable molecule that undergoes reversible *trans*-to-*cis* isomerization upon UV irradiation, inducing destabilization of the lipid bilayer and ultimately leading to the complete disruption of the vesicular compartment.
The developed approach enables precise spatiotemporal control over the release of GUV contents, allowing selective activation of individual vesicles or defined populations via localized UV irradiation. ATP and histamine were loaded into GUVs as model signaling molecules, given their role as agonists of calcium-mediated signaling pathways [2]. Upon UV-triggered isomerization of the photoswitchable molecule, membrane destabilization caused rapid release of the cargo into the extracellular microenvironment of HeLa cells, where receptor binding elicited a measurable increase in cytosolic calcium (Figure 1). These results demonstrate that photoswitch-functionalized lipid vesicles represent a versatile platform for interfacing synthetic compartments with living cells, opening new perspectives in protocell engineering, synthetic cell-to-cell communication, and targeted drug delivery.

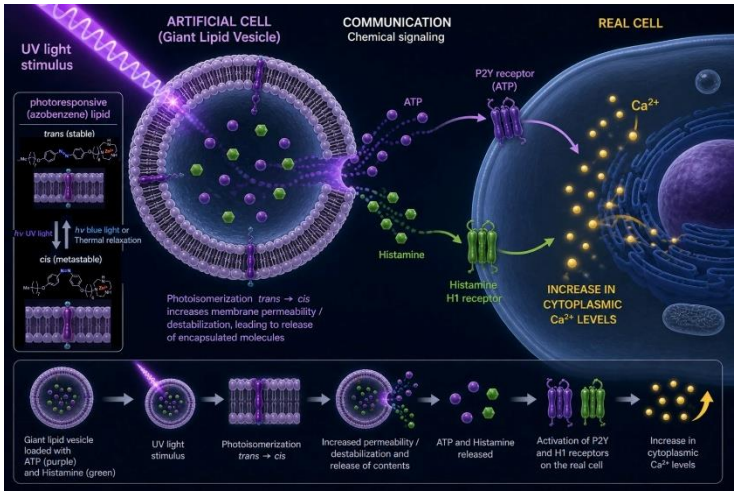

Figure1. Schematic representation of light-controlled communication between an artificial and a living cell. UV-induced trans→cis isomerization of azobenzene lipids incorporated in GUV membranes triggers cargo release (ATP and histamine), which activates P2Y and H1 receptors on target cells, leading to intracellular calcium mobilization.

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-D P2-

A Combined EPR Spectroscopy and Metabolomic Approach for Evaluating Oxidative Stability in Wines

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The oxidative stability of white wines depends on the ability of the matrix to control reactive oxidant species and prevent quality deterioration, such as aroma loss and browning. Unlike red wines, where phenolics dominate antioxidant activity, the molecular basis of oxidative stability in white wines remains less understood. Recent studies indicate that nitrogen- and sulfur-containing compounds, including amino acids and peptides, play a key role by acting as nucleophiles and radical scavengers, thereby limiting oxidation processes. Understanding these mechanisms is crucial for predicting wine aging potential and identifying effective alternatives to sulfites [1]. In this context, spin-trapping electron paramagnetic resonance (EPR) technique represents a powerful tool to directly monitor radical formation and evaluate oxidative stability [2,3]. In this study, oxidative stability was assessed by inducing radical formation through accelerated oxidative induction and monitoring the radical adducts formation with PBN (N-tert-butyl-a-phenylnitrone) spin trap [4]. A total of 14 samples from Favorita grape, produced under different microvinification conditions, were analyzed. The study validates EPR spectroscopy as a rapid and effective tool for assessing oxidative stability and discriminating among different winemaking treatments. EPR data were integrated with metabolomic analyses, revealing a strong and statistically significant correlation with results obtained from climatic chamber tests, in which samples were subjected to prolonged thermal stress to accelerate aging, monitored through color variation (ΔE). The statistically significant correlation ($p < 0.01$) between ΔE values and EPR-derived oxidative stability markers further supports the use of EPR as a predictive tool for shelf life assessment, confirming its suitability as a rapid and reliable method for evaluating oxidative stability in white wines.

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[2] M. Nikolantonaki et al. Food Chem. 2019, 270, 156.
[3] P. Han et al. CRFS 2026, 12, 101276.
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-D P3-

Investigation into the Sustainable Recovery of Bioactive Extracts from Turnip Greens Waste and Preliminary Encapsulation in Liposomes

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The agri-food industry plays a significant role in terms of environmental impact, mainly due to the high energy consumption, intensive use of water and massive production of waste. Thus, the valorization of agri-food residues is essential to promote the circular economy and enhance the sustainability of this sector. Among horticultural crops, members of the Brassicaceae family, including cabbage, cauliflower, and broccoli, hold considerable economic importance. Nevertheless, waste and by-products from such crops vary between 30 and 50 per cent of production [1], posing a significant economic and environmental concern. These byproducts still represent a resource of low-cost bioactive compounds that can be recovered and valorized. Among these, phenolic constituents represent the most abundant fraction of secondary plant metabolites and are of particular interest due to their antioxidant, anti-inflammatory, and antimicrobial properties [2].
This work proposes the valorization of wastes from turnip greens (*Brassica rapa* subsp. *sylvestris*), a typical cruciferous vegetable grown primarily in southern Italy, in the aim of obtaining bioactive extracts, rich in polyphenols, with antioxidant ant antimicrobial properties. Traditional methods of extracting Brassicaceae typically use aqueous alcohol solvents (mainly methanol-water). However, in line with the principles of green chemistry and to obtain extracts safer for the human health and the environment, in this study, methanol was replaced with ethanol. Furthermore, considering the compromise between its performance and the simplicity of the equipment, ultrasound-assisted extraction (UAE) was preferred over other emerging extraction methods and compared with conventional silent maceration (SM) on two different fractions of turnip greens waste. The Design of Experiments approach was used to evaluate the impact of solvent composition, solvent/matrix ratio, extraction technique and extraction time on the Total Phenolic Content and Trolox Equivalent Antioxidant Capacity of leaf and stems extracts, independently. Selected extracts were subsequently characterized for phenolic acid profile through HPLC analysis and tested for antibiofilm activity against six pathogenic strains, showing promising results in both biofilm formation and mature stages. Finally, preliminary tests were carried out on encapsulating the extracts in liposomes for potential applications in the nutraceutical field. The liposomes prepared were characterized from a physico-chemical standpoint and their antioxidant activity was assessed.

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-D P4-

Thylakoid Membranes as Biomaterial for in situ Oxygen Generation Against Ischemia- Reperfusion Injury

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Myocardial ischemia-reperfusion injury (IRI) remains a major cause of cardiomyocyte loss despite timely restoration of blood flow. While reperfusion is essential to salvage ischemic tissue, it also triggers oxidative stress, mitochondrial dysfunction and apoptosis [1], highlighting the need for innovative cardioprotective strategies. Here, we investigated isolated spinach-derived thylakoid membranes as a cell-free photosynthetic biomaterial for oxygen delivery in a human cardiomyocyte model of oxygen-glucose deprivation and reperfusion (OGD/R) [2][3]. Thylakoids were extracted from Spinacia oleracea leaves and characterized for light-driven oxygen evolution. Under optimized conditions, illuminated thylakoids generated up to ~600 nmol mL^{-1} oxygen and maintained photosynthetic activity for over 3 h at 25 °C. Because oxygen evolution rapidly declined at 37 °C, a spatially separated platform was developed in which thylakoids were maintained in external illuminated compartments connected to AC16 human cardiomyocytes through a shared gaseous phase, enabling oxygen transfer without direct contact between the photosynthetic material and cells. During OGD/R experiments, photosynthetic oxygen supplementation was applied during the final hour of ischemia. Assessment of delayed apoptosis after 48 h of reperfusion revealed a marked reduction in cleaved caspase-3-positive cells in thylakoid-treated cultures compared with untreated OGD/R controls, indicating significant attenuation of reperfusion-associated apoptotic injury. These findings demonstrate that isolated thylakoid membranes can function as light-responsive oxygen-generating biomaterials capable of modulating cardiomyocyte fate after ischemic stress. Although thermal instability at physiological temperature currently limits direct application, this work provides proof of concept for the use of simplified photosynthetic biomaterials as controllable oxygen delivery systems and supports further development of thermally robust photosynthetic platforms for ischemic tissue protection. (Figure 1).

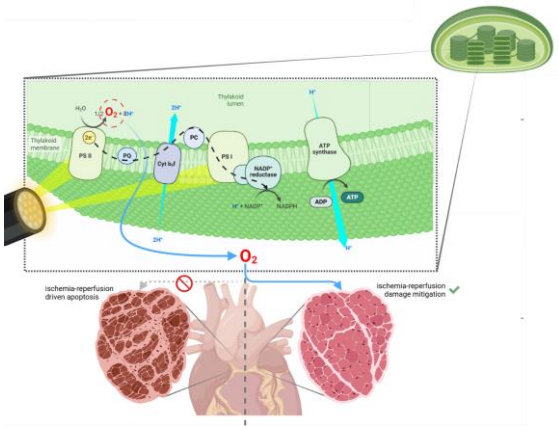

Figure1. Concept of the spatially separated thylakoid–cardiomyocyte platform. Schematic illustration of the therapeutic concept, where isolated spinach thylakoid membranes serve as a light-responsive biomaterial to generate molecular oxygen under illumination and mitigate ischemia-reperfusion injury.

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[3] Y.B. Lv et al. Nat. Commun. 2025, 16, 7678.

-D P5-

SERS Nanostructures with Engineered Active Peptides against an Immune Checkpoint 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.
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].

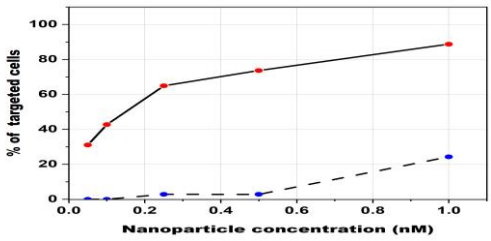

Figure1. Activity of the SERS nanostructure for the targeting of MDA-MB-231 over-expressing PD-L1. The % of the cell with a positive targeting, obtained with SERS signals for each single cell, is plotted against the concentration of nanoparticles used for incubation (HS-PEG-Lys3-Gly2-CLP002-NH2: continuous line, HS-PEG-Lys3-Gly2-sCLP002-NH2: dashed line).

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-D P6-

Advanced Nanoplatforms for Targeted Drug Delivery to Circulating Tumor Cells in Pancreatic Cancer

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[4]Laboratory of Molecular Medicine, National Institute of Gastroenterology, IRCCS "S. deBellis", 70013 Bari, Italy
[5]CNR-NANOTEC, Institute of Nanotechnology, National Research Council, Campus Ecotekne, Lecce 73100, Italy
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Pancreatic ductal adenocarcinoma (PDAC) remains one of the most lethal solid tumors, with a five-year survival rate below 10%. Its poor prognosis is driven by aggressive biology, including rapid progression, intrinsic chemoresistance, and early metastatic dissemination. Increasing evidence indicates that tumor spread occurs at the early stages through the release of circulating tumor cells (CTCs). particularly mesenchymal-like sub-populations that play a key role in invasiveness, therapy resistance, and metastatic colonization [1]. Targeting CTCs therefore represents a promising strategy to limit disease progression and intercept metastasis. However, conventional chemotherapy is often ineffective due to poor bioavailability, rapid systemic degradation, a non-specific distribution, ultimately leading to reduced therapeutic efficacy.
In this context, nanotechnology-based drug delivery systems offer attractive opportunities to improve therapeutic efficacy by enhancing drug stability, bioavailability, and selective delivery. To address these challenges, three distinct nanocarrier platforms were investigated: lipid-based nanoparticles (NPs), polymeric NPs and mesoporous silica NPs (MSNs). These systems were specifically loaded with thalidomide (TAL), a potent immunomodulatory drug whose clinical potential is often limited by poor solubility and systemic side effects [2].
To identify the most promising nano formulation for targeting both primary tumour and CTCs, a comprehensive physical-chemical characterization was performed, including size, morphology, encapsulation efficiency and drug loading. *In vitro* studies were conducted on both normal and tumor cell models, in 2D and 3D culture systems, to evaluate the biological performance of the nano formulations, in terms of biocompatibility, cellular uptake, and therapeutic efficacy.
In addition, extracellular vesicle (EVs) membranes extracted from CTC cultures were explored as next-generation physiological delivery systems with enhanced biological compatibility. EVs were isolated, characterized and loaded with a chemotherapy agent, namely 5-fluorouracil (5-FU), *via* electroporation. These results provide a proof-of-concept for the integration of CTC-derived EV membranes with synthetic nanocarriers in the design of biomimetic hybrid nanoplatforms for PDAC.

Acknowledgments. This work was supported by PNRR(MCNT2-2023-12377885): "Handling of mesenchymal-like circulating pancreatic cancer cells as an innovative approach to restrain disease progression".

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-D P7-

Characterization of Extracellular Vesicles and Circulating Tumor Cells from Pancreatic Cancer Patients

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Pancreatic ductal adenocarcinoma (PDAC) remains one of the most aggressive tumour [1], with limited options for early detection and monitoring. Circulating tumor cells (CTCs) and their secreted extracellular vesicles (EVs) represent promising sources of minimally invasive biomarkers [2]. However, the molecular and functional features of EVs specifically derived from CTCs (CTC-EVs) in PDAC are still poorly understood.
This study aimed to isolate and characterize CTCs and their EVs obtained from the peripheral blood of pancreatic cancer patients, and explore their potential as disease-specific biomarkers.
CTCs were isolated using an EpCAM-based immunomagnetic beads from blood samples of PDAC patients. After short-term culture, CTCs underwent citofluorimetry and immunofluorescence. EVs released into the conditioned medium were collected and characterized by Dynamic Light Scattering analysis (DLS), Scanning electron microscopy (SEM), and Western blot for canonical EV markers and tumor-related proteins. Comparative analyses were performed with EVs derived from tumor and non-tumor pancreatic cell lines (MIA-PaCa-2, PANC-1, HPDE).
Flow cytometry confirmed tumor origin of cells (EpCAM+). They displayed a hybrid phenotype, co-expressing epithelial markers (EpCAM, CK18, CK19) and epithelial-to-mesenchymal transition drivers Vimentin and TWIST, indicating marked plasticity and metastatic potential. Preliminary data indicate that CTCs from PDAC patients release a heterogeneous population of EVs with an average size of 100–150 nm. Scanning electron microscopy revealed CTC surface architectures distinct from pancreatic cancer lines (MIA-PaCa-2, PANC-1), suggesting adaptations for haematogenous survival, while EVs exhibited intact, well-defined morphology. CTC-EVs express both general EV markers and tumor-associated proteins.
Our findings suggest that extracellular vesicles released by circulating tumor cells carry molecular and phenotypic signatures reflective of the metastatic behavior of pancreatic cancer.
Further validation in larger cohorts could establish CTC-EVs as a novel liquid biopsy tool for disease monitoring and therapeutic stratification in PDAC

Figure1. 3D model of CTC-derived EVs in PDAC, showing EMT markers and liquid biopsy potential.

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-D P8-

Enhancing the Sensitivity of LFIA for Ferritin Quantification via LIBS

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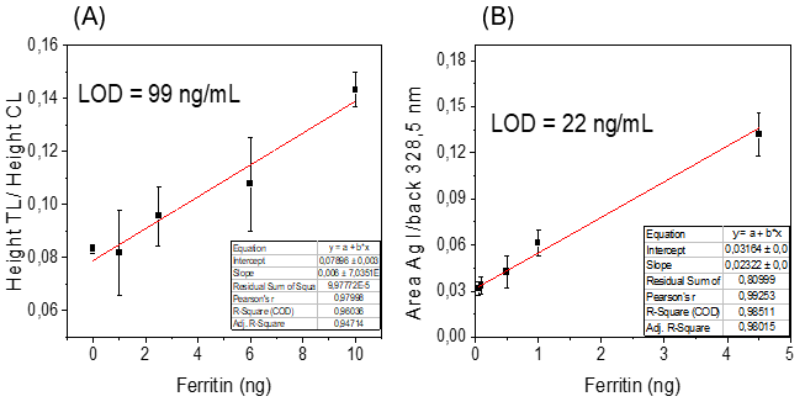
Iron is an essential element for almost all living organisms by participating in a wide variety of metabolic processes. Disorders of iron metabolism are among the most common diseases of humans and encompass a broad spectrum of conditions with diverse clinical manifestations, ranging from anemia to iron overload-induced chronic inflammation. Ferritin is a highly conserved iron-binding protein that consists of heavy chain (FTH) and light chain (FTL) ferritin. Together, these subunits self-assemble to form the cage-like structure responsible for sequestering iron within the core in a non-toxic form [1]. Serum ferritin levels are widely used to measure the quantity of iron accumulation in the body, with ferritin levels directly proportional to the amount of iron reserves. Various laboratory methods are used to measure ferritin concentrations, e.g., enzyme-linked immunosorbent assay (ELISA), immunoturbidimetric assays and microarray-based technologies. Despite their widespread utility, these methodologies present notable trade-offs between cost and complexity; highly automated, sensitive systems often incur prohibitive equipment and reagent costs, whereas more economical alternatives frequently suffer from labor-intensive workflows or lower analytical sensitivity. The objective of this study is to develop a novel ferritin detection method by coupling lateral flow immunoassay (LFIA) technology with laser-induced breakdown spectroscopy (LIBS). By integrating simplicity, rapid turnaround time, and low cost of LFIA with the high analytical sensitivity and multi-elemental capability of LIBS, this hybrid approach aims to provide a highly efficient alternative for routine ferritin quantification. Following LFIA development, the test strips were scanned to construct an initial calibration curve based on optical density measurements (Fig. 1A). Subsequently, direct LIBS analysis was performed on the same strips to establish a secondary spectroscopic calibration curve (Fig. 1B). Notably, the integration of LIBS led to a significant enhancement in analytical sensitivity, drastically lowering the limit of detection (LOD) compared to the optical density approach. This spectroscopic refinement brought the detection threshold down to 22 ng/mL, closely approaching the clinical threshold defined by the World Health Organization (WHO) for iron deficiency (15 ng/mL). This advancement demonstrates the high sensitivity of this dual-quantification strategy and its potential viability for routine screening.



Ferritin calibration curves obtained via LFIA (A) and LIBS (B).

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Session E

Electrochemistry, Catalysis, and Energy Conversion

-E O1-

Combined Atomic Layer Deposition and Sputtering of ZnO/Cu Coatings for CO_2 Electroreduction

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Over the last century, the intensification of human activities has amplified anthropogenic impact on the environment, increasing greenhouse gas emissions, in particular CO_2, and highlighting the finite nature of fossil energy resources. The reduction of CO_2 to value-added products offers a promising solution to both environmental issues. In this frame, electrocatalytic CO_2 reduction (CO_2R) represents a valuable approach for the production of C_1-C_3 molecules, but the design of a suitable catalyst with optimized activity and selectivity is crucial to obtain a competitive process.

Among CO_2R electrocatalysts, Cu/ZnO nanocomposites has been widely investigated for their remarkable performances. Indeed, metal oxides are often used in combination with metal nanoparticles (NPs) since the selectivity and performance of the electrocatalyst are mainly controlled by the metal/metal oxide interface and by the synergistic effect between different phases of the catalysts rather than by the metal NPs alone [1]. A further improvement of the CO_2R yield can be determined by the choice of a porous gas diffusion layer (GDL) electrode, as it allows an increase the CO_2 concentration at the electrode surface, lowering the competitive hydrogen evolution reaction (HER) [2]. However, minimizing the catalyst loading without affecting the overall efficiency of the electrocatalytic process represents still a major challenge in the field. In this framework, Atomic Layer Deposition (ALD) with its precise control over the deposited film thickness and conformality represents a choice of election, enabling the preservation of the porous, high-surface-area structure of the GDL.

In this work, ALD coupled with RF magnetron sputtering for the deposition of a ZnO/Cu coating on carbon paper (CP) is reported. Electrodes were prepared at a process temperature of 100°C by alternating the deposition of a variable number of ZnO and Cu layers on CP: the total thickness of the catalyst layer was kept constant at 60 nm and 80 nm, while the Cu/ZnO ratio in the coating was variated between 0.12 and 0.58. The morphology and chemical composition of the resulting samples were thoroughly characterized. Scanning Electron Microscopy shows the retention of the porous structure of the CP, confirming the conformality of the deposited catalyst layer. X-Ray Photoelectron Spectroscopy analyses highlight the presence of both ZnO and Cu (Cu(I) and Cu(II) oxides). Additionally, Cu/Zn ratio for all samples is determined by Energy Dispersive X-Ray Spectroscopy. In order to investigate the electrochemical CO_2R performance of the electrodes, open circuit voltage, linear sweep voltammetry and chronopotentiometry measurements were conducted in a zero-gap cell where a humidified CO_2 flow (30 NmL/min) was streamed. The fabricated electrodes were used as cathodes in the cell, while a Ni mesh served as the anode. Preliminary results show promising selectivity towards CO and the production of trace amount of alcohols, while HER remains negligible. Post operation analyses are ongoing to rationalize the results obtained. This eCO2RR system is compatible with PV energy input requiring < 2.5V of applied cell potential, offering an affordable solution for solar fuels production with high CO_2 conversion efficiencies.

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-E O2-

Spectroelectrochemical Insights into Heterogeneous Catalysts for the CO_2 Reduction Reaction

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Electrochemical CO_2 reduction (CO_2ER) represents a promising strategy for carbon capture and utilization, enabling the conversion of CO_2 into value-added products [1]. Layered Double Hydroxides (LDHs) have emerged as promising candidates, although the nature of their active sites and surface processes for CO_2 activation remain poorly understood [2,3].
This work investigates Zn-Al LDHs with different Zn^{2+}/Al^{3+} molar ratios (2:1, 1:1, and 1:2) as electrocatalysts for the CO_2 reduction to CO. The catalysts were characterized using various characterization methods such as XRD, STEM-EDX, and volumetry analysis. Infrared (IR) spectroscopy, in absence of applied potential, was employed to investigate surface carbonate species by using a Pike HATR cell, in which a CO_2-saturared H_2O flow was sent in contact with the sample previously deposited on the ATR crystal. The catalytic performances were evaluated under applied potential using a Pike Technologies VeeMAX III accessory coupled with a modified Pike-Jackfish II cell to perform electrochemical tests (Figure 1a). Experiments were performed in 1 M $KHCO_3$ electrolyte using a Pt wire as counter electrode and an Ag/AgCl electrode as reference electrode. Electrochemical measurements revealed that CO selectivity increased with Al content, indeed the Zn–Al LDH 1:2 sample showed the best performance, reaching 40% selectivity toward CO at −1.4 V vs RHE. IR measurements revealed that, upon applying potentials from -0.3V to -1.6V vs Ag/AgCl, the original carbonate bands progressively disappeared, while an intense band at 1390 cm^{-1} grew, indicating the formation of key reaction intermediates (Figure 1b).
In conclusion, these results highlight the influence of Zn-Al LDH composition on catalytic selectivity and demonstrate how the combination of electrochemical measurements and IR spectroscopy can provide molecular insights into surface species involved in CO_2 conversion.

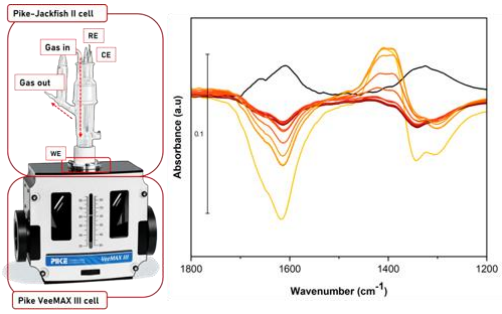

Figure 1. Schematic representation of the IR-SEC cell (a); ATR-IR spectra in difference in the 1800-1200 cm^{-1} range of Zn-Al LDH 1:2 under CO_2-saturared H_2O flow and application of potential (b).

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-E O3-

Structural Insights on FeZnCuK Catalysts for Mild Photothermal CO_2-to-Hydrocarbons

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This work investigates the catalytic performance of FeZnCuK mixed-metal oxide, a catalyst derived from non-critical raw materials, for the photothermal conversion of CO_2 into light hydrocarbons under mild conditions (250°C and 1bar of pressure) [1]. Light irradiation promotes the redox activity of catalytic sites, mitigating the conventional thermocatalytic conditions of the process.The catalyst in its final form will be embedded in a Double-Active Membrane (DAM), enabling simultaneous CO_2 capture and catalytic conversion within a single device. Within the "DAM4CO2" EIC-Pathfinder project [2], the system aims to perform Reverse Water-Gas Shift (RWGS) and Fischer–Tropsch synthesis (FTS) reactions in cascade using CO_2 separated from flue gas streams. Structural and physicochemical characterization of the catalyst was carried out on both its powder and membrane form using Powder X-Ray Diffraction, UV-Vis spectroscopy, N_2 adsorption/desorption, in situ IR and Raman spectroscopy, CO_2 adsorption isotherms, and H_2-TPR analyses. Based on the information collected by characterization data, thermocatalytic tests were performed with different activation approaches to highlight the importance of the balance between metal oxides, such as magnetite, that catalyze the RWGS reaction, and metal carbides, used for the FTs reaction in order to maximize the longer-chain hydrocarbons products in mild conditions[3,4]. The reaction conditions were selected to ensure compatibility with the polymeric membrane (based on a polymer of intrinsic microporosity [5]). Three activation protocols were evaluated: direct activation under reaction conditions (orange bars in Figure 1), H_2 reduction at 325 °C (light blue bars in Figure 1), and carburization in syngas ($CO:H_2$ = 1:2) at 270 °C. (green bars in Figure 1). Between them the syngas carburization provided the highest productivity, indicating a sweet spot between oxide and carbide phases. Spectroscopic analyses revealed that the membrane-embedded catalyst could not fully reach the active phase observed in the powder material. Although pre-carburization prior to membrane incorporation slightly decreased productivity, the catalyst exhibited remarkable stability (violet bars in Figure 1), maintaining identical activity after three months. These results highlight the potential of FeZnCuK-based catalysts for integration into DAM systems for combined CO_2 capture and catalytic utilization under mild conditions.

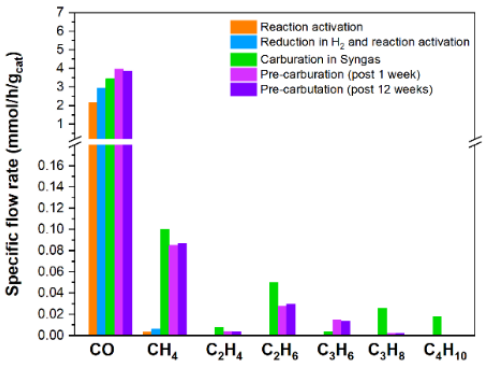

Figure 1. Catalytic test at 250°C.

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-E O4-

Tuning Bacteria-Electrode Interfaces for Biohybrid Electrochemical Systems

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Bacteria-electrode interfaces in biohybrid electrochemical systems employing anoxygenic photosynthetic bacteria offer the unique feature to accomplish semi-artificial photosynthesis, where sunlight energy conversion is coupled to current generation, removal of organic compounds, and solar fuel production [1,2,3]. The complex enzymatic machinery of photosynthetic purple bacteria combines light-induced reactions to their respiratory metabolism, making these processes possible, however, the bacterial cells must be efficiently wired to an electrode surface, and the electron transfer process must be tuned to avoid altering the fragile redox balance of the biological organisms [4].
This work will present the approaches undertaken by our group to tackle these challenges, with the implementation of biocompatible polymers and inorganic nanomaterials towards facilitating the extracellular electron transfer and drive a desired process while avoiding redox imbalance [5,6]. The engineering approaches implemented allowed obtaining systems capable of H_2 and syngas production, enhanced current generation, waste treatment and self-powered monitoring of contaminants [7]. Finally, the current and future challenges for the implementation of these devices for distributed, low cost, waste reuse and environmental monitoring will be discussed.

Acknowledgements. This work has been developed within the project "Photoactivated scalable diffuse production of Green Hydrogen through sustainable materials and processes" SOLE-H2 2025-2026 (Project code. RSH2A_000004) funded by the European Union – NextGenerationEU through MASE within National Recovery and Resilience Plan Mission 2 "Green revolution and ecological transition", Component 2 "Renewable energy, hydrogen, network and sustainable mobility", Investment 3.5 "Research and Development on Hydrogen". This work was made possible thanks to funding provided under the bilateral agreement between CNR and FAPESP (Italy-Brazil), as part of the project NATURE, for the 2024–2025 biennium.

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-E O5-

Stability and Electrochemical Properties in Multi–Doped Sr Ferrates

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Solid Oxide Fuel and Electrolysis Cells (SOFCs and SOECs, respectively) are promising technologies for efficient energy conversion and storage. Consequently, the development of advanced materials for these devices remains a central topic in materials science. Among the most promising candidates, $SrFeO_3$–based systems, belonging to the ABO_3 cubic perovskite family, have emerged as potential fuel electrodes, due to their mixed ionic–electronic conductivity, catalytic activity and structural stability under H_2–atmospheres.
In this work, six multi-doped Sr ferrates were synthesized via solution combustion synthesis, incorporating Ce^{4+}, Y^{3+} or Sm^{3+} at the A-site and Ti^{4+}, Al^{3+} or Mo^{4+} at the B-site, with the aim of exploiting the synergistic effects of simultaneous A and B sites doping to finely tune catalytic, ionic and electronic transport properties [1]. A systematic investigation of the resulting $Sr_{0.9}Ce_{0.1}Fe_{0.9}Ti_{0.1}O_{3-\delta}$ (SCFT), $Sr_{0.9}Y_{0.1}Fe_{0.9}Ti_{0.1}O_{3-\delta}$ (SYFT), $Sr_{0.9}Sm_{0.1}Fe_{0.9}Ti_{0.1}O_{3-\delta}$ (SSFT), $Sr_{0.9}Ce_{0.1}Fe_{0.9}Al_{0.1}O_{3-\delta}$ (SCFA), $Sr_{0.9}Ce_{0.1}Fe_{0.9}Mo_{0.1}O_{3-\delta}$ (SCFM), and $Sr_{0.9}Y_{0.1}Fe_{0.9}Mo_{0.1}O_{3-\delta}$ (SYFM) systems was performed by electrochemical impedance spectroscopy (EIS) on symmetrical cells fabricated by depositing the electrode powders onto a Sm-doped ceria supporting electrolyte and tested under a H_2/N_2 = 20/80 atmosphere (2% humidity). These analyses were complemented by scanning electron microscopy (SEM), X-ray diffraction (XRD), H_2-Temperature programmed reduction (TPR), thermogravimetric analysis (TGA) and µ-Raman spectroscopy studies on both pristine powders and electrodes after electrochemical testing. The results indicate that Ce^{4+} substitution at the A-site provides the best compromise between polarisation resistance (Rp) and activation energy (Ea), especially when combined with Mo and Al at B-site (Figure 1).

Acknowledgements. The project "Ricerca e sviluppo di tecnologie per la filiera dell'idrogeno (POR H_2)", AdP ENEA CNR CUP: B93C22000630006 is acknowledged for financial support.

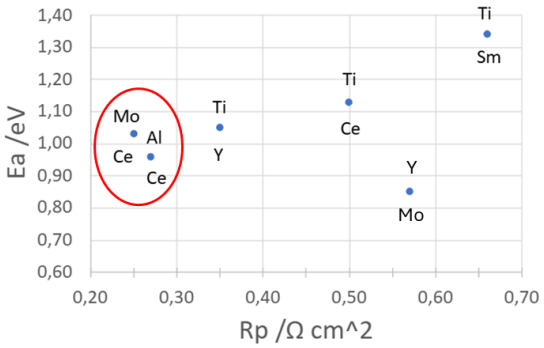

Figure 1. Activation Energy (E_a) vs. polarization resistance (R_p) for the six multi-doped Sr ferrates.

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-E O6-

The Gilded Cage: Towards High Thermoelectric Efficiency in Single-Filled Skutterudites

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In the quest for the transition to novel and clean energy sources, a fundamental step is the minimization of wasted energy, both in energy production and industry. A promising approach to this problem is the conversion of the product of wasted energy – waste heat – into usable electricity; this process, called heat harvesting, can be performed by thermoelectric generators (TEGs), thanks to the Seebeck effect.
In order to make large scale heat harvesting a reality, efficient TEGs are needed, and therefore more suitable thermoelectric materials ought to be developed; this means lowering their cost and improving their efficiency; the latter is defined by the figure of merit ZT [1].

$$ZT = \frac{S^2\sigma}{k}T$$

with *S* being the Seebeck coefficient, *σ* the electrical conductivity, *k* the thermal conductivity, *T* the absolute temperature, and ZT = 1 the conventional threshold for being considered a promising material.
Among the materials currently studied for thermoelectric applications, (Fe,Ni)-based filled skutterudites represent a relevant family [1-3]. In this work samples belonging to the filled skutterudite system $Nd_y(Fe_xNi_{1-x})_4Sb_{12}$ were studied as thermoelectric materials. This system is interesting due to the presence of a large cavity in the centre of the unit cell, which can host a large ion, called filler, able to strongly vibrate [2,3], thus reducing the phonon contribution to thermal conductivity.
The synthesized samples were studied with a variety of techniques of structural and thermoelectric characterization, along with the EXAFS study of the Nd, Fe and Ni absorption edges, so as to better investigate the filler vibration.
What resulted from this study is that Nd appears as an optimal filler, allowing for a high occupancy of the cavity, and a strong suppression of thermal conductivity, which results in a maximum ZT of ~1 for *p*-type compositions and ~0.5 for *n*-type ones.

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-E O7-

Interference and Plasmonic Effects in Dielectric/Metal/Dielectric Multilayers for Semi-Transparent Perovskite Solar Cells

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Semi-transparent perovskite solar cells (ST-PSCs) are an emerging photovoltaic technology combining high efficiency with semi-transparency, that open up new applications such as building-integrated photovoltaics and tandem cells [1]. Key element in ST-PSCs is the top electrode, which should ensure efficient charge collection while maintaining high optical transmission [2]. Conventional ultrathin metallic films provide good electrical conductivity but often suffer from significant optical losses. Dielectric/metal/dielectric (D/M/D) multilayers represent an effective strategy to overcome these limitations [3-4]. In these structures, an ultrathin metallic layer is sandwiched between two dielectric films, enabling a balance between high conductivity and optical transparency. Their optical response is governed by the interplay between multiple interferences within the multilayer stack and plasmonic effects associated with the surface electrons in the metallic layer, which together enable spectral tuning of transmittance and reflectance in the visible and near-infrared range [2]. In this work, symmetric and asymmetric Au-based D/M/D multilayers were investigated and integrated as transparent electrodes in ST-PSCs. MoO_3 and WO_3 were selected as dielectric layers (D) due to their suitable optical properties and compatibility with device fabrication. Multilayer stacks with architecture D_1 (6 nm) / Au (10 nm) / D_2 (0–70 nm) were deposited by thermal evaporation and characterized using a multi-technique approach including Secondary Ion Mass Spectrometry (SIMS), X-ray Photoelectron Spectroscopy (XPS) depth profiling, UV–Vis–NIR spectroscopy, and Atomic Force Microscopy (AFM). The optimized D_1/ Au/D_2 multilayers were successfully integrated into ST-PSCs, yielding devices with performance comparable to standard cells and independently tunable optical transmission in visible and NIR range.

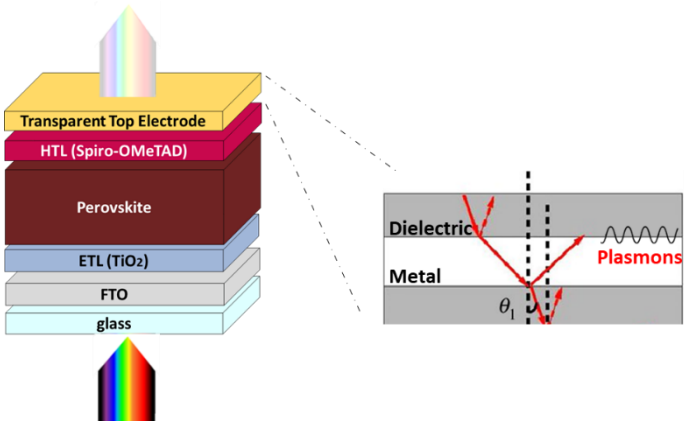

Figure 1. Schematic representation of ST-PSC integrated with D/M/D top electrodes characterized by optical properties tuned through a combination of interference and plasmonic effects.

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-E O8-

Controlling Energy Flow in *Rhodobacter Sphaeroides* Chromatophores via Selective Electron Transfer Inhibition

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The APACE project aims to exploit the light-harvesting capacity of natural photosynthetic antenna complexes to develop a bio-inspired, sunlight-pumped laser for space applications. The central strategy relies on harvesting solar radiation through biological antenna systems and redirecting the collected excitation energy toward an optical gain medium.
The purple bacterium *Rhodobacter sphaeroides* was selected as the primary biological model due to its highly organized photosynthetic apparatus, localized in the intracytoplasmic membrane. Upon controlled mechanical disruption, this membrane fraction can be isolated as sealed vesicles known as chromatophores [1], which preserve the native supramolecular organization of the photosynthetic machinery. Each chromatophore contains four main functional components: the Reaction Center (RC), where primary charge separation occurs; Light Harvesting Complex 1 (LH1), which surrounds the RC; Light Harvesting Complex 2 (LH2), peripheral antenna rings whose expression is regulated by light intensity; and the Cytochrome bc_1 complex, responsible for cyclic electron transport and proton gradient formation. Together, these pigment-protein assemblies absorb solar radiation and funnel excitation energy to the RC with near-unity internal efficiency.
In the context of APACE project, the native electron transport chain represents a competing quenching pathway that must be selectively suppressed to maximize the radiative output of the antenna. Several inhibitors targeting distinct points of the chain were employed, for example o-phenanthroline, which blocks electron transfer. The functional response of isolated chromatophores was monitored by absorption spectroscopy, steady-state fluorescence emission, and time-resolved fluorescence kinetics.
These results establish a robust and reproducible experimental platform for the functional characterization of bacterial photosynthetic membranes and provide a quantitative foundation for the rational design of the bio-hybrid photonic architecture at the core of the APACE project.

Acknowledgements. this work is financed by the project APACE (Towards a bio-mimetic sunlight pumped laser based on photosynthetic antenna complexes) ID 101161312, HORIZON-EIC-2023 PATHFINDERCHALLENGES-01-05.

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-E O9-

Boosted Ionic Conductivity in $Na_2B_{12}H_{12}/SiO_2$ Nanocomposite Electrolyte for Solid-State Sodium Batteries

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All-solid-state sodium metal batteries are an attractive alternative to Li-ion batteries due to their high energy density, improved safety, and the lower price of sodium. A major bottleneck is the development of suitable solid electrolytes with sufficient ionic conductivity and electrochemical stability [1]. Recently, the class of *closo*-borates demonstrated promising properties, such as high thermal stability, wide electrochemical window and low density [2,3]. However, fast ion motion occurs far from room temperature, triggered by a polymorphic phase transition [4]. Anion substitution, high-energy ball-milling and nanostructuring are effective strategies to favour the stabilization down to room temperature of the conductive crystalline phase in *closo*-borate salts [5,6]. Here, we report new all-solid-state sodium metal batteries based on sodium *closo*-dodecahydridoborate ($Na_2B_{12}H_{12}$) electrolyte and both Prussian white ($Na_2MnFe(CN)_6$) and TiS_2 as positive electrodes [7]. Although the pristine $Na_2B_{12}H_{12}$ has a low ionic conductivity at room temperature, the conductivity increases by more than three orders of magnitude upon nanocomposite formation, with mesoporous SiO_2, via high-energy ball-milling (Figure 1). The high ionic conductivity ($5 \cdot 10^{-4}$ S cm^{-1}, 30 °C) and oxidative stability (3.9 V *vs.* Na^+/Na) of $Na_2B_{12}H_{12}/SiO_2$ enable room-temperature battery operation with good capacity retention. Using a variety of techniques, including X-ray Raman scattering and electron energy loss spectroscopy, the presence of an interphase formed by an interfacial reaction between $Na_2B_{12}H_{12}$ and SiO_2 has been highlighted. The observed interface effects are highly influenced by the morphology of the oxidic framework and the preparation conditions of the nanocomposite.

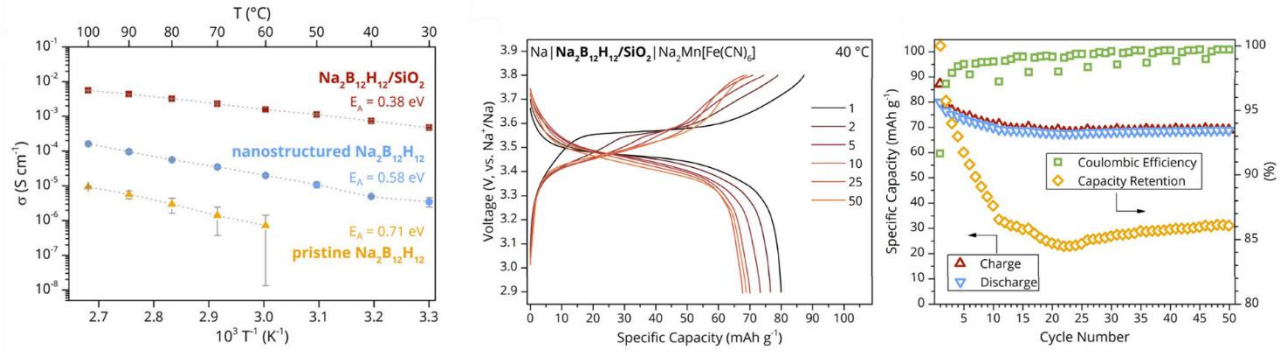

Figure 1. Ionic conductivity of $Na_2B_{12}H_{12}/SiO_2$ vs. pristine and electrochemical performance in solid-state cell.

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-E O10-

Enhanced Biophotocurrent Generation via Tailored Nano-Biointerfaces in *Rhodobacter Capsulatus* Biohybrids

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The combination of photosynthetic microorganisms and tailored nanomaterials represents a promising strategy for addressing the intrinsic performance limitations of energy conversion processes[1]. Coupling biological entities with carbon-based or inorganic nanostructures allows circumventing the narrow light-absorption ranges and slow extracellular electron transfer (EET) rates that generally constrain unmodified biological systems. This work explores the fabrication of resilient biohybrid architectures by modifying the purple non-sulfur bacterium *Rhodobacter capsulatus* with diverse nanostructures, including gold nanoparticles (Au NPs) and carbon dots (CDs). We specifically investigate the role of metallic NPs morphology in influencing electrochemical performance, testing Au spherical nanoparticles or nanostars, synthesized through simple colloidal approaches in aqueous solution[2]. This comparison provides a methodical assessment of how sharp-tip geometry, surface chemistry and localized surface plasmon resonance (LSPR) govern the charge transfer dynamics at the biotic-abiotic interface. Furthermore, the study investigates the utility of CDs - synthesized via a gycothermal solution phase approach from Resorcinol[3] - as biocompatible, light-harvesting components designed to augment the bacterial antenna complex and potentially enhance EET at the bacterium/electrode interface by leveraging π-electron delocalization inherent in their aromatic systems. Structural characterization via TEM elucidates the spatial organization and attachment of these nanostructures on the bacterial cells, while the integrity of the living scaffold is confirmed through viability tests performed over time. A pivotal aspect of this research involves the electrochemical interrogation of the biohybrid systems under anodic polarization using cyclic voltammetry (CV), chronoamperometry (CA) and electrochemical impedance spectroscopy (EIS) tests. Ultimately, this study allows for a comprehensive mapping of electron transfer mechanisms and proves how rational nano-biointerface engineering can enhance biophotocurrent harvesting, offering a robust solar-to-electricity platform that supports the global shift toward sustainable, carbon-neutral energy cycles.

Acknowledgements. This work has been developed within the project "Photoactivated scalable diffuse production of Green Hydrogen through sustainable materials and processes" SOLE-H2 2025-2026 (Project code. RSH2A_000004) funded by the European Union – NextGenerationEU through MASE within National Recovery and Resilience Plan Mission 2 "Green revolution and ecological transition", Component 2 "Renewable energy, hydrogen, network and sustainable mobility", Investment 3.5 "Research and Development on Hydrogen".

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-E O11-

The SIGNE Project: Composite Silicon Nanowire on Graphite Anodes with Ni-Rich Cathodes and Safe Ether based Electrolytes for High-Capacity Li-ion Batteries

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The EU-funded SiGNE project aims to develop advanced lithium-ion battery technology with higher energy density, optimized chemistry and faster charging time compared to state of the art. To achieve their goals, researchers will use a certain amount of silicon in the anode and electrically connect it to the graphite material. Nanowires will improve silicon's beneficial properties by increasing the amount of available surface area in contact with the electrolyte. A sustainable fiber-based separator will be developed, acting as an isolation layer between the anode and cathode. Researchers will demonstrate the innovative battery at scale to enable its adoption in electric vehicles. Furthermore, they will consider circular economic principles to address second-life applications once the lifespan of the battery comes to an end. Signe Project's partners include 7 research performing organizations (UL, KIT, ZSW, DLR, CID, FSU-Jena, U Roma) and 10 industry partners (Ferrari, TES-AMM, CRF-Stellantis, Analog Devices, TMEC, Sidrabe, Delfort and Solvionic) across 8 countries in Europe – Ireland, Germany, Spain, France, Italy, Austria, Poland, Ukraine and Latvia.
The research group at the University of Roma La Sapienza is contributing to the SIGNE project in respect to the advanced characterization of positive electrodes, novel electrolytes and separators, combining experiments and modeling. Moreover, the analysis of the gas release upon cycling is tackled to provide insights into the degradation chemistry of a novel NMC811 vs Si/C Li-ion battery formulation with liquid electrolyte based on ethereal solvents, with enhanced performance and safety [1-3].

Figure 1. Logo of the SIGNE project

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-E O12-

A Comprehensive DFT Study of the Mechanism of Selective PE Oxidation with a Ruthenium-Porphyrin Catalyst

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Petroleum-based plastics, particularly polyethylene (PE), are among the most widely produced polymers and play a central role in modern society. However, their high chemical inertness results in severe environmental persistence, creating major challenges for waste management and sustainability. Introducing controlled functional groups into polyethylene chains is therefore an attractive strategy to improve material properties and enable more efficient recycling or upcycling processes [1].
Selective oxidation represents a promising approach, as it allows the incorporation of polar functional groups (–OH and –C=O) into the polymer backbone without significantly affecting its molecular weight. This modification improves surface adhesion and expands the potential applications of polyethylene. In addition, isolated carbonyl groups within the polymer chain can promote programmed photodegradation, offering further sustainability advantages [2].
Among the catalytic systems explored for this transformation, ruthenium (Ru)-based catalysts have shown remarkable efficiency and selectivity [3], although the reaction mechanism remains poorly understood. In this work, Density Functional Theory (DFT) calculations were employed to investigate the electronic structure and reaction mechanism of a Ru-based catalytic system for polyethylene oxidation. The catalyst precursor, carbonylruthenium(II) tetrakispentafluorophenylporphyrin [Ru(II)(TPFPP)(CO)], is activated by a stoichiometric oxidant to generate an oxo-ruthenium species responsible for the selective introduction of –OH and –C=O functional groups [4].
Our simulations indicate that the active species is a Ru(V)(TPFPP)(O)(Cl) complex. The reaction proceeds through a concerted pathway in which C–H bond cleavage occurs simultaneously with C–O and O–H bond formation, without radical intermediates, providing a mechanistic explanation for the high selectivity observed experimentally. This work provides the first evidence of a "side-on" concerted mechanism in C–H activation mediated by oxo-ruthenium porphyrins and offers insights for the rational design of improved catalysts for polyethylene functionalization [5].

Acknowledgements. I would like to express my sincere gratitude to Giuseppe Santoriello and Michele Tommasini, members of the Computational Chemistry Team at the University of Salerno, for their valuable discussions, which played a crucial role in bringing this work to completion.

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-E O13-

Photoinduced Surface-Driven Bromination of Electron-Rich Arenes on Lead-Free $Cs_2AgBiBr_6$ Microcrystals under Sustainable Conditions

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Metal halide perovskites have emerged as versatile photoactive materials beyond photovoltaics, owing to their unique optoelectronic properties and tunable surface chemistry [1].

Here, we investigate the photocatalytic behavior of the lead-free Ag–Bi double perovskite $Cs_2AgBiBr_6$, focusing on how surface processes govern reactivity under visible-light irradiation. This system enables the selective bromination of aromatic substrates using hydrobromic acid as the bromine source, achieving high activity and selectivity under mild conditions.

Mechanistic investigations reveal that bromine radicals are generated directly at the perovskite surface and continuously regenerated through interaction with HBr, highlighting the critical role of surface chemistry in controlling charge separation and reactive intermediate formation (Figure 1). Radical-trapping and control experiments further support a surface-mediated catalytic cycle involving bromide species [2].

Compared to benchmark perovskite and perovskite-like materials (e.g., $CsPbBr_3$ and $Cs_3Bi_2Br_9$), $Cs_2AgBiBr_6$ exhibits superior photocatalytic performance and stability, maintaining activity over multiple cycles with minimal structural degradation.

These findings underscore the central role of perovskite surface chemistry in directing radical generation and photocatalytic function, providing new insights for the design of lead-free photoactive materials.

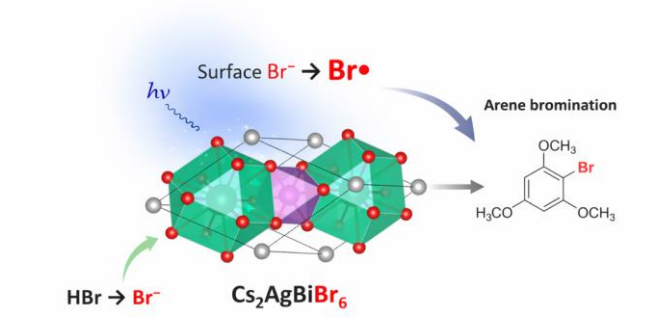

Figure 1. Surface-mediated generation and regeneration of bromine radicals over $Cs_2AgBiBr_6$ under visible-light irradiation, enabling photocatalytic arene bromination.

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-E O14-

Ultrafast Piezo-Assisted Engineering of Metal-ZnO Interfaces for Catalytic Applications

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Hybrid semiconductor/metal nanostructures have attracted considerable attention due to their enhanced optical, electronic, and catalytic properties arising from metal–semiconductor synergy [1–2]. In particular, decorating semiconductor photocatalysts with metal nanoparticles improves charge separation and interfacial transfer, boosting catalytic performance. Herein, we report a rapid (one minute) and sustainable piezo-assisted strategy for the synthesis of metal-decorated ZnO nanostructures via ultrasonic stimulation [3]. This approach exploits the intrinsic piezoelectric response of ZnO to directly reduce metal precursors on its surface, enabling nanoparticle nucleation without external reducing agents. By tuning the precursor concentration, nanoparticle size and surface density can be precisely controlled. TEM analysis (Fig. 1) confirms successful nanoparticles nucleation and size tunability. A key aspect of this work is the demonstration of the method's versatility toward different metal species, including Pd and Pt, underscoring its general applicability for the rational engineering of functional metal–semiconductor interfaces. Structural and spectroscopic analyses (TEM, XRD, XPS) confirm hybrid formation and clarify the interfacial structure–performance relationship. The optimized metal–ZnO systems exhibit remarkable activity in photo- and electrocatalytic processes, with promising results in environmental remediation and hydrogen production. Overall, piezo-assisted interfacial engineering emerges as a powerful and broadly applicable strategy for the rapid fabrication of metal–semiconductor hybrid catalysts for sustainable energy applications.

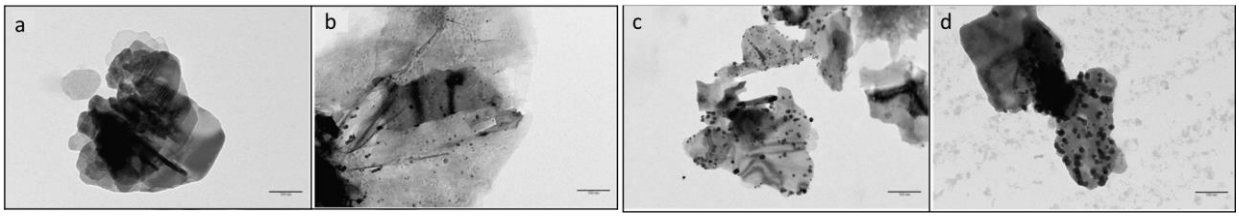

Figure 1. TEM images acquired for ZnO pristine (a) and ZnO with increasing concentration of Au nanoparticles (b-d).

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-E P1-

First-Principles Study of Perovskite Oxide for Solid Oxide Electrochemical Cells: Effects of Cation Substitution on Oxygen Ion Diffusion in $Sr_2Fe_{2-x}Mo_xO_{6-\delta}$

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Solid oxide fuel cells (SOFCs) and their reversible counterparts, solid oxide electrolyzer cells (SOECs), offer efficient routes for clean energy conversion water splitting and hydrogen storage [1]. However, efficient transport of oxygen ions and electrons in state-of-the-art solid-state electrolytes and electrodes typically requires high temperatures, which limit device durability and slow start-up times.
Lowering the operating temperature necessitates advanced electrode materials, particularly mixed ionic-electronic conductors (MIECs) [2]. Among these, perovskite oxides have emerged as promising electrodes for both the oxygen evolution and reduction reactions (OER/ORR), though the efficiency of the two opposite reactions being usually largely different. $Sr_2Fe_{2-x}Mo_xO_{6-\delta}$ (SFMO) has attracted attention as a potentially bifunctional system due to its high electronic conductivity, redox-active B-site cations (Fe/Mo), and capacity to accommodate oxygen vacancies. Following previous works [3,4], in this study, we investigate the impact of cationic substitution on oxygen vacancy formation and migration in SFMO via first-principles calculations, targeting improved oxygen ion transport.
Two Fe:Mo ratios (1:1 and Fe-rich 3:1) are considered to assess the effect of B-site composition, while partial substitution of A-site cation (Sr) with smaller (Ca) and larger (Ba) cations at two Sr:Ca:Ba ratio (6:1:1 and 4:2:2) allowed us to probe the role of lattice strain. Structural, electronic and energetic properties are investigated using Density Functional Theory (DFT+U), revealing trends relevant to the optimization of SFMO as a bifunctional electrode material for low-temperature solid oxide technologies.

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-E P2-

Peptide-based Materials as Active Components in Dye-Sensitized Solar Cells: Macrodipole-Mediated Electron Transfer and Amyloid Fibril Gel Electrolytes

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Protein and peptide-based materials are emerging as versatile and sustainable functional components in photoelectrochemical energy conversion devices. In this contribution, we present two complementary strategies for the integration of peptide-based materials in dye-sensitized solar cells (DSSCs), addressing both the molecular engineering of the photoelectrode interface and the development of bio-inspired gel electrolytes.

In the first part, we explore the use of helical peptides as molecular modifiers of photoelectrode surfaces. Helical peptides carry a permanent macrodipole along their backbone axis, arising from the cooperative alignment of amide bond dipoles. When anchored to an electrode surface, this macrodipole generates a local electric field at the interface that can actively modulate the rate and efficiency of interfacial electron transfer [1][2]. Building on previous work from our group on nucleobase pairing as a supramolecular assembly strategy [3], we designed a well-defined architecture in which a helical peptide, covalently modified with thymine at one terminus and adenine at the other, is anchored to a gold electrode through base pairing with a lipoadenine monolayer, and coupled to a thymine-functionalized ruthenium photoactive dye through adenine-thymine pairing at the opposite end. Photoelectrochemical measurements demonstrate that the system generates anodic photocurrent on both gold and TiO_2 electrodes extending the nucleobase pairing approach, previously used in our group to generate cathodic photocurrent with porphyrins [4], to anodic photocurrent generation.

In the second part, we present a bio-inspired gel electrolyte based on amyloid fibrils self-assembled from whey protein. Fibrillation is induced under acidic conditions, yielding elongated nanostructures that further associate upon exposure to high ionic strength to form a self-supporting hydrogel. The fibrils are characterized morphologically by AFM, and the gels mechanically by oscillatory rheology. The iodide/triiodide redox couple is incorporated directly into the fibril network without disrupting the gel structure, yielding a functional gel electrolyte suitable for integration into DSSC devices.

Taken together, these results demonstrate that peptide-based materials can play an active and multifunctional role in solar energy conversion opening new avenues for the development of bio-inspired photoelectrochemical devices.

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-E P3-

Carbon Dots-Modified TiO_2 and Bacterial Interfaces for (Bio)Photoelectrochemical Applications

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Over the past decade, European Union energy transition strategies have prioritized the development of sustainable hydrogen production to replace carbon-intensive fossil fuel reforming.
Solar driven-photocatalytic production of H_2 can be attained, among others approaches, by water splitting promoted by suitably designed all-inorganic photocatalysts or by photosynthetic bacteria, acting as hydrogen bioreactors converting organic substrate through their metabolism and enzymatic systems [1,2]. However, wide-bandgap semiconductors and biological systems often suffer from limited light harvesting and inefficient charge carrier transfer. In this context, Carbon Dots (CDs) are of interest as sensitizers due to their tunable optical properties and excellent electron transfer capabilities.
Herein, we explored two distinct (bio)nanocomposite systems for H_2 production: CD-sensitized mesoporous titanium dioxide (TiO_2) and CD-functionalized photosynthetic bacteria, *Rhodobacter capsulatus* (R. caps). Specifically, CDs synthesized via glycothermal solution-phase methods [3] were coupled with sol-gel derived TiO_2 [4] using both in situ and ex situ approaches. These materials were successfully deposited onto conductive platforms to evaluate their photo-electrocatalytic performance. Parallelly, the functionalization of *R. caps* with CDs to create high-performance bio-hybrid interfaces [5] was investigated through electrochemical measurements to evaluate the bio-photocurrent response. This allowed us to assess how CDs influence the extracellular electron transfer (EET) from the bacterial photosynthetic metabolism to the electrode surface.
These results aim to clarify the role of CDs within the composite system, providing a flexible framework for the design of stable and efficient systems for solar-to-hydrogen conversion.

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-E P4-

Biohybrid Photoelectrochemical Systems Based on *Rhodobacter capsulatus* Functionalized with Inorganic Nanoparticles for Green Hydrogen Production

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Green hydrogen is a key pillar of decarbonization strategies; however, its large-scale deployment requires the development of sustainable production technologies that can be integrated into real-world systems. In this context, biohybrid photoelectrochemical systems offer an innovative approach by combining the high versatility of biological processes with the functional properties of advanced materials [1]. This work investigates the development of biohybrid electrochemical systems based on the anoxygenic purple photosynthetic bacterium *Rhodobacter capsulatus*, either in its native form or functionalized with inorganic nanoparticles (NPs), coupled with a cathode electrode to drive bioelectrochemical H_2 production. Nanomaterials were utilized to tune the performance of these biohybrids [2]. Accordingly, gold NPs, owing to their high electrical conductivity, chemical stability, and biocompatibility, were employed to enhance electron transfer efficiency at the bio–electrode interface and ceria NPs were explored as functional materials for regulating electron fluxes and improving system stability under operating conditions. The obtained biohybrids were coupled to a polyhydroxybutyrate-carbon nanofiber electrode to develop electroactive biofilms performing H_2 production over a time scale of several days. Photoelectrochemical analyses indicated that nanostructural functionalization of the bacteria improves the cathodic response of the system compared with non-modified configurations, highlighting the potential of bio–nano hybrid platforms for solar-driven energy conversion. Advantages and challenges of the proposed approach will be discussed, laying the groundwork for the future development and characterization of cost-effective photoelectrochemical cells performing water treatment and the valorization of waste streams.

Acknowledgements. This work has been developed within the project "Photoactivated scalable diffuse production of Green Hydrogen through sustainable materials and processes" SOLE-H2 2025-2026 (Project code. RSH2A_000004) funded by the European Union – NextGenerationEU through MASE within National Recovery and Resilience Plan Mission 2 "Green revolution and ecological transition", Component 2 "Renewable energy, hydrogen, network and sustainable mobility", Investment 3.5 "Research and Development on Hydrogen".

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Session F

Materials and Nanoscience for Sustainable Technologies

-F O1-

Low-Temperature Formation of BCZT Piezoceramics: Kinetic Pathways and Structure– Property Relationships

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Lead-free piezoceramics, particularly $(Ba_{0.92}Ca_{0.08})(Ti_{0.95}Zr_{0.05})O_3$ (BCZT), have emerged as promising alternatives to PZT-based materials due to their excellent electromechanical properties [1]. However, conventional solid-state synthesis requires high calcination temperatures (>1200 °C), limiting scalability and increasing energy consumption. In this work, two innovative and sustainable approaches to BCZT synthesis are explored: (i) a water-assisted solid-state route combining high-energy ball milling and freeze-drying, enabling phase formation at ultra-low temperatures (700 °C) [2]; and (ii) a modified Pechini method employing ethylenediaminetetraacetic acid (EDTA) and glycerol as chelating and esterifying agents, achieving complete phase formation at 900 °C—about 300 °C lower than conventional chemical routes [3]. The water-based method, followed by an optimized two-step sintering process (900 °C for 3 h and 1280 °C for 6 h), yields dense ceramics with a pure tetragonal perovskite phase and excellent piezoelectric properties (d_{33} = 320 pC N^{-1}, k_p = 31.45%, ε_r = 3670, tanδ = 0.036 at 1 kHz). The Pechini-derived system, consolidated at 1400 °C with 91% relative density, exhibits a homogeneous grain size distribution (~10 µm) and superior electromechanical performance (d_{33} = 451 pC N^{-1}, k_p = 0.40, ε'_{33} = 4790), as summarized in Figure 1.

Structural analysis by synchrotron X-ray diffraction (SR-XRD) combined with Rietveld refinement confirms the high phase purity achieved in both systems. Differential scanning calorimetry (DSC) reveals that BCZT nucleation in the mechanochemical route follows an Avrami–Erofeev A3/2-type kinetic model, with a relatively low activation energy of 185 kJ mol^{-1}, highlighting the role of mechanochemical activation in enhancing reactivity. These results demonstrate the effectiveness of low-temperature and chemically assisted strategies for BCZT synthesis and provide insight into the relationship between processing conditions, crystallization kinetics, and functional properties, paving the way for more energy-efficient manufacturing of high-performance lead-free piezoceramics.

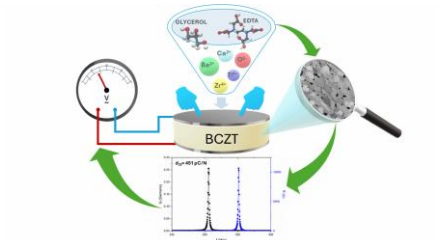

Figure 1. Synthesis and characterization of BCZT piezoceramics via the modified Pechini method, highlighting the role of EDTA and glycerol in enhancing microstructure and electromechanical properties.

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-F O2-

Spin Disorder in Hollow Nanoarchitectures: Beyond Geometric Surface Effects

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At the nanometer scale, the surface-to-volume ratio (R = S/V) of nanoparticles increases significantly, playing a crucial role in altering or introducing novel magnetic properties compared to their bulk counterparts. Among these, hollow nanoparticles (NPs) stand out as a particularly intriguing class, as they possess both internal and external surfaces, further enhancing the surface-to-volume ratio and amplifying their unique magnetic behaviour [1]. Here, we present a comparative study of the morpho-structural and magnetic properties of full and hollow maghemite (γ-Fe2O3) nanoparticles, characterized by a big surface to volume ratio, of corresponding sizes 5.0(5) nm, 7.4(7) nm and 13(1) nm. These systems have been thoroughly characterized by means of DC and AC magnetization measurement and in field ^{57}Fe Mössbauer spectrometry. The in-field hyperfine structure analysis suggested the presence of a non-collinear spin structure (i.e., spin casting) for both hollow NPs originated from the increased surface effects due to presence of inner surface (IS) and outer surface (OS) t (i.e., hollow morphology) Interestingly, after field cooling, a horizontal shift of the hysteresis loop was observed. Monte Carlo (MC) simulations show that the spin canted in the OS and IS are strongly antiferromagnetically exchange coupled leading to the decrease of its saturation magnetization (Ms). At the interface, this strong exchange coupling results in a strong exchange bias inducing an increase of the coercive field, in agreement with the experimental and Mössbauer findings.

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-F O3-

Enhanced Physico-Chemical Characterization of Complex Hybrid Nanocomposites: an O_2-GCIB TOF-SIMS Depth Profiling Approach

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Hybrid nanocomposites are complex systems characterized by the integration of organic and inorganic moieties, at the nanoscale, within their architectures. Materials exhibiting such compositions are gaining significant prominence in the microelectronic and high-tech industries representing a novel class of materials possessing unique synergistic properties that exceed those of their individual constituents. Given their growing importance, the availability of advanced physico-chemical characterization techniques capable of providing in-depth investigations into both chemical and structural configurations, along with degradation patterns and device failures analysis are essential. Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) effectively addresses these requirements providing the capability to acquire both mass spectra and depth profiles, making it a versatile tool for the characterization of inorganic and organic materials. However, while inorganic substrates necessitate monoatomic primary ion beams at high impact kinetic energies to facilitate erosion and secondary ion generation, organic materials require far more gentle sputtering conditions to prevent chemical damage or the carbonization of the sample during analysis, such as those provided by Gas Cluster Ion Beam (GCIB) sources. Due to the previously mentioned motivations, a significant challenge remains regarding the simultaneous ToF-SIMS characterization of hybrid nanocomposites; specifically, the difficulty lies in analyzing samples composed of both organic and inorganic materials with a single sputter beam. Within this framework, our research investigates the efficacy of high energy per molecule O_2-GCIB sputtering sources as a versatile tool to bridge the gap between these disparate material requirements [1]. We achieved an increase in the energy per incident molecule by selecting the smallest available cluster distribution combined with the highest kinetic energy; this approach significantly enhances the sputtering efficiency when eroding resilient inorganic materials. Conversely, the inherent reactivity of oxygen clusters provides a mechanism to mitigate ion beam induced chemical reactions within the organic moieties (such as cross-linking) which typically led to carbonization and the loss of molecular information. Specifically, oxygen species are presumed to act either as radical scavengers, promoting reactions with transient radical species generated during sputtering and preventing them to react with their chemical surroundings, or generating volatile CO_x species resulting in a less amount of damaged material at the crater surface. These findings demonstrate that, for such complex hybrid systems, optimized O_2-GCIB setups offer a viable approach for reliable depth profile characterization. By successfully balancing sputtering efficiency with the preservation of molecular information, this methodology overcomes longstanding instrumental limitations, establishing a robust analytical framework for the study of heterogeneous nanocomposites.

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-F O4-

Physico-Chemical Insights into the Stepwise Assembly of Copper-Based Metal-Organic Frameworks Thin Films on Functionalized Silicon Oxide

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Metal–organic frameworks (MOFs) represent a versatile class of hybrid porous materials composed of metal nodes interconnected by organic linkers. Their exceptional surface area, chemical and structural tunability make them attractive candidates for applications in gas storage, pollutant capture, heterogeneous catalysis, and sensing. For practical implementation in devices, however, controlled immobilization of MOFs onto solid substrates is essential.
In this work, we examine the interfacial physico-chemical processes governing the layer-by-layer assembly of a copper-based MOF on thermally grown SiO_2 substrates functionalized with a zirconium phosphate anchoring layer. The use of a well-defined oxide support enables systematic investigation of nucleation, coordination bonding, and film growth mechanisms.
The evolution of the surface composition and chemical states was monitored after each deposition step by X-ray photoelectron spectroscopy, providing semi-quantitative elemental analysis and insight into metal–ligand coordination. Time-of-flight secondary ion mass spectrometry enabled molecular-level identification of characteristic framework fragments and interfacial species. Morphological development and surface roughness were assessed using atomic force microscopy.
The combined analytical approach provides a detailed picture of interfacial reactions, growth progression, and film homogeneity.
These findings contribute to a deeper physico-chemical understanding of MOF thin-film formation and support the rational design of functional porous coatings for applications in environmental remediation and sustainable energy technologies.

Acknowledgments. This work was partially supported by the project PRIDE (MASE Prog. n. RSH2A_000037 - CUP: F57G25000320006), the European Union's Horizon Europe research and innovation programme under the EIC Pathfinder Open project ERMES – Information Transfer Between Medical Doctors and Implanted Medical Devices via Artificial Molecular Communication (Grant Agreement No. 101185661) and the research project PIACERI 2024-2026 - Linea 1.

-F O5-

From Cultural Heritage to Fundamental Magnetism: Insights from Nanostructured Hematite

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Hematite (α-Fe_2O_3) is a model antiferromagnetic material whose Morin transition (T_m) is strongly influenced by particle size, surface effects, composition, and microstructural defects. Here, we present a combined magnetic and morpho-structural investigation of hematite nanostructures with different origins and thermal histories, including natural (geologically extracted) and synthetic samples prepared via an auto-combustion sol–gel method and subsequent annealing. Thermal treatments were designed to reproduce color variations typical of hematite-based archaeological pigments. Structural and magnetic properties were investigated through synchrotron X-ray powder diffraction (XRPD), neutron powder diffraction (NPD), DC magnetization, and Mössbauer spectroscopy. Magnetic measurements enable a clear discrimination of hematite origin based on distinct magnetic signatures. At 300 K, NPD data are consistent with a canted antiferromagnetic structure (Γ_3), while upon cooling a transition to an antiferromagnetic state (Γ_1) occurs around ~265 K. However, low-temperature NPD data show that the (003) magnetic reflection is only partially suppressed and remains finite at 1.5 K, indicating the coexistence of antiferromagnetic and weakly ferromagnetic domains below T_m. Domain size analysis reveals that crystallographic domains exceed magnetic ones, suggesting that nanoparticles do not behave as single magnetic entities. This behavior supports a core–shell-like magnetic configuration, with an antiferromagnetic core and a surface region sustaining weak ferromagnetic canting. Mössbauer spectroscopy under applied field confirms the coexistence of two magnetic components and shows that thermal treatment reduces both the weak ferromagnetic fraction and canting angle, stabilizing the bulk antiferromagnetic phase. Overall, these results demonstrate how origin, thermal history, and nanoscale heterogeneity govern the magnetic behavior of hematite nanostructures, with implications for both fundamental studies and archaeological pigment analysis [1].

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-F O6-

The NanoLuBC Project: a Join Chairs on Innovative Nanostructured Materials with Luminescent Properties for Cultural Heritage

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This work presents the research activity carried out within the framework of the NanoLuBC project, supported by the National Research Council (CNR) through the Joint Chair call. The project involves a collaboration between the Institute for Chemical-Physical Processes (IPCF) of CNR in Messina and the University of Palermo. The project focuses on the development of nanostructured materials for Cultural Heritage applications, particularly luminescent sensors designed for anti-counterfeiting systems and for the non-invasive identification of molecules such as pigments and lakes.
During the first year, the research was dedicated to the development of anti-counterfeiting inks, which demonstrated effectiveness on a range of substrates, including paper, wood, and mortars [1-3]. In detail, rare earths doped materials were used in combination with ancient blue pigments to generate distinct optical signals in visible and infrared region depending on the excitation wavelength. By combining luminescent materials with different chemical compositions and physical properties, synergistic effects are obtained. Furthermore, the potential use of these pigments as markers for assessing the consolidation of lime-based materials and mortars is explored [1].
Such luminescent systems represent promising tools for anti-counterfeiting strategies and authenticity verification in the field of cultural heritage.

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Figure 1. Logo of the NanoLuBC Project.

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-F O7-

Microbial Photosynthesis for Space Applications

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The development of robust biological systems for space applications requires a comprehensive understanding of how key environmental stressors, particularly ultraviolet (UV) and ionizing radiation and microgravity, affect cellular structure and function. In this study, the photosynthetic bacterium *Rhodobacter sphaeroides* was employed as a model organism to investigate the stability and resilience of microbial light-harvesting systems under simulated space conditions, namely microgravity and UV radiation.
A combined experimental approach was adopted, integrating controlled irradiation assays and simulated microgravity experiments, with *in vivo* absorption spectroscopy used as the primary analytical tool.
Radiation experiments were conducted using a Xenon-enhanced UV lamp (185–2000 nm), enabling the reproduction of spectral conditions comparable to those on Low Earth Orbit.
Simulated microgravity experiments were performed using a clinostat system, which effectively averages the gravitational vector through continuous rotation, mimicking a reduced-gravity environment.
The findings demonstrate that while radiation induces measurable, pigment-specific degradation (modulated by carotenoid content), microgravity instead exerts negligible short-term effects on photosynthetic structure and function.
These results underscore the intrinsic resilience of *R. sphaeroides* and support its potential application in bio-regenerative life-support systems for long-duration space missions.

Acknowledgments. Project APACE - Towards a bio-mimetic sunlight pumped laser based on photosynthetic antenna complexes (Project n. 101161312) funded by Horizon-European Innovation Council is acknowledged.

-F O8-

Next-Generation Sustainable Membranes: Nanostructured Platforms for Environmental and Energy Challenges

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Membrane-based technologies play a crucial role in addressing some of the most pressing environmental and energy challenges of modern society. They are widely employed in processes such as water purification, pollutant removal, desalination, gas separation, and electrochemical energy conversion systems. In particular, membrane processes are increasingly recognized as efficient and versatile solutions for wastewater treatment and environmental remediation, thanks to their high selectivity, modularity, and relatively low energy consumption [1]. At the same time, membranes represent key components in several emerging energy technologies, including fuel cells and water electrolysis systems for hydrogen production [2].
Therefore, the development of advanced and sustainable membrane materials is critical to overcome the inherent limitations of current systems. Conventional fossil- and fluoro-based polymers and membranes, widely used in water filtration and electrochemical devices for hydrogen production, offer high chemical stability and ionic conductivity but are hindered by high cost, limited long-term durability under harsh conditions, and environmental concerns due to their petrochemical origin and persistence. These challenges highlight the urgent need for alternative non-fluorinated and bio-based membranes capable of combining performance, durability, and sustainability. In this context, nanotechnology offers promising solutions, as the incorporation of functional nanofillers can enhance ionic transport, mechanical properties, and overall membrane performance while improving sustainability.
In this work, innovative and eco-friendly polymeric membranes were designed, developed, and characterized using functional polymer and bio-polymer blends processed through techniques such as non-solvent induced phase separation and electrospinning [3, 4]. To enhance adsorption capacity and transport properties, the membranes were functionalized with eco-friendly nanofillers, as functionalized clays (i.e., halloysite), able to modulate surface reactivity and physicochemical interactions with target species. Moreover, particular attention was devoted to the integration of high-value-added materials derived from lignocellulosic biomass residues, including biochar and crystalline micro- and nanocellulose [5]. These fillers were incorporated into sustainable polymer matrices to obtain mixed matrix membranes with enhanced mechanical stability, tunable swelling behavior, and improved functional performance. Comprehensive characterization of both nanofillers and membranes was carried out using chemical-physical, structural, and morphological techniques, combined with adsorption tests of model organic dyes to evaluate the performance of the developed membranes.

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-F O9-

Innovative Hybrid Nanocomposites Based on Soot Carbon Nanoparticles Decorated with Au Nanoparticles for Electroanalytical Sensors

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Soot carbon nanoparticles (NPs), a by-product from incomplete hydrocarbon combustion, have garnered significant attention due to their adverse effects on environment and human health [1]. However, their unique properties, such as a high surface to volume ratio, excellent electrical conductivity and remarkable thermal stability, have prompted interest in their reuse as a cost-effective graphitic alternative to commercial graphene derivatives. This upcycling into high added value nanocomposites offers a sustainable pathway for innovation in materials science [2]. Among various approaches, decorating soot NPs with Au NPs by chemical approaches, a strategy that has never been explored so far, can be effective, yielding hybrid materials with enhanced surface area, electrical conductivity and electrocatalytic performance. While extensive research exists on similar hybridization with carbon nanotubes, carbon black and graphene derivatives [3], very few studies have explored the decoration of soot carbon NPs with inorganic NPs [2]. In this work, soot carbon NPs were synthesized using a nitrogen-quenched ethylene diffusion flame, producing graphitic NPs of tens of nm in size, which formed fractal-like aggregates and a sustainable colloidal chemical approach was implemented to decorate soot carbon NPs with Au NPs. The structural, spectroscopic, morphological and electrochemical properties of the achieved original nanocomposites were characterized, and their electroanalytical properties were tested in the detection of H_2O_2 and diclofenac (DFC) drug. The soot NPs were characterized by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), before and after decoration with the Au NPs. The CV results indicated an increase in the $[Fe(CN)_6]^{3-/4-}$ redox peaks compared to those observed at the bare SPCE electrode, and EIS data revealed a significant enhancement in the electrocatalytic activity and faster electron transfer kinetics at the electrodes modified with the soot NPs and the soot/Au NPs samples, underscoring the potential of the developed materials for electroanalytical applications. Preliminary tests for H_2O_2 and DCF detection showed promising results. The soot NPs demonstrated an improvement of the electrode performance in H_2O_2 and DCF detection, that further enhanced in the soot/Au NPs sample synthesized with citrate. For H_2O_2, a linear limit of detection of 71 µM (sensitivity of 0.28 µA/mM) was reached in the soot/Au NPs sample synthesized by spontaneous reduction of the Au precursor. For DFC, a shift in its characteristic oxidation peak towards lower potentials was observed at both the soot/Au NPs modified electrodes. These findings underscore the potential of the soot/Au NPs hybrid nanocomposites in the development of enzymatic biosensors, for clinical diagnostics, in oxidative stress assessment and electrocatalytic sensors.

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-F O10-

Modulating the Morphology of Lignin Microparticles via Green Solvent-Shifting

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The development of functional lignin particles (LPs) represents a fundamental challenge in the valorization of industrial byproducts through the lens of colloid science. In this study, the formation of LPs is controlled via a solvent-shifting process utilizing levulinic acid (LA) and its derivatives—specifically its ethyl ester (EL) and the ketal (K) obtained from EL and glycerol—as sustainable solvent media. The physicochemical driving forces governing the nucleation and growth of these colloids are systematically investigated to establish a correlation between solvent nature and the resulting supramolecular architecture.

It is demonstrated that the choice of solvent fundamentally modulates the internal organization of lignin macromolecules, specifically influencing the degree of π- π stacking between aromatic moieties. This molecular-level control translates into distinct morphological transitions: LA promotes the formation of irregular particle clusters (Figure 1a), whereas EL induces the assembly of compact well-defined spheres (Figure 1b), and the ketal derivative leads to the generation of planar fragments (Figure 1c). Such structural diversity is linked to the varying solubility parameters and the specific interactions between the lignin backbone and the solvent molecules during the anti-solvent addition.

The characterization of these LPs reveals that the composite structure and high surface area achieved through LA-mediated synthesis result in enhanced functional properties, such as antioxidant capacity. Furthermore, the understanding of these assembly mechanisms is essential for governing the interfacial behaviour of lignin in multiphase systems. These tailored LPs are successfully employed as stabilizers for high-performance Pickering emulsions, platforms for the encapsulation of bioactive compounds, and as reinforcing agents in functional composite hydrogels based on polysaccharides such as alginate and chitosan. This work provides a robust framework for the design of bio-based soft materials with tunable properties for advanced interfacial applications.

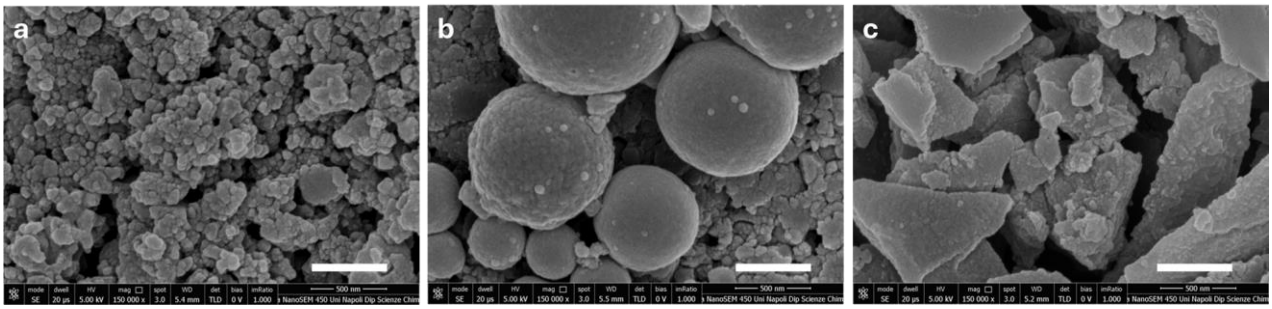

*Figure 1. SEM micrographs at room temperature of the samples LA-LP (**a**); EL-LP (**b**); K-LP (**c**). The bottom part of each panel shows the operative parameters with scalebar (white line in the bottom right of the micrographs) fixed at 500 nm.*

-F O11-

Activated Carbon Derived from Agro-Industrial Waste for H_2 Storage

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The preparation of highly porous activated carbons (ACs) has attracted considerable attention due to their remarkable performance in a wide range of emerging applications, including water remediation, CO_2 capture and H_2 storage. In the latter case, the use of activated carbons with high micropore volumes is particularly advantageous as they enable effective H_2 adsorption within narrow cavities (< 2 nm) leading to a substantial increase in its density and enhancing the overall storage capacity. In this contribution a cost-effective strategy for the production of ultraporous activated carbon based on the chemical activation of agro-industrial residues is reported. A hyper-cross-linked polystyrene-divinylbenzene resin was tested as model system of exhausted resins from water treatment application while hazelnut shells, together with the corresponding hydrochar, was selected as a representative lignocellulosic waste. ACs were prepared by pyrolysis using KOH and an environmental benign eutectic mixture of K_2CO_3/KCl, respectively; exploiting a solvent-free procedure, different mixtures with precursor:activator weight ratios ranging from 1:1 to 1:3 were pyrolyzed under N_2 at 800°C [1]. The produced ACs were in-depth characterized by multi-technique approach using N_2 and CO_2 physisorption analysis at 77K and 273K, and Raman spectroscopy. Furthermore, thermogravimetric analysis (TGA) was conducted on the pyrolysis mixtures to assess the principal temperature range in which the activators are involved in the degradation of the carbon matrix and XRPD analysis were exploited to follow the evolution of inorganic components. The ACs obtained from resin exhibit remarkably high specific surface area and pore volume (above 3000 m^2/g and ca. 1.3 cm^3/g, Figure 1a), which increase with the precursor : activator weight ratio, whereas for biomass-derived samples, hydrochar based ACs show slightly enhanced porosity development along with higher solid yields. The H_2 adsorption capacity was measured at 77 K up to 80 bar, with the highest excess volumetric uptake of 35 g/L (19 mol/kg) observed for the 1:1 sample (Figure 1b) at 25 bar. An innovative method called PoLA (porosity local analysis) developed by our research group was adopted for the simulation of H_2 adsorption isotherms and an absolute volumetric adsorption capacity up to 50 g/L at 120 bar was determined.

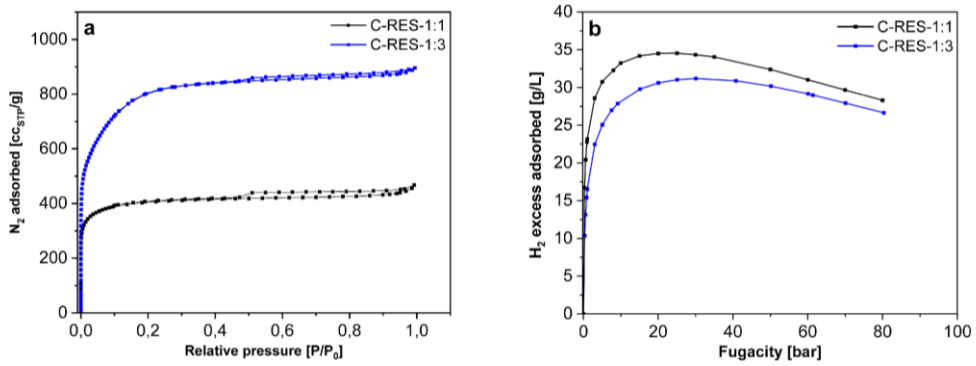

Figure 1. N_2 adsorption isotherm (a) and excess H_2 excess volumetric adsorption isotherm (b) registered at 77 K.

[1] M. Sevilla et al. ChemSusChem 2021, 14, 94.

-F O12-

3D-Printable Bioreceptive M–S–H Cements Containing Large Quantities of Marble Dust Waste

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Climate change is severely threatening Earth's ecosystems and calls for urgent reductions in anthropogenic CO_2 emissions. In this context, the cement industry—among the major emitters—is pursuing multiple decarbonization strategies, including the development of alternative binders and the reuse of industrial by-products. Among low-carbon systems, magnesium silicate hydrate (M–S–H) cements —that can be prepared through the hydration reaction of MgO in the presence of silica and water—are promising due to their durability and chemical stability, particularly in aggressive environments [1]. In parallel, mineral-waste valorization is becoming central to circular construction, yet marble dust, a fine carbonate-rich waste from stone cutting and polishing, is still often improperly landfilled. Nonetheless, high loadings of marble powder can be used to reduce the use of conventional cementitious materials while improving different physico-chemical properties, acting as a functional filler [2]. Besides, 3D printing of cement-based materials —despite being extremely challenging—can allow the preparation of complex geometry and porosity, key features for bioreceptive materials, where surface chemistry, texture, and pore networks can be tuned to promote biological colonization (e.g., biofilms, algae, lichens) [3].
In this work, we developed 3D-printable, bioreceptive M–S–H cements containing large quantities of marble dust waste (Figure 1). The formulations were optimized to balance extrudability, hardening, and shape retention by incorporating sodium alginate (a brown-algae-derived biopolymer used to adjust paste viscosity) and glycerol (a naturally derived compound affecting setting behavior and inspired by symbiotic processes in coral reef ecosystems). Selected systems were characterized in terms of setting, phase composition, microstructure, porosity, morphology, and mechanical performances. Finally, bioreceptivity was evaluated through biological assays with different algal cultures, confirming attachment and growth and demonstrating the feasibility of 3D-printable, biocompatible, waste-based M-S-H cementitious materials.

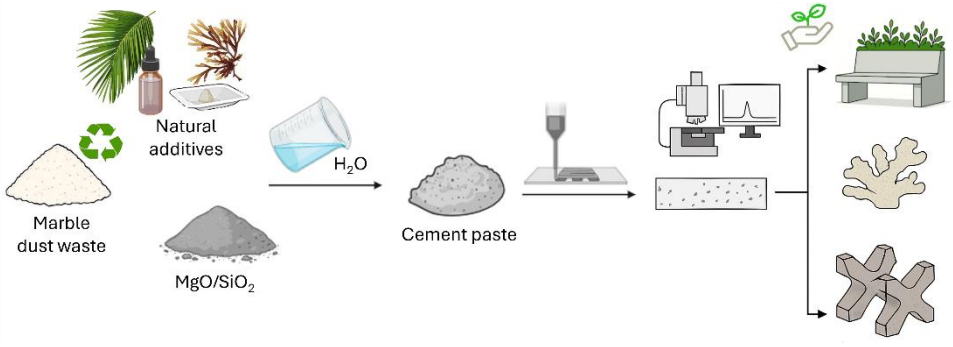

Figure 1. Schematic diagram of the samples' preparation, characterization and fields of applications.

[1] S. Sreenivasan et al. Cem. Concr. Res. 2024, 178, 107462.
[2] P. Prakash et al. Constr. Build. Mater. 2023, 401, 132887.
[3] F. Tonelli et al. J. Colloid Interface Sci. 2021, 598, 24.

-F O13-

Flexible Synthesis of Copper, Iodine – Based Coordination Polymers with Modulable Luminescent Emission

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Coordination polymers (CPs) are structures built from metal clusters or ions coordinated to exodentate organic ligands, which extend into one, two, or three dimensions forming infinite chains or networks. Among CPs, Cu(I) CPs find several applications within the fields of sensing, catalysis, and luminescence [1, 2]. Most of them are constituted by Cu(I) halide chains externally functionalized with organic ligands. In this work we present the synthesis and physico-chemical characterization (PXRD, FTIR, DRS, PL / PLE) of six CPs based on a Cu, I double chain externally functionalized with pyridinic ester ligands. We demonstrate the possibility to modulate their optical properties, by reacting CuI and isonicotinic acid (INA), in presence of titanium isopropoxide (TTIP), in six different alcoholic solvents: methanol, ethanol, iso-propanol, 1-butanol, tert-butanol, and 1-pentanol. According to PXRD results (Figure 1a), in presence of MeOH, i-PrOH or EtOH, TTIP is able to catalyze an esterification reaction between the carboxylic group of the isonicotinic acid and the alcoholic solvent employed since these products exhibit a crystallographic structure analogue to the coordination polymer described in the literature [3], which results from the direct reaction of copper iodide and etil - isonicotinate. By contrast, the synthesis performed in t-BuOH is unsuccessful, as the collected product is an amorphous solid containing unreacted CuI. Surprisingly, the CPs synthesized in 1-BuOH and 1-PeOH have a different crystalline structure respect to the previously two samples, which probably involves titanium atoms coordinated to the carboxyl functionality of isonicotinate groups. All the crystalline CPs, upon excitation at 350 nm, exhibit a strong luminescent emission (Figure 1b), whose maximum wavelength is shifted according to the solvent employed for the synthesis, together with a weaker emission centered around 420 nm, due to the presence of unreacted CuI. The amorphous compound exclusively exhibits the emission at 420 nm. These preliminary results suggest the involvement of the ester chain towards the mechanism of the excitation – emission process. Further investigations will assess the effective role of titanium in the structure of these CPs and so in their optical behavior.

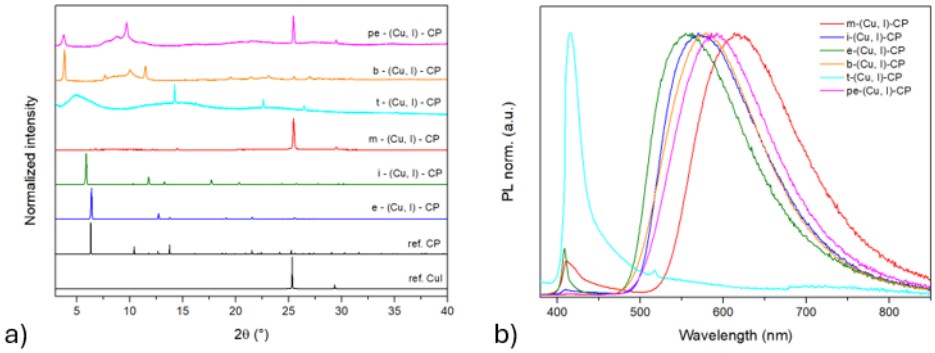

Figure 1. a) PXRD experimental patterns, reference patterns of CuI and CP (CCDC 1047309); b) PL spectra (λ_{exc} = 350 nm) of (Cu, I)– CPs synthesized in: MeOH (m–(Cu, I)-CP), EtOH (e–(Cu, I)-CP, i-PrOH (i-(Cu, I)-CP), 1-BuOH (b-(Cu, I)-CP), t - BuOH (t - (Cu, I) CP), and 1-PeOH (pe-(Cu, I)-CP).

[1] H. Kargar et al. Inorg. Chim. Acta 2026, 589, 122910.
[2] J.S. Kim et al. Inorg. Chem. Commun. 2007, 10, 717.
[3] K. Hassanein et al. Chem. Eur. J. 2015, 21, 17282.

-F P1-

Sustainable Valorization of Artichoke Leaves into K_2CO_3-Activated Biochars for Efficient CO_2 Capture

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There is increasing interest in developing biomass-derived adsorbents due to their potential for diverse environmental applications, including CO_2 capture. In this study, K_2CO_3-activated biochars were prepared from artichoke leaves through physical mixing followed by single-step pyrolysis within the temperature range of 500 to 800 °C. The chemical composition, structural features, and textural properties of the resulting biochars were investigated using appropriate spectroscopic and analytical techniques. Among all samples, the biochar activated at 800 °C (K-LE800) exhibited the highest specific surface area (1,439 $m^2\ g^{-1}$), micropore volume (0.53 $cm^3\ g^{-1}$), and total pore volume (0.67 $cm^3\ g^{-1}$). Furthermore, ultimate analysis revealed that nitrogen content decreased progressively as the pyrolysis temperature is increased, with K-LE800 containing the least nitrogen. Notably, the sample activated at 700 °C (K-LE700) and 800 °C showed similar CO_2 uptakes achieving 3.83 mmol g^{-1} and 3.73 mmol g^{-1} at 1 bar and 24 °C, demonstrating their suitability for CO_2 capture. Equilibrium adsorption data were modelled using Langmuir, Freundlich, Sips, and Toth isotherm models, with the Toth model showing the best fittings, indicating heterogeneous interactions between CO_2 molecules and the activated biochar surfaces. The isosteric heat of adsorption evaluated from Toth model fittings of experimental data, ranged from 23.28-30.54 kJ mol^{-1}, confirming a predominantly physisorption-driven mechanism. Overall, these results suggest the potential of artichoke leaves derived biochars as low-cost, sustainable and effective adsorbents for CO_2 capture.

-F P2-

Inside the Structure of Historical Red Cadmium Pigments

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Cadmium-based pigments, introduced in the 19th century, marked a fundamental turning point in art history by revolutionizing the color palette available to painters. The primary constituent of these substances is cadmium sulfide (CdS), characterized by an orange hue, from which ternary compounds were later developed to achieve a range of adjustable tones [1,2]. Through the addition of increasing amounts of zinc, it is possible to shift the color toward yellow, while the substitution of sulfur with selenium allows for the production of red pigments. Extensive research has demonstrated that cadmium-based materials are distinguished by a high degree of heterogeneity, which manifests in color variability, the presence of impurities, the coexistence of different phases, and varying particle sizes. This heterogeneity is attributable to the diversity of synthetic methods employed by various manufacturing companies, a factor that directly influences the long-term stability of these compounds. Ultimately, the lack of precise information regarding the composition of pigments derived from specific historical syntheses constitutes a significant limitation for predicting the deterioration processes that may affect real paintings [3].
In this study, a series of $CdS_{1-x}Se_x$ pigments were synthesized following established historical formulations. The synthesized pigments progressively change their hues according to the selenium content; however, a detailed structural characterization revealed the presence of two different crystal phases. Detailed electron microscopy analyses and synchrotron radiation investigations suggested the formation of core-shell heterostructure, where the shell is selenium rich. Photodegradation tests were conducted to check the stability of the pigments according to the environmental conditions, evidencing an increased stability conferred by the selenium.

Figure 1. Variation of the hue of the pigments $CdS_{1-x}Se_x$ pigments increasing the selenium amount (from the left).

[1] I. Fiedler et al. Artist's Pigments 1986, 1, 65.
[2] P. Dunning et al. High Perform. Pigment. 2009, 2, 13.
[3] E. Castagnotto et al. Chem. Mater. 2025, 37, 2749.

-F P3-

Colloidal Synthesis of BiOX Nanocrystals

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In this work, we present the controlled synthesis of BiOX nanocrystals, belonging to the MEX family of heavy pnictogen chalcohalides (MEX, where M = Sb or Bi, E = O, S, Se, and X = Cl, Br, I), a class of mixed-anion materials that has recently attracted significant attention for optoelectronic and energy storage applications due to their unique combination of chemical stability and low toxicity. Nanocrystals are synthesized via a hot-injection method under inert atmosphere using a Schlenk-line. In particular, Bi–carboxylate complex is first formed and subsequently reacted with the halogen precursor upon its injection. By tuning parameters such as temperature and growth time, precise control over nanoparticle size and morphology is achieved [1]. Bismuth oxyhalides crystallize in a layered tetragonal matlockite structure, consisting of alternating $[Bi_2O_2]^{2+}$ slabs and halide layers [2]. This architecture is particularly promising for the intercalation of metal cations, a key mechanism for energy storage applications.
Finally, we address the scalability of the colloidal approach, demonstrating its potential for reproducible and transferable large-scale synthesis, enabling the industrial implementation of MEX materials.

[1] D. Quarta et al. Angew. Chem. Int. Ed. 2022, 61.
[2] S. Li et al. Adv. Funct. Mater. 2024, 34.

-F P4-

Atomic Layer Deposition of ZnO on Laser-Induced Graphene: A Photoactive Nanocomposite for Water Remediation

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Among n-type semiconductors, zinc oxide (ZnO) has been widely investigated due to its low cost, biocompatibility, environmental safety and photoactivity. Despite its wide band gap of 3.37 eV that enables strong absorption in the UV region, its photocatalytic performance is hindered by a fast electron–hole recombination rate. To address this drawback, ZnO–carbon nanomaterial (CNM) nanocomposites represent an effective strategy to enhance charge separation and improve performance in various photocatalytic applications, including wastewater treatment and degradation of organic pollutants. A particularly innovative and promising carbon nanomaterial candidate that can be combined with ZnO is Laser-Induced Graphene (LIG), first reported by Lin et al. in 2014 [1]. LIG is especially attractive for the development of photoactive nanocomposites as it acts as an efficient electron sink, thereby suppressing charge recombination, and as a high-surface-area porous scaffold for ZnO deposition. This dual functionality facilitates the recovery and reuse of the photocatalyst, making LIG-based systems attractive for scalable and sustainable environmental applications.
Building on this framework, we investigated the thermal Atomic Layer Deposition of ZnO onto polyimide-derived LIG with two distinct porosity levels [2]. Structural and compositional analyses (X-Ray Photoelectron Spectroscopy and X-Ray Diffraction) confirm that ZnO grown on LIG is both stoichiometric and crystalline. Scanning Electron Microscopy and Energy Dispersive X-Ray results reveal the conformality of the deposited ZnO layer throughout the porous network down to the bottom of the pores, and hence the preservation of the initial 3D structure of the LIG support. Moreover, Zno coverage increases with an increasing number of ALD cycles. The photocatalytic performance of the ZnO/LIG nanocomposites was evaluated by monitoring the discoloration of a methylene blue (MB) solution under UV irradiation (λ = 365 nm) over 120 min. The results show that the photocatalytic activity improves with increasing ZnO deposition time, regardless of the initial porosity of the LIG substrate, reaching a maximum of 70% for both substrates after 400 deposition cycles. Conversely, MB adsorption capacity of the samples decreases upon ZnO deposition, owing to the reduced accessible porosity and the increased hydrophobicity of the nanocomposites, as confirmed by WCA measurements.

[1] S. Stuart et al. Phys. Rev. B 2009, 60, 3320.
[2] P. Morris et al. Phys. Rev. Lett. 2008, 70, 214.

-F P5-

Persistent Luminescence in Cr-Doped Zinc Gallogermanate Nanocrystals

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Persistent luminescent materials (PeLMs) are characterized by their property to continue emitting light for a prolonged time after the excitation source—such as X-rays, electrons, or ultraviolet/visible radiation—has been removed. Owing to this property, they have attracted considerable interest for numerous applications, including emergency lighting, road safety signaling, bioimaging, photocatalysis, optical data storage, and anti-counterfeiting systems. For several of these applications, nanocrystalline PeLMs are required; however, decreasing the particle size often results in a marked reduction or even a complete suppression of Persistent Luminescence (PeL) at room temperature.[1]

An exception to this is for $Zn_{1+x}Ga_{2-2x}Ge_xO_4$:Cr (ZGGO:Cr) nanocrystals (NCs). These materials exhibit PeL in the near-infrared region (NIR) lasting several hours after excitation with UV or visible radiation.

Experimentally, partial substitution of Ga^{3+} for Ge^{4+} significantly modifies the photoluminescence (PL) intensity and the PeL duration. However, the underlying mechanism remains unclear.[2]

In this work, we investigate the effect of the progressive substitution of Ga^{3+} with Ge^{4+} on both the structural and optical properties. Structural changes are analyzed by X-ray diffraction (XRD) (Figure 1a), while the optical response is studied through PL (Figure 1b), photoluminescence excitation (PLE), and persistent luminescence (PeL) measurements.

Preliminary results indicate that the material is typically characterized by NIR emission associated with Cr^{3+}, but at higher Ge concentrations ($x \geq 0.4$) a significant additional PL contribution emerges in the visible region. Further investigations are currently ongoing to clarify the origin of this effect, but the present results point to a possible strategy for tuning the emission properties of ZGGO:Cr NCs and potentially extending their PeL toward the visible range.

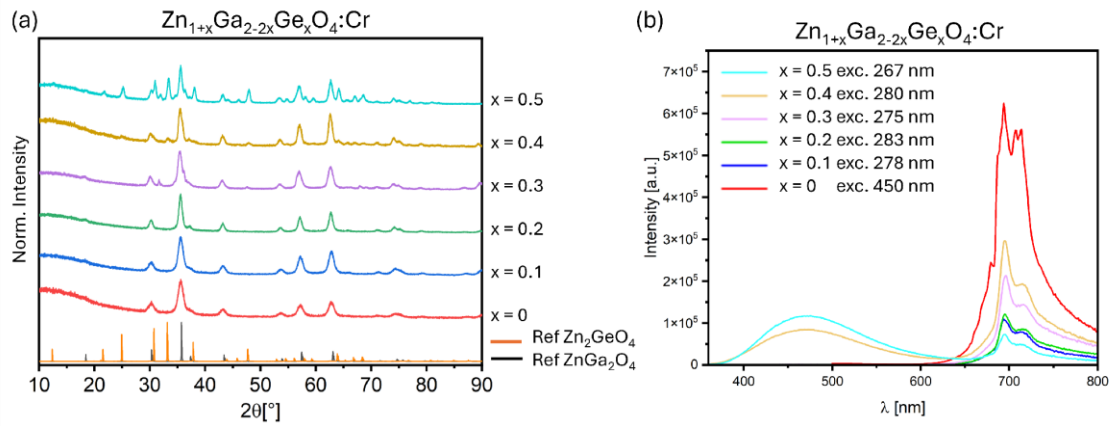

Figure 1. (a) XRD for $0 \leq x \leq 0.5$ samples, Zn_2GeO_4 and $ZnGa_2O_4$ references; (b) PL for $0 \leq x \leq 0.5$ samples at their best excitation.

[1] E. Di Giorgio et al. Cryst. Growth Des. 2024, 24, 4271.
[2] J. Wang et al. ACS Nano 2017, 11, 8010.

-F P6-

Promising Advanced Properties of Bio-Based Non-Isocyanate Polyhydroxyurethanes from Resorcinol Bis(Cyclocarbonate)

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The transition towards sustainable polymers is a central challenge in modern materials science, particularly within circular economy strategies that aim to reduce reliance on fossil-based feedstocks and minimize environmental impact. Bio-based polymers offer the potential to combine high performance with environmental responsibility, and among them, non-isocyanate polyhydroxyurethanes (PHUs) have gained increasing attention due to their safer synthetic routes and versatile functional properties.[1]
In this work, bio-based PHUs were synthesized via solvent and catalyst-free polymerization of resorcinol bis(cyclocarbonate) (RCC) with diamine monomers.[2] The reaction proceeded efficiently under mild conditions, achieving high monomer conversion (>95%) and yielding polymers with weight-average molecular weights (M_w) in the range of 15–25 kDa. FTIR and NMR analyses confirmed the formation of urethane linkages and hydroxyl groups along the polymer backbone, indicating successful PHU formation. Thermal characterization revealed glass transition temperatures (T_g) between 60–85 °C and thermal stability up to 250 °C, demonstrating promising suitability for high-performance applications. Adhesion tests performed on model substrates demonstrated that the bio-derived PHUs exhibit strong interfacial interactions, with adhesion values comparable to conventional polyurethane systems.
These results indicate that the combination of renewable feedstocks, good mechanical performance, and inherent adhesion capability underscores the potential of these PHUs as sustainable alternatives in advanced polymer design. Overall, this study highlights their applicability in material platforms aligned with circular economy principles and environmentally responsible manufacturing.

Acknowledgments. This project acknowledge funding within the Horizon Europe Grant Agreement 101060941 for GREENART (“GREen ENdeavor in Art ResToration”).

[1] G. Rokicki et al. Polym. Adv. Technol. 2015, 26, 707.
[2] F. Olivieri et al. Macromol. Mater. Eng. 2026, e00352.

-F P7-

Melanin-Driven Engineering of Silver Nanostructures for Ultrasensitive SERS Detection

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Hybrid interfaces based on eumelanin thin films and electrochemically deposited silver nanostructures (Mel@Ag) are developed as reproducible platforms for ultrasensitive surface-enhanced Raman scattering (SERS). Natural eumelanin, extracted from sepia pigment and deposited on indium tin oxide (ITO) via dip-coating, acts as a redox-active and metal-chelating interlayer that modulates Ag^+ electroreduction, inducing an anodic shift up to 120 mV and enabling controlled nanoparticle nucleation and growth. [1]

The physicochemical properties of the system were investigated by UV–Vis spectroscopy, FT-IR, Raman spectroscopy, X-ray diffraction, and electron microscopy, providing a comprehensive correlation between structure, plasmonic response, and SERS activity. The resulting Mel@Ag substrates exhibit improved nanostructure uniformity and enhanced plasmonic behavior compared to bare Ag films.

Finite-element simulations combined with experimental data identify nanoparticle dimers as the dominant contributors to electromagnetic enhancement, particularly under 638 nm excitation, where a larger effective near-field enhancement volume is observed (Figure 1A).

The platform enables detection of L-Dopa down to 10^{-11} M, with a response governed by heterogeneous adsorption (Figure 1B). The melanin layer plays a dual role, directing nanostructure growth and promoting analyte preconcentration via π–π interactions. [2]

Measurable SERS signals are retained in complex biological media, indicating partial resistance to biofouling and highlighting the potential of melanin-based hybrid architectures for sensing in biologically relevant environments.

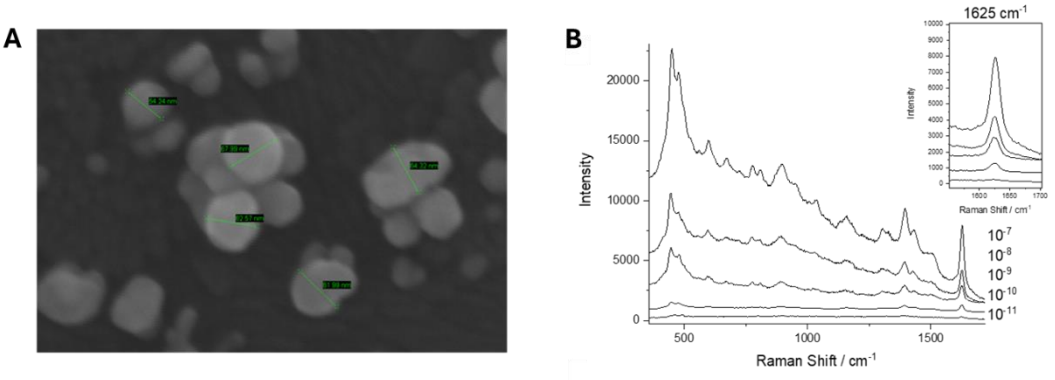

Figure 1. (A) SEM image of Mel@Ag nanostructures showing nanoparticle organization and dimer formation. (B) SERS spectra of L-Dopa at decreasing concentrations, demonstrating detection down to 10^{-11} M.

[1] G. Hasan et al. Ferroelectrics 602, 121.
[2] A. Mavridi-Printezi et al. Int. J. Mol. Sci. 2023, 24, 9689.

-F P8-

A Sustainable Sers Platform for Cultural Heritage and Environmental Applications

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Within the framework of the SAMOTHRACE project, the IPCF-CNR (Messina) developed an eco-sustainable and flexible Surface-Enhanced Raman Spectroscopy (SERS) platform based on recycled cellulose substrates decorated with nanostructured silver or gold nanoparticles obtained by Pulsed Laser Deposition [1]. The morphology of the substrate, along with the size, distribution, and density of the nanostructures, plays a crucial role in SERS sensing efficiency. Surface and optical characterization by SEM, UV–Vis spectroscopy, and profilometry enabled the identification of the best-performing substrate configuration. The analytical performance of the sensing system was validated using Rhodamine 6G as a probe molecule, achieving a lower detection limit of 10^{-10} M, while additional tests were explored with violacein, a natural non-toxic microbial pigment (Fig. 1) [2].

The platform was initially conceived for the non-invasive detection of pigments, dyes, and degradation products in Cultural Heritage materials, where its flexibility makes it particularly suitable for nano-sampling on fragile and irregular surfaces. However, the same technology is being extended to other application fields requiring rapid trace-molecule detection directly on complex surfaces. In this perspective, a strong potential is the detection of analytes of environmental and safety interest, including pollutant residues, molecular markers of contamination, and other trace compounds. The portability, low cost, and disposable nature of the devices make them promising candidates for rapid in situ screening. The proposed approach therefore represents a versatile sensing technology at the interface of Cultural Heritage science and environmental monitoring, and food safety diagnostics.

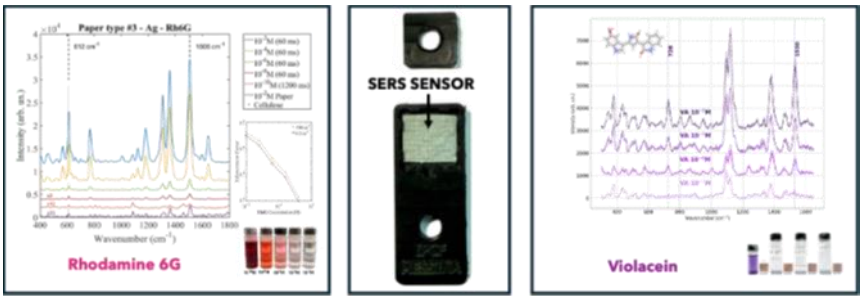

Figure 1. Detection of Rhodamine 6G at different concentrations (left panel), prototype of the SERS sensing system (center panel), and detection of violacein at different concentration levels (right panel).

Acknowledgments. We thank European Union (NextGeneration EU), through the MUR-PNRR project SAMOTHRACE — Sicilian Micro and Nano Technology Research and Innovation Center (ECS00000022).

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-F P9-

Kinetic and Morphological Aspects of Ettringite Formation in Low-Clinker Cement Systems

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The development of low-carbon cementitious materials is a key challenge for sustainable construction, as ordinary Portland cement production is a major source of global CO_2 emissions. Reducing clinker content through supplementary cementitious materials and fillers is an effective strategy, but significantly alters hydration pathways, phase assemblage, and microstructural evolution [1]. Cement hydration involves coupled dissolution, transport, nucleation and growth processes that remain only partially understood [2]. A detailed physicochemical description of these mechanisms is therefore essential, particularly in low-clinker systems where phase assemblage and kinetics are strongly modified [3,4].

Physical chemistry provides a fundamental framework to investigate early-age hydration, involving dissolution–precipitation reactions, ion transport, and nucleation and growth phenomena. Ettringite formation plays a key role in controlling fresh-state properties and early microstructure in multicomponent systems and is highly sensitive to sulphate availability and chemical admixtures.

This contribution presents an experimental investigation of early-age hydration and ettringite formation in a low-clinker ternary cementitious system, characterized by high filler content, reduced clinker fraction, and ground granulated blast-furnace slag. The combined effects of sulphate source and dosage, together with superplasticizer (SP) chemistry, were systematically examined. Rheological measurements were used to characterize paste flow behavior in the presence of two SPs and to determine optimal dosage. Isothermal calorimetry provided insights into early hydration kinetics, while DSC extended the analysis to longer times, allowing reconstruction of hydration evolution. SEM enabled investigation of hydrated phase morphology, with particular focus on ettringite.

The results show that sulphate chemistry critically controls both the kinetics and mechanisms of ettringite formation. Increasing sulphate content progressively delays precipitation, with a retardation effect following the order hemihydrate > gypsum > anhydrite, consistent with differences in dissolution rates and sulphate release. Significant variations in ettringite morphology were observed: low sulphate contents promote fine needle-like crystals at early ages, whereas higher dosages favour thicker, rod-like structures, indicating a shift from nucleation- to growth-controlled regimes. SP chemistry further modulates crystal habit, suggesting specific interactions with growing phases.

Overall, these findings highlight the complex interplay between sulphate speciation and chemical admixtures in controlling early hydration and microstructural development in low-clinker systems. The physicochemical insights gained contribute to a deeper understanding of the mechanisms governing phase formation, particularly ettringite, in low-carbon cementitious materials.

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-F P10-

Green-Emitting Carbon Dots Synthesized in Deep Eutectic Solvents as sustainable photosensitizer for (bio)photoelectrochemical hydrogen Production

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Carbon dots (CDs) have gained significant attention owing to their remarkable properties, such as strong fluorescence, biocompatibility, and environmental friendliness. They are characterized by low toxicity, tunable optical properties, with light absorption covering the visible region. Since their discovery, CDs have evolved into versatile platforms with applications spanning bioimaging, sensing, photocatalysis, photonics, and energy storage [1]. Recently, increasing attention has been devoted to the development of sustainable synthetic strategies for the preparation of CDs [2]. In this context, deep eutectic solvents (DESs) are emerging as green reaction media in materials chemistry due to their low toxicity, low cost, and ability to promote the formation and stabilization of nanoscale carbon-based nanomaterials with favourable photophysical properties [3]. In particular, DESs as Choline Chloride/Urea (1:2 mol/mol) and Choline Chloride/Ethylene glycol (1:2 mol/mol) can be explored as sustainable synthetic media for the preparation of CDs.
In this work, starting from a well-established synthetic procedure involving the thermal carbonization of Resorcinol in ethylene glycol in air at atmospheric condition, new synthetic strategies of fluorescent CDs in DESs are developed aiming to obtain CDs showing intriguing optical properties in the visible range for material integration as photosensitizer in (bio)photoelectrochemical systems for hydrogen production. Aromatic precursors are purposely selected to effectively undergo to polycondensation under the reaction condition, enabling the formation of polyaromatic structures regulating the CDs emission [2]. A systematic investigation of reaction conditions, including the proper selection of precursors, and spectroscopical properties is carried out via UV-vis absorption and steady-state and time-resolved fluorescence emission spectroscopy to select the approaches able to provide the best performing material in terms of optical properties, such as broad absorption and bright emission in the visible region. Life cycle assessment study of the synthetic procedures is also developed to compare and understand the environmental impacts of the developed routes towards sustainable approaches.

Acknowledgements. This work has been developed within the project "Photoactivated scalable diffuse production of Green Hydrogen through sustainable materials and processes" SOLE-H2 2025-2026 (Project code. RSH2A_000004) funded by the European Union – NextGenerationEU through MASE within National Recovery and Resilience Plan Mission 2 "Green revolution and ecological transition", Component 2 "Renewable energy, hydrogen, network and sustainable mobility", Investment 3.5 "Research and Development on Hydrogen".

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-F P11-

Spectroscopic Characterization and Photocurrent Generation of a Novel Erythrosine B-Peptide Conjugate System for Dye Sensitized Solar Cells (DSSCs)

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Dye Sensitized Solar Cells (DSSCs) are a third-generation photovoltaic technology, developed to enable simple fabrication processes, low production costs, and efficient operation under low-light and indoor conditions [1]. In our research group, we have previously exploited the photocurrent generation capabilities of self-assembled monolayers (SAMs) formed by conformationally constrained peptides, which play a crucial role in mediating charge-transfer processes [2,3]. The incorporation of peptides in DSSCs offers a pathway toward more sustainable solar energy technologies. In this work, we have explored and characterized a novel system consisting of an Erythrosine B-peptide conjugate anchored to a TiO_2 substrate. The structure of the SAM is shown in Figure 1, with the sequence: EB-Sar [Leu-Aib]$_4$-Leu-Cyclohexyl-COOH [MW: 1937.4087]. The system was first characterized spectroscopically in solution to investigate its photophysical properties. Subsequently, the SAM deposited on the TiO_2 substrate was studied for photocurrent generation under different excitation wavelengths. The photocurrent action spectrum closely follows the absorption spectrum in solution (Figure 2) showing preliminary promising results, with the photocurrent reaching 600 nA/cm^2 at the absorption maximum of Erythrosine B dye.

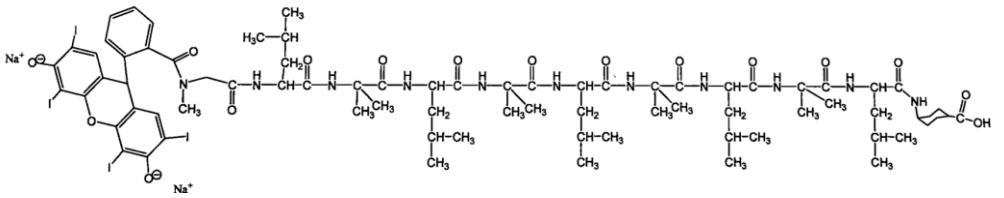

Figure 1. Chemical structure of SAM Erythrosine B System.

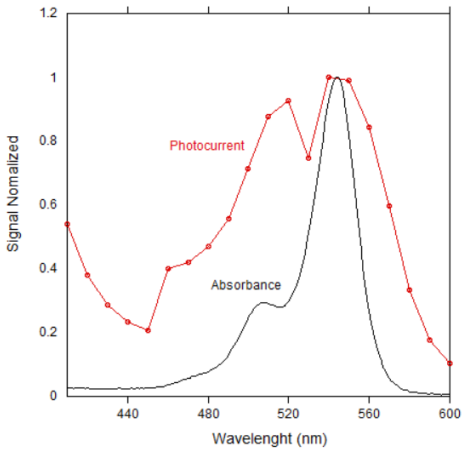

Figure 2. The action photocurrent spectrum and absorbance spectrum of SAM Erythrosine B system.

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-F P12-

Monolithic g-C_3N_4/Activated Carbon as Photocatalyst for Nitrogen Fixation under UV- Visible Irradiation

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The sustainable production of ammonia (NH_3) represents one of the most critical challenges in modern chemical engineering. The traditional Haber-Bosch process, while efficient, remains a massive source of CO_2 emissions due to its extreme operating conditions. Heterogeneous photocatalysis for atmospheric N_2 fixation emerges as a transformative alternative, enabling the reduction of nitrogen under ambient conditions through photon-driven processes in the UV-Visible range. However, the intrinsic stability of the N≡N triple bond (941 kJ/mol) requires highly efficient catalytic systems capable of both activating the molecule and suppressing charge recombination.

Among visible-light-responsive materials, graphitic carbon nitride (g-C_3N_4) stands out for its suitable band structure for N_2 reduction [1]. In this work, the photocatalytic performance of g-C_3N_4 is significantly enhanced through its integration with a high-surface-area activated carbon (AC) matrix. The synthesis involves the thermal condensation of melamine directly onto the carbonaceous support, a process that leads to the nanonization of the g-C_3N_4 phase [2]. In this composite system, the activated carbon plays a dual synergistic role:

1. Structural Dispersing Agent**:** The AC, by providing a vast and porous surface (≈3000 m^2/g), effectively prevents the thermal agglomeration of g-C_3N_4 during calcination, ensuring a uniform distribution and maximizing the exposure of catalytic sites.
2. Electronic Co-catalyst: The AC matrix facilitates the separation of photogenerated carriers. It acts as an electron sink, effectively trapping electrons from the g-C_3N_4 conduction band, thereby suppressing charge recombination and prolonging the lifetime of the reactive species involved in N_2 reduction.

A key focus of this study is the comparison between conventional powder catalysts to a structured monolithic reactor. While slurry-based systems often suffer from catalyst loss and environmentally taxing recovery procedures, the proposed monolithic design addresses these engineering advantages:

- **Mass Transfer and Photon Harvesting:** The three-dimensional porous architecture of the monolith ensures excellent accessibility to the active sites.
- **Stability and Recyclability:** The immobilization of the AC/g-C_3N_4 composite within a self-supporting structure prevents the leaching of the catalytic active phase and eliminates the need for environmentally taxing filtration or centrifugation steps.
- **Scalability:** By bridging the gap between material science and chemical engineering, the monolithic system offers a simplified and robust configuration suitable for continuous-flow applications.

This work demonstrates a synergistic approach to N_2 fixation by combining the photo-activity of nanonized g-C_3N_4 with the structural and electronic advantages of an activated carbon monolith. The resulting material provides a stable, easy-to-handle, and efficient platform for the photon-driven synthesis of value-added nitrogen compounds, representing a significant step toward the practical implementation of structured photocatalytic reactors.

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-F P13-

Temperature-driven phase engineering of WO_3 nanoparticles for enhanced photochromic nanocomposites

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Tungsten oxide (WO_3) is a promising inorganic photochromic material for smart optical devices, owing to its reversible light-induced coloration, governed by crystal structure and proton diffusion pathways [1–3]. Here, WO_3 nanoparticles (NPs) are synthesized via sol-gel route to establish the relationship between synthesis conditions, crystalline phase and photochromic response. Effect of solution pH and reaction temperature (from 45 to 90°C) are investigated by TEM, XRD and DRS. While pH mainly yields orthorhombic WO_3 NPs characterized by a rounded shape and by an intense yellow color, reaction temperature governs the crystallographic phase, enabling selective formation of different WO_3 polymorphs with rodlike structure. Under UV irradiation, orthorhombic WO_3 NPs deposited in thin films demonstrate negligible photochromic response, whereas hexagonal NPs reach an intense blue coloration after few minutes of UV irradiation, confirming the role of the hexagonal framework in promoting proton intercalation [2,3]. (Fig.1)

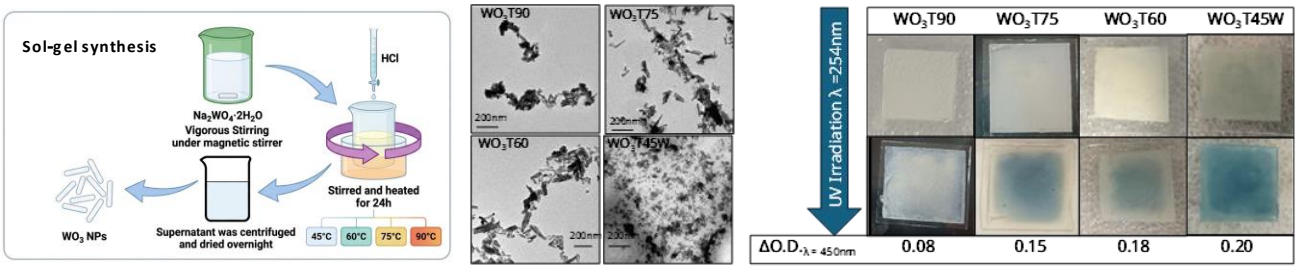

Figure 1. Synthesis, characterization and photochromic response of WO_3 NPs deposited in thin films.

Incorporating the optimized nanoparticles into PVP films preserves the photochromic response at higher WO_3 loadings, highlighting the potential of polymer-assisted architectures for flexible photochromic coatings.[4] Overall, the reaction temperature is identified as the key factor controlling WO_3 phase development and photochromic behavior, providing a solid guideline for the rational design of high-performance photochromic materials.

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Session G

Environmental Physical Chemistry

-G O1-

Cellulose-Based Nanocomposites Embedding Metal Oxides Nanoparticles for Dye Removal from Wastewater by Synergistic Adsorption and Photocatalytic Processes

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The development of efficient and sustainable strategies for water remediation is a pressing global need. Adsorption has grabbed the attention as a versatile, cost-effective option for relatively effortless large-scale water treatment. Recently cellulose-based adsorbents (CA) represent an eco-friendly alternative addressing environmental concerns [1]. However, their high performances in the removal of cationic dyes are limited in the case of anionic dyes. To fill this gap, here, CA modified with metal oxides nanophotocatalysts are developed towards water treatment processes that synergistically combined adsorption and photocatalysis for efficient pollutants removal. Colloidal metal oxide nanoparticles, including TiO_2 and CeO_2, tested as efficient photocatalysts, were synthesized through water-based low-temperature procedures and incorporated into cellulose-based matrices obtained from carboxymethyl cellulose or cellulose fibrils crosslinked with citric acid. The resulting nanocomposites were structurally, morphologically and optically characterized. Nanocomposites confirmed their transparency in the visible range, allowing prompt spectrophotometric monitoring of the adsorption and photocatalytic processes of cationic and anionic dyes used as model pollutants under selected pH conditions. Adsorption isotherms, kinetic studies and photocatalytic experiments were performed to evaluate dye removal performances. Bare CA showed fast adsorption of cationic dyes, thanks to robust electrostatic interactions among dye and cellulose surface, which follows Langmuir model and kinetic described by the pseudo-second order model. Poor removal of anionic dyes has been confirmed. Nanocomposites, based on CA containing photocatalytic nanoparticles, are demonstrated to preserve fast adsorption of cationic dyes, characteristic of the CA, concomitantly providing photocatalytic decoloration of anion dyes in solution upon light irradiation. The convergence of adsorption and photocatalysis in a novel hybrid composites has offered a sustainable and energy-efficient strategy for the removal of pollutants from water systems.

Acknowledgments. This work has been funded by European Union through Next Generation EU, Mission 4 Component 1, for the financial support to MUR within PRIN call 2022 PNRR, project title: Photocatalytically-regenerable hierarchically porous adsorbents for efficient water treatment PHOTOPAD, P2022FP2W4, 2023-2025CUP B53D23027540001.

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-G O2-

Thiol-Functionalized Chitosan Derivative as a Novel Bioadsorbent for Selective Mercury Remediation

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Mercury pollution in aquatic environments represents a critical environmental problem, posing a severe threat to both human health and ecosystems [1]. Consequently, the removal of mercury from contaminated water is of primary importance. Among the various remediation techniques developed, adsorption stands out as a highly efficient solution, offering a combination of high removal efficiency, cost-effectiveness, and environmental sustainability [2]. Polysaccharide-based bioadsorbents have garnered significant attention due to their natural abundance and chemical versatility, which allows for structural functionalization to enhance their adsorption performance [3,4]. In this work, a chitosan derivative containing ethylene sulfide groups, namely mercapto-ethylchitosan (MECS), was synthesized through a nucleophilic substitution reaction. In particular, the hydroxyl groups of chitosan were first activated by treatment with NaH and subsequently reacted with thiirane, enabling the introduction of mercaptoethyl moieties into the polymer backbone and resulting in the formation of the modified chitosan derivative [5]. This modification aims to exploit the well-known high affinity of thiol groups for mercury to promote its adsorption. The resulting material was comprehensively characterized using elemental analysis, point of zero charge (PZC) determination, FTIR, TGA, SEM-EDX, and BET analysis. Results demonstrated that MECS exhibits excellent adsorption capacity, comparable to those of pristine chitosan (CS), but distinguishes itself through key operational advantages. Crucially, MECS remains completely insoluble and maintains its high adsorption efficiency even under acidic conditions, successfully overcoming a major chemical limitation of native CS. Furthermore, a distinct improvement in the adsorption capacity of MECS compared to CS emerges at higher mercury concentrations. Most importantly, under competitive conditions in multi-metal solutions (e.g., in the presence of lead), MECS exhibits remarkable selectivity towards mercury. These findings suggest that MECS is a highly promising, sustainable, and robust bioadsorbent for the efficient and selective remediation of mercury-contaminated water.

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-G O3-

Synthesis and Preparation of Cyclodextrin Modified Carbon Nanotube Buckypapers for the Efficient Removal of Carbofuran from Water

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Carbofuran (CB) occurrence into aquatic sources represents a serious threat to terrestrial ecosystem safeguard due to its toxicity to birds, fish, mammals, wildlife and humans. As a consequence, a prompt action, based on cleaning up CB contaminated environments, is urgently required. Here, we report the realization of a new adsorption system, based on the development of buckypaper membranes (BP), well-known for their high thermal and chemical stability, from β-cyclodextrin (β-CD) functionalized carbon nanotubes (SWCNT-CD), with the aim of capturing CB from aqueous solutions. This material contemporaneously enjoys from both the covalently attachment of β-CD units, acting as a cage for carbofuran, onto carbon nanotubes' surface, and from the possibility to organize β-CD functionalized CNTs in structured membranes (BP-CD), where no other supporting polymers are incorporated, having the advantage of being ease to handle and recycle (Figure 1). BP-CDs membranes were tested on a wide range of CB concentration values (0.5 – 50 ppm) and at two temperatures (298, 313 K). Experimental data were thermodynamically and kinetically treated, finding that at room temperature CB adsorption is a spontaneous endothermic process (ΔG = -31.6 kJ mol^{-1}), with a maximum adsorption capacity of 48.4 mg g^{-1}. As confirmed by the high value of Langmuir constant (K_L = 1.57), a strong affinity between CB and BP-CD has been observed, assessing the great potentiality of BP-CDs in the capture of carbofuran from water.

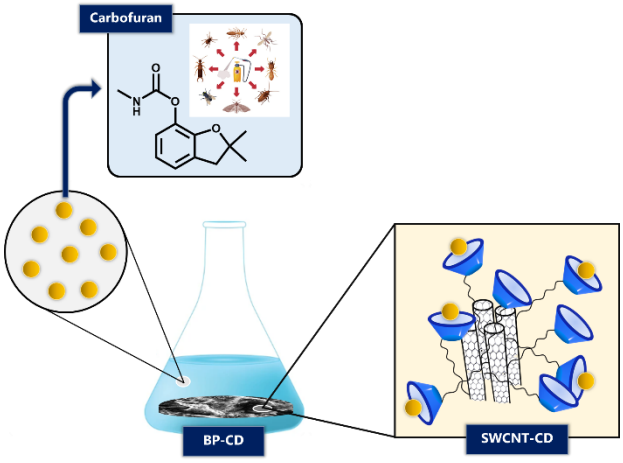

Figure 1. Schematic representation of BP-CD membranes employment for Carbofuran removal from water.

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-G O4-

Magnetic Fe_3O_4/BiOBr for Sunlight Degradation of Tetracycline Antibiotic

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A layer-structure bismuth oxybromide (BiOBr) has gain much attention assigning to its benefits of optimal energy gap, stability, inexpensive and the promising photocatalytic activity. Several strategies have been used to prepared BiOBr. However, a major difficulty dealing with the bare BiOBr is based on its low sunlight-responsive photocatalytic performance attributing to the fast electron-hole recombination rate. To overcome the problems, the fabrication of BiOBr with a promising solar-light-driven efficiency is of high concern. In this work, magnetic Fe_3O_4/BiOBr, synthesized via an ultrasonic route, was applied for detoxification of tetracycline (TC). BiOBr exhibited E_g of 2.71 eV while Fe_3O_4/BiOBr showed E_g of 2.04 eV. The Fe_3O_4/BiOBr displayed lower photoluminescence signal than BiOBr, suggesting improved electron-hole separation speed. The promising photocatalytic efficiency of 100% with improved rate constant of 0.0732 min^{-1} was achieved. The synthesized Fe_3O_4/BiOBr exhibited promising performance and stability after five cycles. The promising performance, compared to the pristine Fe_3O_4 and the bare BiOBr, is mainly due to the drastic decrease of carrier recombination velocity and the remarkable improvement in the absorbance within the visible light regime after construction of the binary Fe_3O_4/BiOBr. The superoxide anion radicals are the main active species. The present paper demonstrates a novel way to fabricate the sunlight-responsive photocatalyst, with magnetic separable property, for decontamination of TC drug in aqueous phase. This research emphasizes a promising strategy to remove toxic pollutant by utilizing the economical solar light.

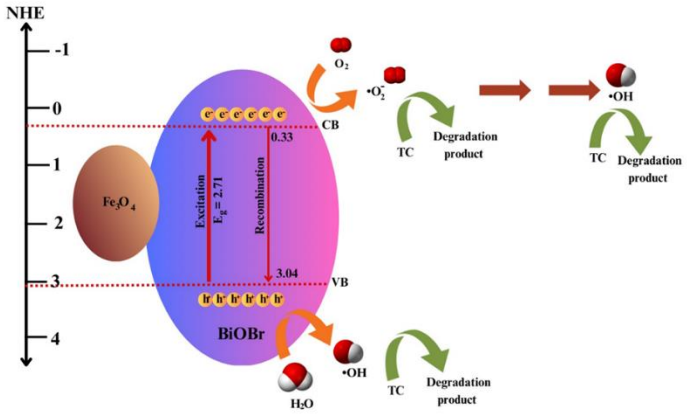

Figure 1. Photodegradation mechanism of TC in the presence of the magnetic Fe_3O_4/BiOBr photocatalyst.

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-G O5-

Probing Aluminum Speciation and Surface Acidity in Mesostructured Aluminosilicates: Structure–Acidity Insights for CO_2-to-DME Conversion

Fausto Secci[1], Valentina Mameli[1], Patrícia A. Russo[2], Paula Soares-Santos[3], Mauro Mureddu[4], Nicola Pinna[2], João Rocha[3], Carla Cannas[1]

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Nowadays, research is increasingly focusing on green fuels produced from captured CO_2 (e-fuels). One of the most promising candidates is dimethyl ether (DME), a substitute for diesel fuel. DME can be synthesized from CO_2 via two consecutive reactions: the first, catalyzed by Cu-based reduction catalysts, involves the reduction of CO_2 to methanol; the second, promoted by solid acid catalysts, is the dehydration of methanol to DME. Here, three mesostructured aluminosilicates (Al-MCM-41, Al-SBA-15, and Al-SBA-16 (Figure 1a)) each one with three Si/Al ratios (10, 15, and 20) are presented as methanol dehydration catalysts for the one pot-CO_2-to-DME conversion. The catalysts have been tested and characterized with a particular focus on the correlation of their structural properties with their acid features and their catalytic performance. Al-MCM-41, Al-SBA-15, and Al-SBA-16 samples were obtained, respectively, with a conventional sol-gel, a hydrothermal sol-gel approach, and by an Evaporation-Induced Self-Assembly (EISA) method. The samples were studied with a wide range of techniques to determine their structural (XRD, ^{27}Al- and ^{29}Si-SS-NMR), textural (N_2-physisorption), morphological (TEM-EDX), acid (pyridine-adsorption FTIR), and compositional properties (ICP-OES) and tested to determine their catalytic performance. Catalytic results (Figure 1b) show that increasing Al content enhances DME selectivity, particularly in samples exhibiting lower surface area and thus higher surface density of acid sites, in agreement with pyridine-FTIR acid site characterization (Figure 1c), which shows a moderate increase in acid site number with decreasing Si/Al ratios. This trend highlights the relevance of acid site density rather than total acidity in steering product distribution. Aluminum speciation was probed by ^{27}Al solid-state NMR (Figure 1d), alongside with ^{29}Si-SS-NMR, and correlated with acid features derived from pyridine-adsorption FTIR. ^{27}Al MAS NMR reveals the coexistence of framework tetrahedral Al and extra-framework five- and six-coordinated species. Higher Al loadings promote partial segregation of Al as amorphous Al_2O_3, with the extent of segregation depending on both synthesis route and mesostructure. ^{29}Si MAS NMR is consistent with partial Si substitution by framework Al. Overall, the results demonstrate that mesostructure topology and aluminum coordination environment jointly determine acid site distribution and surface density, which ultimately govern DME selectivity in CO_2 hydrogenation.

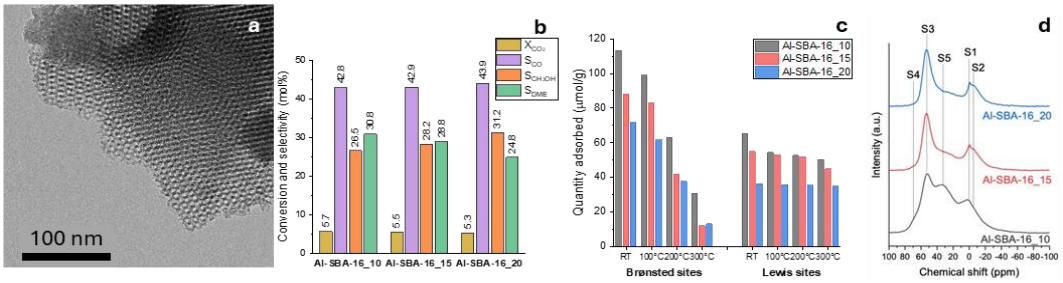

Figure 1. TEM imaging (a), catalytic performance (b), acid sites characterization (c), and ^{27}Al-SS-NMR (d) of Al-SBA-16.

-G O6-

A Sequential Probe Adsorption Approach for the Characterization of Acid Sites in Hierarchical Zeolites

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Hierarchical zeolites, featuring a distinctive architecture of interconnected micro- and mesopores, are widely studied for their tunable acidic properties, whose nature and accessibility play a key role in determining their performance in adsorption and catalytic processes [1,2]. These systems can be obtained either via post-synthetic *top-down* approaches or through *bottom-up* synthesis strategies, and the nature and spatial distribution of Brønsted acid sites (BAS) are crucial for understanding structure–property relationships. FTIR spectroscopy coupled with the adsorption of basic probe molecules is a well-established approach for this purpose. In particular, probes with different kinetic diameters are commonly employed to selectively access BAS located in distinct pore environments. However, conventional methodologies rely on separate single-probe experiments, which are time- and resource-intensive. In this contribution, two *top-down* desilicated commercial zeolites (HZSM5 and natural clinoptilolite, HCLI, with MFI and HEU structures, respectively) and a *bottom-up* synthesized SAPO-34 (CHA structure) were investigated. Their hierarchical architectures were characterized through a multi-technique approach, including 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. Conventional single-probe adsorption experiments (NH_3 and bulkier probes such as 2,4,6-trimethylpyridine 2,4,6-TMPy and 2,4,6-tri-tert-butylpyridine 2,4,6-TTBPy) were performed to assess total BAS concentration in different pore domains. To gain deeper insight into the accessibility of acid sites, a sequential adsorption approach was explored, involving the adsorption of bulky probes and NH_3 under identical conditions, yielding promising results. FTIR difference spectra collected after sequential adsorption show the simultaneous presence of characteristic bands of both probe molecules, confirming the feasibility of the approach (Figure 1). This strategy offers the prospect of determining, within a single experiment, both the total BAS concentration and their spatial distribution across the pore system, thereby substantially reducing experimental time and energy consumption. Moreover, it may provide insights into the interactions between the different basic probe molecules.

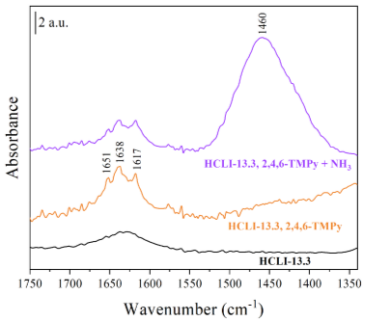

Figure 1. FTIR difference spectra of 2,4,6-TMPy and NH3 probes sequentially adsorbed on HCLI-13.3 sample in the low wavenumber region.

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

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-G O7-

Valuable Waste for CO_2 Conversion and H_2 Evolution Induced by Mechanical Energy

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In the quest for innovative routes for CO_2 removal on large scale application, a smart approach should consider the exploitation of largely available and overlooked materials, such as industrial waste, in mineral carbonation processes [1,2]. Mafic and ultramafic minerals (including olivine, serpentine, talc, etc), as well as metal oxides or hydroxides have gained wide attention due to their low cost and large availability. Further advances, along this line, consider the use of industrial waste possessing similar chemical features, in a recovery-recycle-reuse scenario [2]. In particular, this study demonstrates the feasibility of employing granite waste (GW) as an effective reactive medium for the simultaneous conversion of CO_2, H_2 generation, and CH_4 formation under mechanochemical activation [3-5]. The results reveal that GW, consisting mainly of oligoclase, quartz, and orthoclase together with minor Fe^{2+}-bearing phases such as biotite and chlorite, exhibits measurable reactivity towards CO_2 even under mild conditions of temperature and pressure [3-5].

The experiments highlight a clear dependence of the reaction on the chemical environment, particularly on the pH: the introduction of a carbonate/bicarbonate buffer solution significantly enhances both CO_2 conversion and H_2 evolution. This enhancement is attributed to the increased solubility of CO_2 in the buffered medium and to the improved mobility of cations released from the mineral lattice [6].

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-G O8-

Use of Vis-NIR Spectroscopy for Environmental Monitoring: Potential and Applications

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Visible-near-infrared reflectance spectroscopy (vis-NIR, 350 nm – 2500 nm) is an innovative, versatile, and environmentally sustainable proximal sensing technique for environmental monitoring [1]. Rapid analysis, low cost, and the ability to perform real-time, field-based, and large-scale measurements are crucial for the widespread presence of environmental criticalities. Vis-NIR reflectance spectroscopy helps overcome the limitations of traditional analysis methods, which often rely on destructive techniques that can damage sample integrity and delay environmental emergency responses. Moreover, spectral reflectance measurements, based on the ratio of incident radiation to the reflected radiation from a sample, provide a unique spectral signature that can be correlated with physicochemical parameters using advanced chemometric models. In this context, the vis-NIR spectroscopy demonstrated its effectiveness in assessing soil quality, as part of the application of Ministerial Decree 46/2019 to a potentially contaminated area near the Taranto SIN [2]. From the spectral signatures, the presence of physical (texture) and chemical (water, organic matter, clay minerals, iron oxides, and carbonates) chromophores could be analysed. By combining spectral data with multivariate statistical methods, it was possible to predict the concentrations of inorganic pollutants and heavy metals such as beryllium, vanadium, and thallium, thereby performing a pre-screening function for the creation of reference spectral libraries and maps of the spatial distribution of contaminants, which are crucial for planning long-term environmental remediation interventions. Similarly, by soil colour analysis obtained from spectral data, the presence of PCBs in samples from a former MATRA industrial area in Taranto was predicted [3]. The potential of this technique has also been confirmed by spectral investigations of polluted sediments, aimed at evaluating the ability of some microorganisms to catabolize organic compounds, such as hydrocarbons, in microbial fuel cell applications [4].

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-G P1-

Synthesis and Characterization of Metal Organic Cluster and Frameworks for Energy and Environmental Applications

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Metal-organic frameworks (MOFs) and metal-oxo clusters (MOCs) are porous crystalline structures composed of multiple metal centers linked to each other via bridging oxygen atoms and organic linkers. The properties of both metal ions and linkers determine the physical, structural, and morphological features of MOFs and MOCs [1], and 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, or the fields of optoelectronic and luminescence emission. The construction of Ti-based clusters was carried out, along with the synthesis of Coordination Polymers based on Cu and I, where the presence of Ti has a positive effect on the optoelectronic properties of the material. Titanium based compounds possess the qualities required to face environmental problems, and for this reason they were chosen as candidate precursors to build up environmentally active frameworks. Samples were prepared through a building block approach, by means of a one-pot reaction, 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 and labelled as (PTC-3) [2]. Subsequently, our aim was to operate modifications to the cluster to extend its dimensionality, by using silver nanoparticles, in accordance with Pearson's soft and hard acid-base theory, so that AgNPs could be incorporated within the structure, or by the approach of ligand exchange reactions, using polycarboxylic ligands. 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 The synthesis of both PTC-3 and PTC-3@AgNPs was successfully achieved through the solvothermal method, and AgNPs could be incorporated within the structure. The most promising samples were tested towards the adsorption and the photocatalytic degradation of methylene blue (MB) in aqueous solutions and both samples showed promising results as adsorbents and as catalyst, while in combination with hydrogen peroxide, while the role of silver in the photocatalytic degradation process still needs to be clarified.

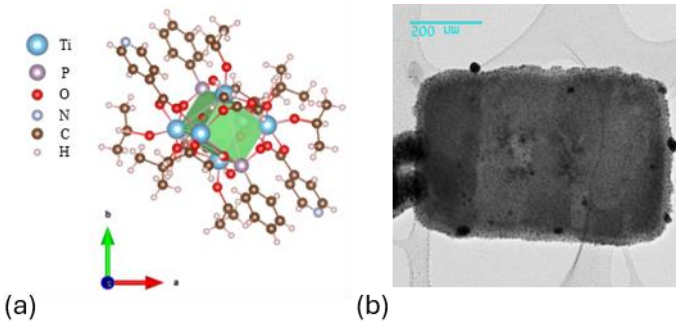

Figure 1. (a) Structure of PTC-3 cluster, (b) TEM image of the PTC-3@AgNPs.

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-G P2-

Bio-Fenton Reaction for the Removal of Persistent Organic Pollutants from Wastewater

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In recent years, numerous innovative strategies have been developed, based on both chemical and biological approaches, for the removal of certain classes of emerging contaminants, including pharmaceuticals, pesticides, household compounds, microplastics, and synthetic dyes. Chemical methods, such as the use of reactive oxygen species, although effective, present environmental and health-related drawbacks, whereas biological methods, which are more sustainable, are limited by sludge production and reduced effectiveness toward toxic compounds. In this context, the present work proposes the use of a treatment system based on the Bio-Fenton reaction, obtained by coupling the enzymatic reaction catalyzed by glucose oxidase enzyme (GOX) with the conventional Fenton process. The enzyme produces hydrogen peroxide (H_2O_2) in situ, which subsequently undergoes redox reactions with Fe^{2+} and Fe^{3+} to yield reactive oxygen species (ROS, e.g. the hydroxyl radical •OH) and promotes the oxidative degradation of organic pollutants until their complete mineralization into carbon dioxide and water. The enzymatic activity of GOX was characterized at different pH and temperature values; under optimal conditions, the kinetic constants Km (42.82 ± 3.30 mM), k_2 (2.08 ± 0.0044 min^{-1}), and Vmax ((93.00 ± 1.94) × 10^{-4} min^{-1}) were determined, and the potential applications in pollutant degradation processes (rate, robustness, and substrate dependence) were evaluated. Furthermore, using o-dianisidine and methyl orange as model substrates for organic dyes, the main operational parameters for field applications (pH, temperature, reagent concentration) were assessed and optimized. In parallel, a kinetic model was developed, including both a purely enzymatic model and one extended to the entire Bio-Fenton system (enzymatic + chemical), useful for describing oxidation and inhibition phenomena and guiding experimental design. The system was finally tested on pollutants from the textile industry, in particular the azo dyes Reactive Black 5 (RB5, tetrasodium 4-amino-5-hydroxy-3,6-bis[[4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]naphthalene-2,7-disulfonate) and Reactive Yellow 201 (RY201, disodium 5-amino-4-hydroxy-3-[4-[[2-(sulfooxy)ethyl]sulfonyl]phenylazo]-6-[(2,4,6-trichloro-1,3,5-triazin-2-yl)amino]naphthalene-2,7-disulfonate), demonstrating good application potential, with removal efficiencies of 60-80% within the first 7 hours of reaction.

The Bio-Fenton reaction represents a promising strategy for wastewater treatment, capable of reducing the use of harmful chemical reagents and the associated environmental risks. In the future, this work may be extended to process optimization and evaluation at an industrial scale. Furthermore, the possibility of confining the reaction within compartmentalized systems, such as cell-mimicking structures, could be explored to enhance its stability and efficiency under complex environmental conditions.

-G P3-

Exploring New Routes for The Valorization of Spent Li-Ion Batteries: the WAVEE Project

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The large demand for lithium-ion batteries (LIBs) and the rising implementation of electrification programs is requiring the development of efficient and sustainable recycling processes aimed at valorizing materials and components of spent batteries and recovering critical metals such as Lithium, Cobalt, Nichel, and Manganese. Whereas currently available industrial technologies, such as pyrometallurgy and hydrometallurgy suffer for severe energy requirement and waste production, more selective, efficient and environmentally friendly separation processes should be developed, focusing on reduction of the energy consumption and application to different electrode materials.
Along these lines is WAVEE, Waste As Valuable Elements for Europe, an MSCA staff exchange action program, funded by EU within the scheme of Horizon Europe, which aims at valorizing skills and know-how coming from academic and industrial scientists operating in the field of waste treatment and material science by the development of cutting-edge and low impact recovery methods for critical raw materials, CRMs from spent Li-ion batteries. Innovative approaches, based on the adoption of microwave radiation and mechanochemical techniques, also in combination with mild organic/metal-organic compounds are expected to replace conventional pyrometallurgy and strong and hazardous acids, providing leap forward safer and greener recovery paths. Work is also addressed to scale-up the developed protocols to pre-industrial level, in order to assess the overall efficiency of the innovative recycling processes and the quality of recovered RMs. In the present work main research lines of the project and preliminary results of research activity are presented

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-G P4-

Complete Degradation of Organic Pollutants in Water by Magnetically Separable Fe_3O_4/CQDs-ZnO Photocatalyst Under Sunlight Irradiation

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The present work is based on the fabrication of solar-light-active photocatalyst for removal of organic dyes and antibiotics in water. The ternary photocatalyst based on Fe_3O_4/CQDs-ZnO was prepared, via a Ultrasonic method, for degradation of levofloxacin (LVX) antibiotic and Rhodamine B (RhB) dye under natural sunlight. The Fe_3O_4/CQDs-ZnO showed the lowest photoluminescence intensity, compared to those of all prepared photocatalysts including the bare ZnO. This agrees with the greatest photocatalytic activity detected in the ternary photocatalyst. The key strategy is based on improvement of electron-hole separation rate and enhancement of the visible light absorption after construction of the ternary photocatalyst. Complete removal of LVX and RhB was achieved within 120 min and 240 min of photo irradiation. The degradation of the pollutant fits nicely with the first-order kinetic model The highest rate constant of about 0.0238 min^{-1} was obtained. The ternary heterojunction still exhibits the promising photocatalytic performance even after five cycles of use indicating its excellent cycling ability. The scavenger experiment reveals that the superoxide anion radicals play a major role in removal of the organic contaminants. This work shows the new avenue to generate the three-component heterostructure, with magnetic separable property, for degradation of harmful LVX antibiotic and RhB dye in the environment.

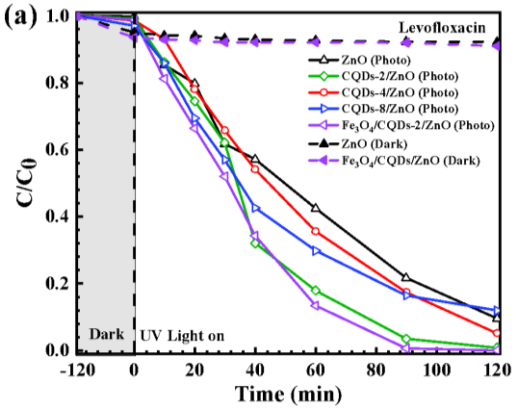

Figure 1. Plots of LVX concentration vs time under UV light (a).

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-G P5-

Physico-Chemical Characterization and Adsorption Performance of Cu- BTC Surface- Supported MOF Thin Films for Water Remediation

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Driven by the urgent demand for effective environmental remediation technologies, this study investigates the development of surface-supported Metal-Organic Framework (Sur-MOF) thin films for the removal of organic pollutants from water.
Sur-MOF films were synthesized using a wet Layer-by-Layer (LbL) approach, employing copper metal nodes and 1,3,5-benzenetricarboxylate (BTC) organic linkers. Owing to their high surface area and intrinsic porosity, the fabricated films were evaluated for the adsorption of Rhodamine B (RhB), a common organic contaminant found in textile industry wastewater.
Comprehensive physico-chemical characterization was conducted using UV–Vis spectroscopy, Atomic Force Microscopy (AFM) and Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) to assess optical properties, surface morphology and chemical composition. This holistic approach enabled a systematic evaluation of adsorption performance as a function of deposition cycles and RhB exposure time. Additionally, desorption and regeneration studies were performed to assess the reusability of the Sur-MOF films.
The findings of this study highlight the potential of Sur-MOF thin films as versatile and efficient platforms for water purification and selective molecular capture.

Acknowledgments. This work is partially funded by the project PRIDE (MASE Prog. n. RSH2A_000037 - CUP: F57G25000320006).

-G P6-

Magnetically Recoverable Swellable Magnetite/SOMS Hybrid Nanocomposites for Rapid Adsorption of Organic Dyes from Water

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The development of efficient and easily recoverable adsorbents is a key challenge in water treatment technologies. In this context, magnetic nanomaterials have attracted significant attention due to their ability to be rapidly separated from aqueous media using an external magnetic field. Among them, magnetite-based hybrid materials offer a promising strategy by combining high adsorption capacity with magnetic responsiveness. Hybrid magnetic adsorbents based on magnetite nanoparticles and Swellable Organically Modified Silica (Mag-SOMS) are synthetized and investigated here to overcome the limited recoverability of absorbents from aqueous media. The materials are synthesized by integrating magnetite nanoparticles, obtained via co-precipitation route, into a SOMS matrix prepared through a sol–gel process. Structural, spectroscopic, textural, and magnetic characterization demonstrate that the magnetite phase retains its crystalline structure and, crucially, preserves its magnetic properties after incorporation into the SOMS framework, ensuring efficient magnetic manipulation. Mag-SOMS system achieves more than 99% removal (1.91 mg g^{-1} adsorbed) of Rhodamine B from water within 10 minutes. Importantly, the preserved magnetic properties enable rapid and efficient recovery of the adsorbents via an external magnetic field. Furthermore, the materials are regenerable and can be reused over multiple adsorption cycles without loss of performance, underscoring the key role of magnetism in enhancing their practical applicability for water treatment.

-G P7-

Upcycling of Cigarette Filters into a High Surface Area Polymer via Hyper-Crosslinking

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Hyper-crosslinked (HCL) polymers represent a class of materials characterized by high specific surface area (SSA), that can be synthesized from a wide range of precursors [1]. However, many of the synthetic processes currently used to produce these materials are environmentally unsustainable, particularly with regard to the solvents involved. In this study, sulfolane was employed as an alternative, green solvent [2] to synthesize high SSA materials starting from cellulose acetate (CA) in presence of a typical Friedel-Crafts catalyst, $FeCl_3$. CA is a polymer widely used in textiles, plastics, films, and in cigarette filters (CF) [3]. In particular, CF represent one of the most abundant and critical waste streams due to the massive scale of littering and the release of toxic chemicals [4].
In this work, the conditions required to promote the aromatization and extensive crosslinking of CA were explored, with the aim of transferring the optimized protocol to the waste CF. Reaction parameters were systematically optimized to minimize environmental impact by balancing reaction yield, reaction time, precursor/solvent and catalyst ratios. Preliminary results confirm the effective aromatization and crosslinking of the precursors and N_2 adsorption analysis shows that the HCL-CA and HCL-CF are characterized by SSA above 1000 m^2/g. Both materials exhibit a highly microporous structure, with about 70% of the pore volume attributed to micropores (Figure 1).

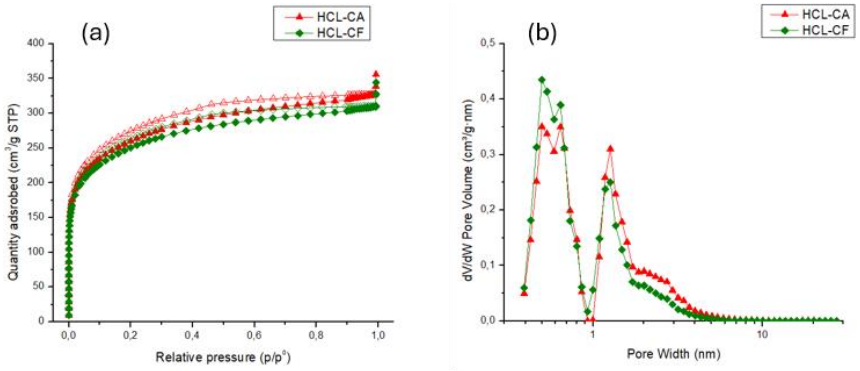

Figure 1. Adsorption-desorption isotherms (a) and Non-Local Density Functional Theory pore side distribution (b) of HCL CA and HCL-CF.

Acknowledgments. The authors acknowledge financial support under the FIS 2 Call funded by the Italian MUR for the project HIPAD (FIS-2023-01686, CUP B53C24009520001, Grant Assignment Decree No. n. 23314 adopted on 11/12/2024 by the Italian MUR).

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