MACCS2

2nd International Workshop on "Modeling and Characterization of Complex Systems"

17 June 2025, University of Cagliari, Campus of Monserrato, Italy

Book of abstract

Aims

The MACCS Workshops – now in their second edition – aim to foster interaction among scientists from UNICA and from other Italian and international institutions, providing a space to share knowledge and perspectives on challenges in chemistry and physics across a range of applications.

The focus is on exploring and explaining the behavior of complex systems relevant to materials science, biotechnology, and green chemistry, through a combination of experimental work and multiscale modeling. By encouraging interdisciplinary collaboration and exchange, MACCS2 contributes to developing new approaches and practical solutions to complex real-world problems.

Scientific and Organizing Committees

Scientific Committee

- Marketa Palocyova – Czech Advanced Technology and Research Institute (CZ)
- Miroslav Medved – Matej Bel University (SK) and Czech Advanced Technology and Research Institute (CZ)
- Leon Engelbrecht – Lulea Technical University (SE)
- Flaminia Cesare Marincola – University of Cagliari (IT)
- Francesca Mocci – University of Cagliari (IT)
- Carlo Maria Carbonaro – University of Cagliari (IT)
- Claudio Melis – University of Cagliari (IT)

Local Organizing Committee

- Francesca Mocci – Department of Chemistry and Geology, University of Cagliari (IT)
- Carlo Maria Carbonaro – Department of Physics, University of Cagliari (IT)
- Maria Francesca Casula – Department of Mechanical, Chemical and Materials Engineering, University of Cagliari (IT)
- Luca Malfatti – Department of Biomedical Sciences, University of Sassari (IT)
- Chiara Olla – Department of Physics, University of Cagliari (IT)
- Luca Pilia – Department of Mechanical, Chemical and Materials Engineering, University of Cagliari (IT)
- Andrea Salis – Department of Chemistry and Geology, University of Cagliari (IT)

Patronage

The event is organized under the patronage of the Department of Chemistry and Geology, the Department of Physics and the Department of Mechanical, Chemical and Materials Engineering of the University of Cagliari and that of the COSY COST ACTION CA21101 – CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS (COSY). The event is also sponsored by the research project "Engineered robust-composite photoelectrodes with enhanced durability and solar-to chemical energy conversion" granted by the Italian Ministry of Universities and Research within the PRIN 2022 call (P2022JRB2Y)

Program

June 17th, 2025 – CITTADELLA UNIVERSITARIA DI MONSERRATO, AULA 110, Block A

9:00 Registration + Coffee & Hanging up Poster

10:00 Welcome and opening

10:10 Michal Otyepka "Inkjet Printing in Electrochemical Biosensing"

10:30 Cristina Carucci "Investigating protein corona formation; BSA interactions with bare and amino functionalized mesoporous silica nanoparticles"

10:50 Seyed H. Mussavi Rizi "Advances in Bioresorbable phospate glass optical fiber fabrication"

11:10 Jela Nociarová "NMR Spectroscopy as a Tool for Characterization of Molecular Fluorophores in Carbon Dots: Challenges and Opportunities"

11:30 Luca Malfatti "Light-activated Carbon dots for functional applications"

11:50 Claudio Melis "Engineering thermal transport in transition metal dichalcogenides: from molecular modifications to defect-engineered superlattices"

12:10 Eva Otyepková "Inverse Gas Chromatography in the Study of Surface Properties of Materials**"**

12:30 Lunch

14:00 Rosangela Mastrangelo "Surface-modified agar microgels as food foams stabilizers**"**

14:20 Miroslav Medved' "Computational Insights into Molecular Photochromism"

14:40 Chiara Olla "Photopolymer-Based Colorimetric Sensors Incorporating Natural Dyes for Detection of Toxic Substances"

15:00 Davide Tocco "Sustainable Carbon Quantum Dots: From Fluorescent pH Sensors to Performance Enhancement in Solar Cells"

15:20 Nicola Melis "Nanoporous Au in Dye-Contaminated Water: A Case Study with Methyl Orange"

15:40 Coffee Break

16:10 Markéta Paloncýová "Simulation Insight into Bio-Nano Interface"

16:30 Annalisa Chiappone "Vat 3D printing of ionically conductive polymers for tactile sensors"

16:50 Riccardo Dettori "Linear Machine-Learning Approaches For Accurate Atomistic Simulations"

17:10 Poster session and coffee break

18:30 Poster prize announcement & Closing remarks

19:00 Transfer to social dinner

19:30 Dinner

Oral Presentations

Vat 3D printing of ionically conductive polymers for tactile sensors

A. Chiappone[1], M.V. Piras[1], G. Mogli [2], F. Secci [1], I. Roppolo[2], S. Stassi[2]

[1]Department of Chemical Science and Geology, University of Cagliari, Cagliari, Italy
[2]Department of Applied Science and Technology, Politecnico di Torino, Torino, Italy

Smart sensors based on conductive soft polymers have shown remarkable potential whenever a link between the "soft" human world needs an interface with the "rigid" electronic one is required, in fields like wearables and soft robotics. [1] However, conventional manufacturing technologies, such as casting processes, limit the obtainable shapes and applications. 3D printing offers a valid alternative for producing customizable and conformable sensors and, among the printing technologies, light-induced ones allow high printing precision and fast production. Nevertheless, developing highly deformable and conductive thermoset photocurable polymers is not trivial; merging these requirements with those linked to the 3D printability of the formulation makes the target challenging. [2] Herein different materials that were successfully tailored to obtain 3D printable tactile sensors will be presented.

On one side photocurable ionic conductive hydrogels based on a semi-interpenetrating polymeric network have been synthesized and 3D printed. The presented photocurable hydrogel, with excellent sensitivity to mechanical deformations, holds remarkable mechanical properties (ultimate tensile strain of 550%) and spontaneous self-healing capabilities, with complete recovery of its strain sensitivity after damages. Furthermore, the developed material can be processed by digital light processing 3D printing technology to fabricate complex-shaped strain sensors, increasing mechanical stress sensitivity with respect to simple sensor geometries, reaching an exceptional pressure detection limit below 1 Pa. [3]

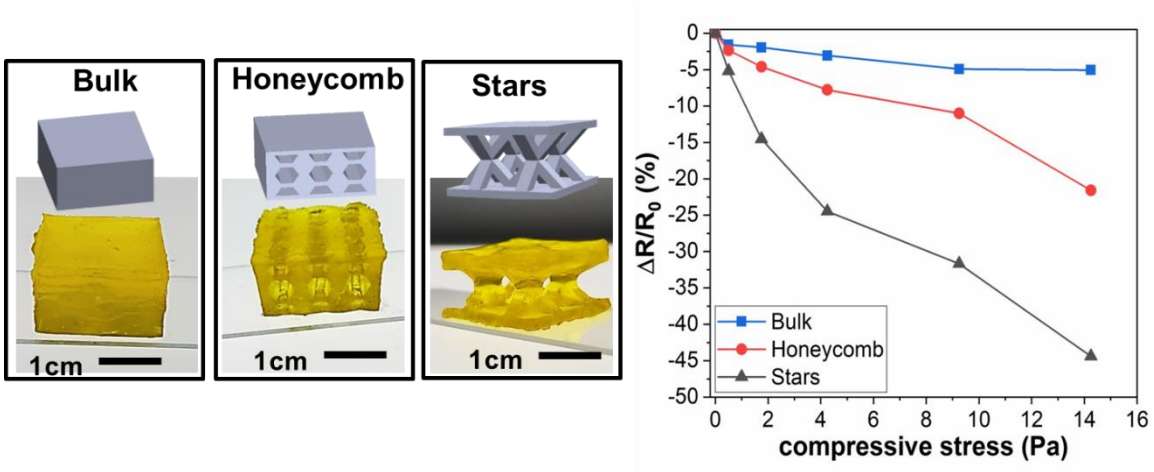


Figure 1- 3D printed hydrogels with different shapes and their resistive response to compression.

Despite the intriguing properties of the presented material, the main drawback of hydrogels is the poor stability due to water evaporation, thus, alternative solutions must be developed.

In a second work, a mixture based on acrylic acid and hydrated salt was used to homogeneously disperse and simultaneously functionalize cellulose pulp extracted from local waste, also enhancing the sustainability of the device. In this way, 3D printable formulations were obtained and the precise printing of highly stretchable structures was achieved.
The resulting material gave extremely good results in terms of sensitivity, demonstrating again the possibility to tune the sensing response by giving different shapes through 3D printing. Furthermore, the developed material showed remarkable stability in time and at different temperatures.

REFERENCES

[1] Pyo S., Lee J., Bae K., Sim S., Kim J. (2021) "Recent progress in flexible tactile sensors for Human-interactive systems: from sensors to advanced applications" *Advanced Materials* 33,47, e2005902.

[2] Payandehjoo B., Kwok T.H. (2023) "Embedding ionic hydrogel in 3D printed humancentric devices for mechanical sensing" *J. Manuf. Process*. 100, 1–10.

[3] Mogli G., Reina M., Chiappone A., Lamberti A., Pirri C.F., Roppolo I., Stassi S.(2024) "Self-Powered Integrated Tactile Sensing System Based on Ultrastretchable, Self-Healing and 3D Printable Ionic Conductive Hydrogel" *Adv Funct. Mater*. 34, 2307133 DOI: 10.1002/adfm.202307133

Linear Machine-Learning Approaches For Accurate Atomistic Simulations

Riccardo Dettori[1]

[1]Universita' degli Studi di Cagliari, Dipartimento di Fisica, riccardo.dettori@dsf.unica.it

Molecular dynamics (MD) simulations are a fundamental tool for investigating the atomistic behavior of complex systems, offering deep insights into reaction mechanisms, phase transitions, and emergent properties in both condensed and soft matter. Recent advances in machine learning (ML) have determined a paradigm shift in atomistic simulations, allowing the development of force-fields that closely mimic quantum mechanical interactions with exceptional accuracy and efficiency—achieving this at a fraction of the computational cost of ab initio methods. However, while standard non-linear ML potentials such as Gaussian Approximation Potentials and Neural Network Potentials deliver excellent descriptions of the atomic environment, their numerous fitting parameters often restrict the size of the systems and the duration of simulations due to increased computational demands from high-dimensional parameter spaces. Furthermore, realizing these potentials is labor-intensive, as they generally require extensive training datasets and are vulnerable to overfitting. In this presentation, I will introduce the Chebyshev Interaction Model for Efficient Simulation (ChIMES) [1], which leverages a linear expansion in Chebyshev polynomials to accurately reproduce atomic forces, energies and stress tensors in molecular and condensed-phase systems while requiring comparatively less data. I will present some of my recent results adopting the ChIMES approach both for approximate quantum mechanical simulations and for classical molecular dynamics calculations, regarding different systems ranging from a meteoritic magnetic material (Fe3P, Schreibersite) [2] to crystalline and amorphous silicon interfaces with hydrogen (c-Si/a-Si:H) for photovoltaics [3].

REFERENCES

[1] Lindsey et al., Journal of Chemical Theory and Computation, 2017, 13, 6222
[2] Dettori R., Melis C., Colombo L. Nanotechnology, 2025, 36(15), 155703
[3] Dettori R., Goldman N. Journal of Physical Chemistry A, 2025, 129(2), 583–595

Light-activated Carbon dots for functional applications

L. Malfatti[1], L.Stagi[1], D. Carboni[1], P. Innocenzi[1], A. Sciortino[2], F. Messina[2]

[1]LMNT, Department of Biomedical Sciences, University of Sassari, Viale San Pietro 43/B, Sassari 07100, Italy
[2]Department of Physics and Chemistry "Emilio Segrè", University of Palermo, Via Archigrafi 36, 90123 Palermo, Italy

Carbon dots (C-dots) are an emerging class of carbon-based nanostructures derived from low-cost raw materials. They exhibit broad absorption in the UV and visible range, tunable photoluminescence, and high quantum yield. Additionally, under specific conditions, C-dots can function as pro-oxidant photosensitizers, enabling antibacterial and antiviral applications [1].

Despite their promising properties, integrating C-dots into solid matrices remains a critical challenge in the development of functional nanocomposites. While C-dots have been extensively studied in solution, their application in solid-state systems is still limited, mainly due to aggregation and optical quenching phenomena that significantly reduce their performance. Sol-gel chemistry, when paired with a carefully designed selection of chemical precursors, plays a crucial role in incorporating luminescent C-dots at high concentrations without inducing aggregation in the matrix [2].

Recently, we developed a simple chemical strategy to synthesize C-dots from dye molecules. This approach enables accurate prediction of the nanoparticles' emission characteristics, preserves the quantum yield of the precursor dyes, and significantly enhances photobleaching resistance [3].

Leveraging this strategy, we synthesized photocurable hybrid organic–inorganic monoliths capable of efficiently producing amplified stimulated emission in the visible red range. Due to the rapid photocuring process of the hybrid matrix, we achieved high C-dot loadings (exceeding 3 OD) without aggregation. Remarkably, the C-dot-based nanocomposites exhibit a lower threshold for amplified stimulated emission (Figure a) compared to analogous monoliths containing only the precursor dye molecules.

Furthermore, the flexibility provided by the materials synthesis allows introducing an innovative one-step strategy to create a medium for random lasing applications. (Figure b). During the photocuring of the hybrid organic–inorganic network, the UV exposure can trigger the nucleation and growth of gold nanoscatterers, featuring controlled size distribution and plasmonic properties. Overall, the optical response of the nanocomposites is compatible with an incoherent random lasing regime, characterized by a low lasing threshold and a spectral emission width of less than 5 nm.

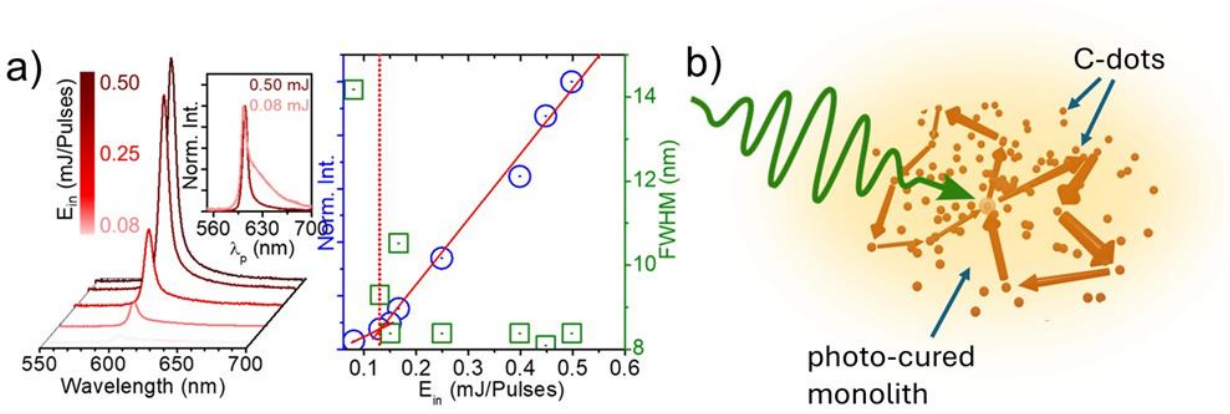


Figure 2 – a) Spectral emission of C-dot-based nanocomposites under pulsed laser at 540 nm below and above the amplification threshold. b) Schematic of solid-state random lasing.

REFERENCES

[1] Malfatti L, Poddighe M, Stagi L, Carboni D, Anedda R, Casula M F, Poddesu B, De Forni D, Lori F, Livraghi S, Zollo A, Calvillo L, Innocenzi P, (2024) "Visible Light Activation of Virucidal Surfaces Empowered by Pro-Oxidant Carbon Dots". *Adv. Funct. Mater.* 2404511. DOI: 10.1002/adfm.202404511

[2] Malfatti L, Innocenzi P, (2018) "Sol-gel chemistry for carbon dots". *Chem. Rec.* 18, 1192-1202. DOI: 10.1002/tcr.201700108
[3] Meloni M, Stagi L, Sanna D, Garroni S, Calvillo L, Terracina A, Cannas M, Messina F, Carbonaro C M, Innocenzi P, Malfatti L, (2022) "Harnessing Molecular Fluorophores in the Carbon Dots Matrix: The Case of Safranin O". *Nanomaterials* 12, 2351. DOI: 10.3390/nano12142351
[4] Stagi L, Carboni D, Anedda R, Popescu R, Eggler Y, Calvillo L, Pramanik A, Sciortino A, Cannas M, Messina F, Malfatti L, (2025) "One-Step Fabrication of Carbon Dot-Based Nanocomposites Powering Solid-State Random Lasing". *Small Struct.* 6, 2400498. DOI: 10.1002/sstr.202400498

Surface-modified Agar Microgels As Food Foams Stabilizers

R. Mastrangelo[1,2,3], V. Guglielmino[2], D. Tocco[2], F. Desogus[1], E. Fratini[2,3]

[1]Department of Mechanical, Chemical and Materials Engineering, University of Cagliari, Via Marengo, 2, Cagliari 09123, Italy, rosangela.mastrangel@unica.it
[2] Department of Chemistry, University of Florence, Via della Lastruccia 3, Sesto Fiorentino (FI) 50019, Italy
[3] Center for Colloid and Surface Science, CSGI, Via della Lastruccia 3, Sesto Fiorentino (FI) 50019, Italy

The formulation and stabilization of foams and emulsions is a central challenge in food engineering and technology [1]. While traditional emulsifiers (e.g. proteins, polysaccharides and surfactants) are widely used to prevent or retard the macroscopic phase separation, due to their ability to adsorb at the interface and reduce the interfacial tension [2], their application in the food industry can be limited by their high cost, possible toxicity or low biocompatibility [3]. The advent of Pickering emulsions [4], including solid particles that irreversibly adsorb at the interface, effectively reduced these drawbacks. The stabilization of foams with particles has regained attention recently, due to the possible applications in critical research fields, including not only food science, but also wastewater treatment, cosmetics and health-care products. The so-called Pickering foams are significantly more stable those stabilized with traditional amphiphiles, due to the high energies linked to the particles adsorption at the interface [5]:

$$-\Delta E=\pi R^2\gamma(1-|\cos\theta|)^2 \quad (1)$$

with θ the contact angle of particles in the aqueous phase, R the particle radius and γ the air-water (A/W) interfacial tension. Larger radii and θ ~ 90° are expected to favor the adsorption at the interface and, thus, the foam stabilization.

In this framework, biopolymers-based microgels have emerged as ideal soft stabilizers. Unlike rigid particles, microgels can deform and swell, adapting to the interface and being less prone to undergo sedimentation when their size exceeds the micron (due the reduced density difference, Δρ, with the continuous phase).

Many natural polymers have been used to obtain microgels, like proteins, starch, gellan, alginate, dextran, agar etc.[1] Among them, agar can be used to obtain thermally reversible physical hydrogels, with tunable rigidity, size and shape [6].

This study aimed at the formulation and characterization of surface-modified agar microgels as Pickering agents. Spherical microgels were obtained by a low-energy method, i.e. the spontaneous water-in-oil (W/O) emulsification of agar, stabilized by the food-grade polymer HCO40 (a polyoxyl hydrogenated castor oil). Emulsions were obtained at 80°C and cooled down at ~4°C allowing the polymer to form the physical microgels. During the agar gelation, the polyoxyl units of HCO40 (constituting the bulky polar head) are expected to get trapped in the microgels core, leaving the castor oil chains (i.e., the hydrophobic tails) exposed to the continuous phase. In this way, the microgels' surface hydrophobicity can be increased safely and irreversibly, without using toxic crosslinkers or simply adsorbing surfactants on the microgels' surface.

The best suitable W/O emulsions (high water:oil ratio, lower polydispersity) were identified by building a pseudo-ternary phase diagram (fig. 1 A) and observing the formed microgels through optical microscopy and Confocal Laser Scanning Microscopy (CLSM images, fig. 1, right panel). Samples with a high aqueous-phase content and different surfactant concentrations were further investigated (3T, 5T and 10T in fig.1 A).

A washing protocol, to remove the oil and the unbound surfactant, was optimized by monitoring the washed product by Confocal Raman Microscopy. Water-based dispersions of microgels were finally obtained ("Washed" samples, fig. 1, right panel).

To verify the possibility of tailoring the microgels' surface hydrophobicity, formulations with increasing HCO concentrations were challenged. Contact angle measurements, performed on dried microgel films, indicated that the surface hydrophobicity increased with the surfactant concentration (fig.1, right panel).

The microgels' ability to stabilize food foams was assessed on a commercial egg white product. In general, some microgels mixtures showed enhanced foam capacity (FC, fig. 1 B) and stability.
Finally, microgels' ability to encapsulate actives was investigated through CLSM imaging: 1 µm fluorescent particles, mimicking specific antimicrobial peptides, were added to the formulation. The particles inclusion and retention within the microgels was confirmed before and after washing, opening to the possibility of combining the enhanced foamability/stability with bioactive components' encapsulation, protection and delivery.

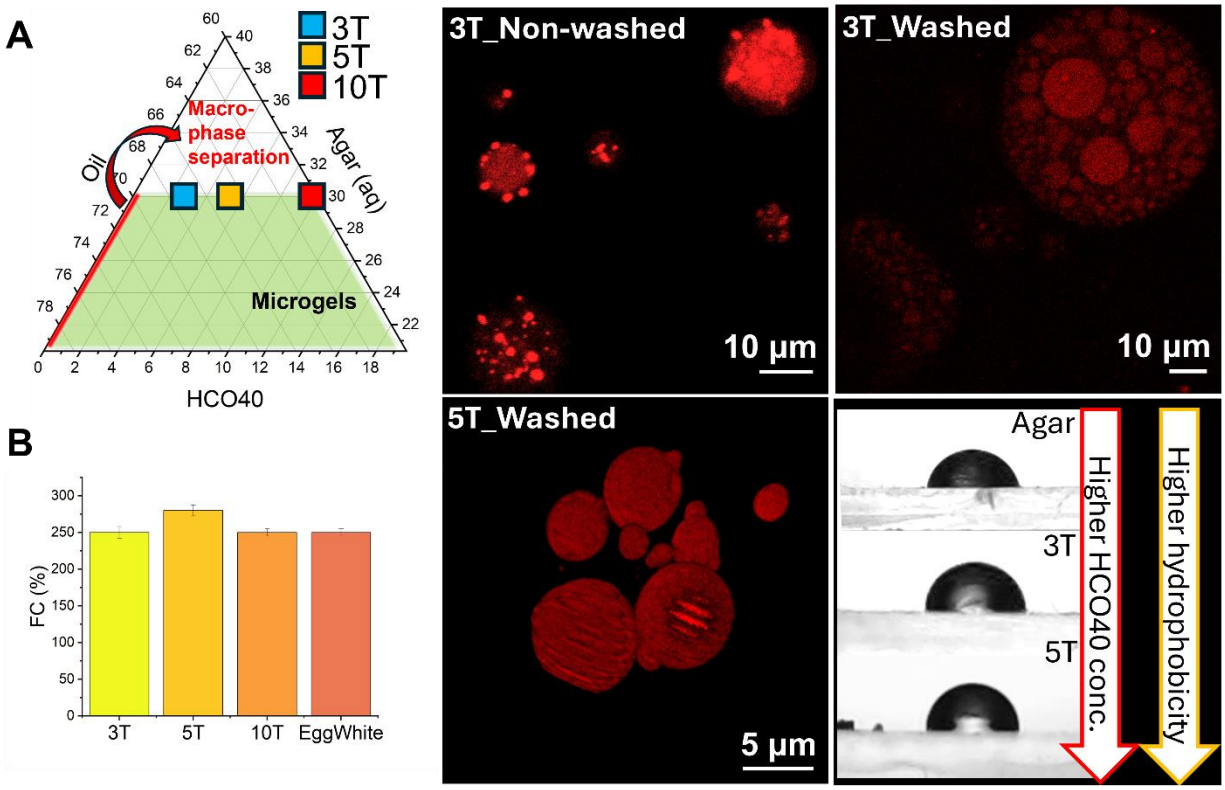


Figure 3 – A) Pseudo-ternary phase diagram showing the area where microgels were obtained (in green) and the samples investigated (3T, 5T and 10T, with increasing HCO40 concentration); B) Foaming Capacity (FC%) of the egg white with and without microgels; Right Panel: Confocal Images of the microgels before and after washing; Contact Angle measurements on dry films.

REFERENCES

[1] Dickinson E. (2015) "Microgels — An alternative colloidal ingredient for stabilization of food emulsions". *Trends Food Sci. Technol.* 43, 178–188. https://doi.org/10.1016/j.tifs.2015.02.006.
[2] McClements D.J. (2004) "Food Emulsions: Principles, Practices, and Techniques". 2nd ed., *CRC Press*, Boca Raton. https://doi.org/10.1201/9781420039436.
[3] Yang Y., Fang Z., Chen X., Zhang W., Xie Y., Chen Y., Liu Z., Yuan W., (2017) "An Overview of Pickering Emulsions: Solid-Particle Materials, Classification, Morphology, and Applications". *Front. Pharmacol.*, 8. https://doi.org/10.3389/fphar.2017.00287.
[4] Chevalier Y., Bolzinger M.-A., (2013) "Emulsions stabilized with solid nanoparticles: Pickering emulsions, Colloids". *Surf. Physicochem. Eng. Asp*., 439, 23–34. https://doi.org/10.1016/j.colsurfa.2013.02.054.
[5] Binks B.P., (2002) "Particles as surfactants—similarities and differences", *Curr. Opin. Colloid Interface Sci*., 7 21–41. https://doi.org/10.1016/S1359-0294(02)00008-0.
[6] Xiao Q., Chen Z., Xie X., Zhang Y., Chen J., Weng H., Chen F., Xiao A., (2022) "A novel Pickering emulsion stabilized solely by hydrophobic agar microgels". *Carbohydr. Polym*. 297 120035. https://doi.org/10.1016/j.carbpol.2022.120035.

Engineering Thermal Transport in Transition Metal Dichalcogenides: From Molecular Modifications to Defect-Engineered Superlattices

Claudio Melis[1], Francesco Siddi[1], Antonio Cappai[1], Riccardo Dettori[1]

[1]Department of Physics University of Cagliari Monserrato, CA 09042, email: claudio.melis@dsf.unica.it

Controlling heat transport in two-dimensional (2D) materials—particularly transition metal dichalcogenides (TMDs)—is crucial for advancing thermoelectric and nanoelectronic technologies. This presentation discusses two atomistic-level studies that demonstrate how phonon behavior can be tailored through chemical functionalization and structural patterning.

In the first study[1], we focus on TaS_2 functionalized with tert-butyl isocyanate, where the covalent bonding of organic side groups leads to a dramatic, nearly 100-fold reduction in in-plane thermal conductivity. Phonon dispersion and lifetime analyses reveal two dominant effects: (1) the suppression of interlayer quasi-acoustic modes due to increased spacing between layers, and (2) the lowering of group velocities caused by the introduction of soft optical modes from the molecular chains.

The second study[2] examines defect-engineered monolayer MoS_2, where sulfur vacancies are arranged into periodic superlattices. Surprisingly, specific defect periodicities can recover the thermal conductivity of pristine MoS_2 by reducing acoustic–optical phonon scattering, effectively mimicking the behavior of phononic metamaterials.

Together, these findings underscore the power of atomic-scale engineering—through chemical modification and structural design—in tuning thermal transport in TMDs. Such approaches offer promising pathways to optimize the performance and stability of future 2D material-based devices.

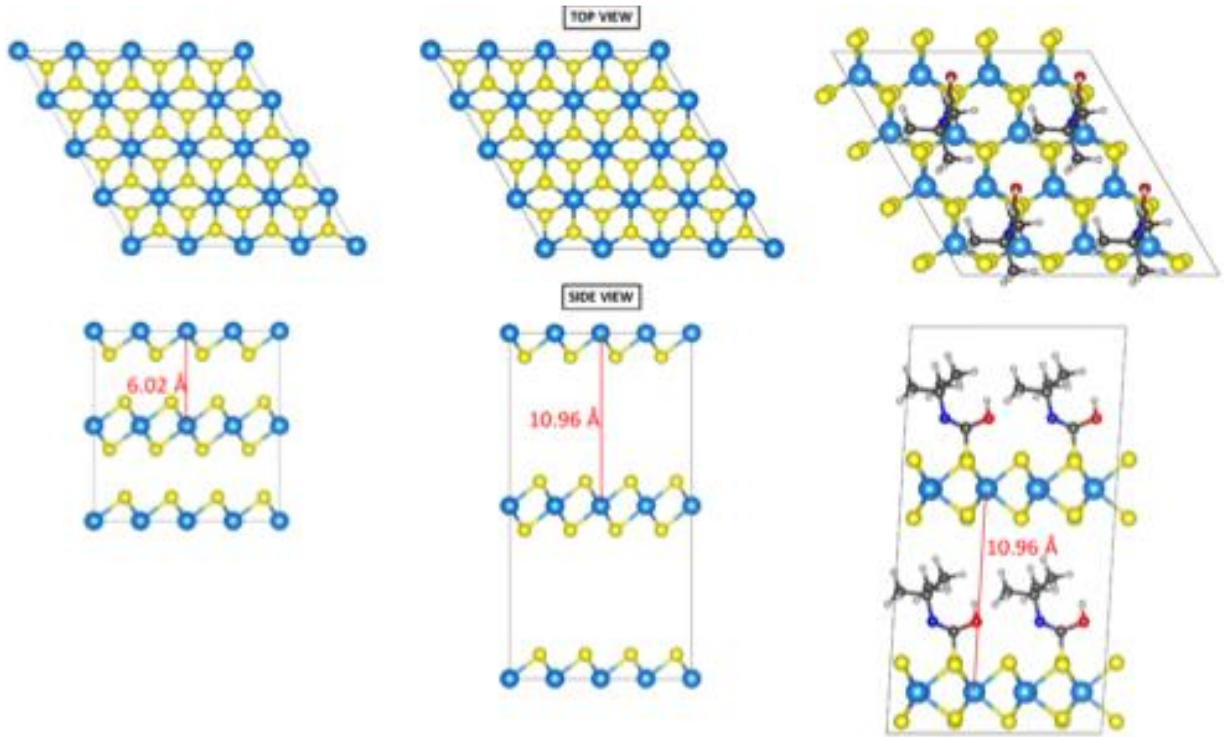


Figure 4 – Stick-and-ball representations of the three geometry-optimized structures considered in this study.

REFERENCES

[1] Siddi F, Cappai A, Colombo L, Melis C, (2024) "An Ab Initio Investigation of Ultra-Low Thermal Conductivity in Organically Functionalized TaS_2". *Advanced Theory and Simulations*, 7, 2400056.
https://doi.org/10.1002/adts.202400056
[2] Dettori R, Siddi F, Colombo L, Melis C, (2024) "Superlattice Thermal Modulation in MoS_2 by Defect Engineering". *Advanced Theory and Simulations*, 2024, 2401199.
https://doi.org/10.1002/adts.202401199

Nanoporous Au in Dye-Contaminated Water: A Case Study with Methyl Orange

N. Melis[1], A. Pinna[1], G. Pia[1], M. Prato[2], M. G. Cutrufello[3], E. Sogne[4], A. Falqui[5], L. Pilia[1].

[1]Dipartimento di Ingegneria Meccanica, Chimica e dei Materiali, Università degli Studi di Cagliari, via Marengo 2, 09123, Cagliari, Italy. e-mail: nicola.melis87@unica.it
[2]Materials Characterization Facility, Italian Institute of Technology, Via Morego 30, 16163 Genoa, Italy
[3]Dipartimento di Scienze Chimica e Geologiche, Università degli Studi di Cagliari, S.S. 554 bivio per Sestu, 09042 Monserrato (CA), Italy
[4]PoliFAB, Polytechnic of Milan, Via Giuseppe Colombo, 81, 20133 Milan, Italy
[5]Department of Physics "Aldo Pontremoli", University of Milan, Via Celoria 16, 20133 Milan, Italy

Nanoporous gold (NP Au) is among the most extensively investigated nanostructured metals due to its high surface area, tunable porosity, chemical stability, and ease of functionalization. These characteristics – particularly its high surface area, biocompatibility, and chemical stability – make NP Au an exceptional candidate for advanced applications, including catalysis, sensing, and energy conversion [1]. Among these, its catalytic performance in key chemical reactions has attracted considerable attention. However, its potential in environmental applications such as the catalytic degradation of water contaminants, remains relatively underexplored. In this context, the degradation of methyl orange (MO), a hazardous azo dye commonly found in industrial wastewater, has been studied using NP Au as a potential catalyst. Early studies suggest that NP Au may facilitate the breakdown of MO, although the underlying mechanism remains not fully understood [2].
The present study focuses on investigating the interaction between NP Au and MO in aqueous solutions, aiming to clarify the nature and extent of this catalytic behavior. NP Au was synthesized starting from a ball-milled AuAg precursor alloy with a gold/silver atomic ratio of 3:7. This alloy was subsequently cold-pressed into a pellet and chemically etched through immersion in concentrated nitric acid for 24 h to selectively leach out silver. SEM and EDS measurements of the resulting NP Au (Figure 1) highlight a bicontinuous structure composed of interconnected ligaments and pores, with ligaments diameter of approximately 15 nm and pore diameter around 14 nm. Additionally, the material retains about 12 % residual silver atomic content.

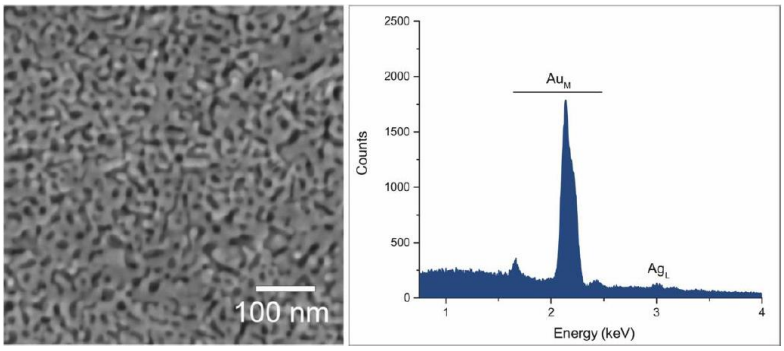


Figure 1 – SEM image and EDS spectrum of NP Au after 24 h of dealloying

Both pellet and powder forms of NP Au were subjected to immersion tests in MO solutions, and the post-reaction solutions were analyzed using UV-Vis absorption spectroscopy and high-performance liquid chromatography (HPLC), as reported in figure 2. Moreover, to gain deeper insight into the changes occurring in the NP Au structure and surface chemistry during exposure, X-ray photoelectron spectroscopy (XPS) and electrochemical impedance spectroscopy (EIS) were also employed.

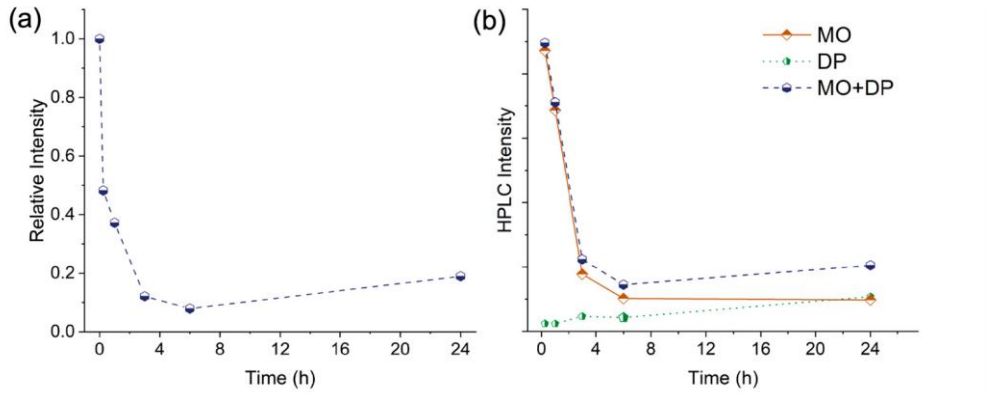


Figure 2 – (a) UV-Vis relative intensity of absorption peak at 463 nm at different times after NP Au powder immersion; (b) HPLC absorption intensities of MO, degradation product (DP) and sum of the two intensities (MO + DP).

The results indicate that the predominant process is the rapid, partially reversible adsorption of MO molecules onto the nanoporous gold surface. In contrast, the actual catalytic degradation of the dye occurs more slowly and to a lesser extent [3]. These findings suggest that, under the explored conditions, adsorption dominates the interaction between NP Au and MO, while catalytic decomposition plays a secondary role. This nuanced understanding provides a foundation for optimizing NP Au systems for future water treatment applications.

REFERENCES

[1] Seker E., Reed M. L., Begley M. R., (2009) "Nanoporous Gold: Fabrication, Characterization, and Applications". *Materials,* 2, 4, 2188-2215. https://doi.org/10.3390/ma2042188

[2] Hakamada M., Hirashima F., Mabuchi M., (2012) "Catalytic decoloration of methyl orange solution by nanoporous metals". *Catal. Sci. Technol. 2,* 1814–1817. https://doi.org/10.1039/c2cy20218b

[3] Pinna A., Pia G., Melis N., Prato M., Cutrufello M. G., Sogne E., Falqui A., Pilia L., (2024) "Nanoporous Au Behavior in Methyl Orange Solutions". *Molecules*, 29,1950. https://doi.org/10.3390/molecules29091950

Computational Insights into Molecular Photochromism

Miroslav Medveď[1,2]

[1]Czech Advanced Technology and Research Institute (CATRIN), Regional Centre of Advanced Technologies and Materials, Palacký University Olomouc, Šlechtitelů 27, Olomouc, 77900 Czech Republic, miroslav.medved@upol.cz
[2] Department of Chemistry, Faculty of Natural Sciences, Matej Bel University, Tajovského 40, 974 00 Banská Bystrica, Slovakia

Light is an exceptional external stimulus offering precise control over the properties and functions of chemical and biological systems. This is enabled through the use of materials exhibiting photochromism, i.e., a reversible change of color upon the light irradiation. This change is typically induced by structural changes (e.g., isomerization, ring opening/closure, breaking of chemical bonds) of molecules (molecular photoswitches) and usually affects the physical properties such as dielectric constants, surface wettability, hydrophilicity, and refractive index. Molecular photoswitches have diverse applications including control of surface properties, surface patterning, data/energy storage, and drug delivery. For each of these applications, there are specific requirements on the photochromic characteristics of the material, with the operational wavelengths of light, photoswitching efficiency, and thermal stability of a metastable form being the key parameters. For example, ideal photoswitches for biological and medicinal applications are responsive to visible light, show large separation of absorption bands, exhibit thermal stability in the range of 0.1-1 s and are functional in various solvents including water. On the other hand, for the data storage use, the high thermal stability is the crucial feature.

In collaboration with experimental groups, we have been involved in research of various classes of molecular photochromes including donor–acceptor Stenhouse adducts (DASAs) [1,2], iminothioindoxyls (ITIs) [3-5], azonium salts [6], and hydrazones (HZs) [7,8]. Employing advanced quantum chemical methods, we explored spectral properties (absorption spectra) and thermal as well as photochemical reaction pathways of these systems. With the help of theory, we proposed structural modifications leading to significant improvement of their photochromic characteristics. For example, in the case of ITIs, which typically thermally relax on a millisecond time scale, we successfully designed derivatives with thermal half-lives exceeding 0.1 s [5]. In the class of triaryl-HZs, a recently discovered subclass of photochromic HZs, our computational analysis of various de-excitation pathways enabled to design derivatives with notably increased quantum yields of the *Z*-to-*E* photoisomerization. In the talk, several examplars of how computational tools can be used to gain insights into molecular photochromism will be provided.

Acknowledgements: Financial support of the Slovak Research and Development Agency (APVV-20-0098), the Scientific Grant Agency of the Slovak Republic (VEGA 1/0647/24) and the ERDF/ESF via project TECHSCALE (No. CZ.02.01.01/00/22_008/0004587) is acknowledged.

REFERENCES

[1] Di Donato M., et al. (2017) *J. Am. Chem. Soc.*, 139, 15596-15599. DOI: 10.1021/jacs.7b09081
[2] Lerch M. M. et al. (2018) *Angew. Chem. Int. Ed.*, 130, 8195 –8200. DOI: 10.1002/anie.201803058
[3] Hoorens M. W. H. et al. (2019) *Nat Commun.* 10, 2390. DOI: 10.1038/s41467-019-10251-8
[4] Medveď M. et al. (2021) *Chem. Sci.* 12, 4588. DOI: 10.1039/d0sc07000a
[5] Boëtius M. E. et al. (2024) *Chem. Sci.* 15, 14379. DOI: 10.1039/d4sc01457j
[6] Medveď M. et al. (2023) *J. Am. Chem. Soc.*, 145, 19894−19902. DOI: 10.1021/jacs.3c06157
[7] Mravec B. et al. (2021) *J. Org. Chem. 86, 11633–11646*. DOI: 10.1021/acs.joc.1c01174
[8] Hegedüsová L. et al. (2024) *Chem. Eur. J. 30, e202303509*. DOI: 10.1002/chem.202303509

Advances in Bioresorbable Phosphate Glass Optical Fiber Fabrication

Seyed Hossein Mussavi Rizi[1], Davide Luca Janner[1], Nadia Boetti[1,2]

[1]Politecnico di Torino, Italy
[2] Links Foundation, Torino, Italy

Bioresorbable phosphate glasses have emerged as a promising alternative to traditional silicate-based glass systems for biomedical applications. These glasses can be customized for their bioresorbability and mechanical properties and are transparent in a wide range of wavelengths (from 300 to 2600 nm), making them particularly suitable for biophotonic devices. Developing new and improved materials for innovative applications requires a multidisciplinary approach that involves glass-based photonics and advanced processing techniques for fiber optic research. Glass-based photonics plays a crucial role in pushing the development of new materials and advanced processing techniques for fiber optic research.
While extrusion is a powerful shaping method, extruding glass is rarely studied. The advantages of extrusion are the ability to vary the size and geometry of the extrudate, having excellent surface quality without any need for further treatments, fabricating complex preforms, and the ability to extrude different glass compositions. However, extrusion can result in distortion of the extrudates. In this thesis work, the soft glass extrusion process was optimized by studying the effects of various parameters on the glass billet and corresponding extrudate.

Preforms with low distortion and high surface quality enable the fiber drawing of microstructured optical fibers. The feasibility of fabricating microstructured bioresorbable optical fibers from phosphate glass with different compositions was investigated through melt-casting glass billets, extruding preforms, and using rod-intube and stack-and-draw assembly techniques. The resulting fiber comprises one microfluidic channel for liquid delivery and one core-cladding section for guiding light.

The fiber diameter dimension ranged from 125 to 250 µm. The performance of the fibers in guiding light and reducing attenuation loss was tested, and the microfluidic channel was evaluated for its ability to deliver liquid. Furthermore, by extruding preform with a very high outer-to-inner ratio diameter, we were able to fabricate singlemode fiber with a 7 µm diameter core size. On the other hand, by extruding preforms with a low outer-to-inner diameter ratio, it was possible to draw multi-mode fiber with a 220 µm diameter core size. These fibers are being studied to realize theranostic devices that can be used for targeted treatment within the body without the need for removal operations [1].

Glass fabrication
The core and the cladding exhibit a difference in refractive index for efficient light guiding within the core part of the microstructured fiber.
Cladding and capillary, PG1: *50 P_2O_5 – 23 MgO – 11.5 Na_2O – 10 CaO – 3 SiO_2 – 2.5 B_2O_3 (mol%)*
Core, PG2*: 50 P_2O_5 – 3 MgO – 11.5 Na_2O – 30 CaO – 3 SiO_2 – 2.5 B_2O_3 (mol%)*

Characterization
The bioresorbability of the fibers from this glass system was assessed in another study of our group using PBS solution at pH = 7.4 and a temperature of 37 °C. Solution volume/sample exposed area was 0.1 ml/mm2. The result was 37% weight loss in 21 days for the PG1 [2].
A set-up was created by injecting colored water into a 20 cm-long section of the 230 µm diameter fiber to examine how the liquid flows inside the 25 µm capillary hole. The liquid flow inside the capillary is visible demonstrating the liquid delivery functionality of the microstructured fiber. This type of microfluidic channel is comparable to standard planar channels and allows for a flow of around 10-50 µl/min which is compatible with the release of drugs or staining agents [1].

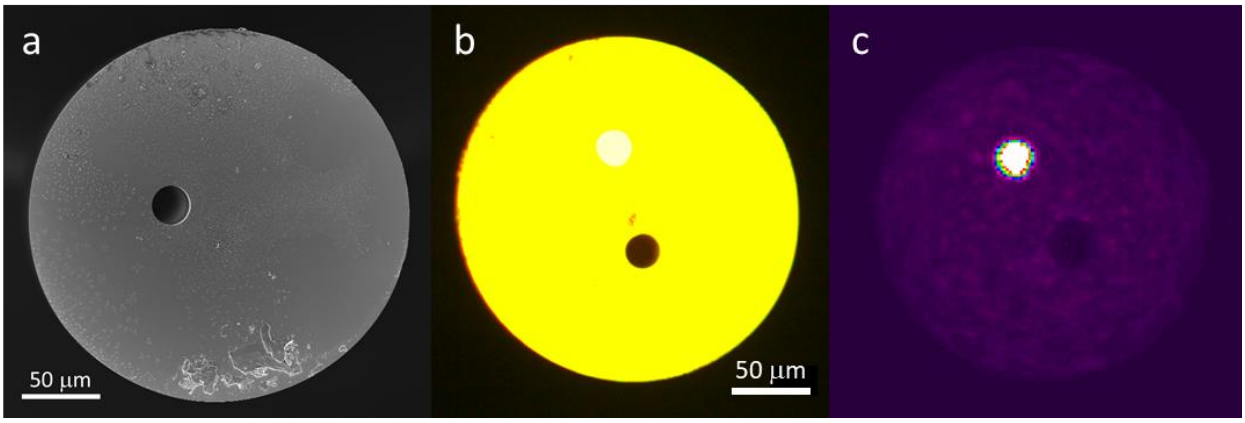


Figure 1. SEM (a) and optical microscope (b) image of the facet of the 230 µm diameter fiber; (c) optical fiber output of guided light at 1300 nm.

Figure 1a and b show a cross-section of the 230 µm fiber under the electron and optical microscopes, respectively, where both the core and the channel are visible. The optical fiber output was characterized by a camera (Xeva XC 130 Camera) by injecting the core with a diode laser at 1300 nm. An objective lens was utilized to acquire an image from a 80 cm-long cross-section of the 130 µm diameter microstructured fiber and to examine the light-guiding performance. Figure 1c shows that the light is well confined into the core. The optical loss of the multimode core-cladding fiber was measured at 1300 nm and was estimated to be 2.4 dB/m. These results are consistent with previous studies on the same glass optical fiber [1].

REFERENCES

[1] S.H. Mussavi Rizi, N.G. Boetti, D. Pugliese, D. Janner, Phosphate glass-based microstructured optical fibers with hole and core for biomedical applications, Opt. Mater. 131 (2022) 112644. https://doi.org/10.1016/j.optmat.2022.112644.

[2] E. Ceci-Ginistrelli, D. Pugliese, N.G. Boetti, G. Novajra, A. Ambrosone, J. Lousteau, C. Vitale-Brovarone, S. Abrate, D. Milanese, Novel biocompatible and resorbable UV-transparent phosphate glass based optical fiber, Opt. Mater. Express. 6 (2016) 2040–2051. https://doi.org/10.1364/ome.6.002040.

NMR Spectroscopy as a Tool for Characterization of Molecular Fluorophores in Carbon Dots: Challenges and Opportunities

Jela Nociarová[1]

[1]Department of Chemistry, Faculty of Natural Sciences, Matej Bel University,
Tajovského 40, 974 01 Banská Bystrica, Slovakia, jela.nociarova@umb.sk.

Carbon dots (CDs) prepared by bottom-up methods from inexpensive and widely available precursors are broadly studied as possible economic and environmentally friendly replacement for traditional organic fluorophores and metal-based catalysts. However, their exact composition and structure remain unknown.

Although liquid-state nuclear magnetic resonance spectroscopy (NMR) is an indispensable tool in characterization of organic compounds, it is not routinely used to study CDs due to the complexity of the studied systems. But should it stay so?

We have recently demonstrated that even the simplest and rapid ^{1}H NMR measurement is an efficient way to monitor the formation of intermediates / molecular fluorophores / more complex systems in the reaction mixtures formed by the hydrothermal treatment of citric acid and ethylenediamine [1]. By combining 1D and 2D NMR techniques with mass spectrometry, we also identified a previously unreported blue emitting derivative of citrazinic acid present in reaction mixtures prepared from citric acid and urea by solvent-free pyrolysis. NMR spectroscopy also allowed us to discover a molecular source of fluorescence in hydrothermally treated mixtures of folic acid, previously attributed solely to the formation of CDs.

However, NMR spectroscopy faces certain challenges in CD research. Even the most sensitive ^{1}H NMR technique has relatively high detection limit [2] and requires sufficient solubility of the analyte, which is not always achieved in standard NMR solvents like $CDCl_3$ or DMSO. In deuterated water, hydrogen-deuterium exchange can occur not only at labile protons (e.g., –OH, $–NH_2$, –COOH), but also at certain aromatic C–H positions, leading to the disappearance of signals relevant for interpretation.

Despite these challenges, ^{1}H and ^{13}C NMR spectroscopy is still useful as a quick proof of the presence or absence of molecular fluorophores in CDs and thus it should become a standard part of their characterisation.

Acknowledgements: Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00428 (CD4UMB – Carbon Dots for Upgrading Molecular Bioimaging).

REFERENCES

[1] Pykal M. et al., (2024) "Thermodynamics and kinetics of early stages of carbon dot formation: a case of citric acid and ethylenediamine reaction". *Nanoscale,* 17, 7780-7789. DOI 10.1039/D4NR04420G

[1] Wysocka A. et al., (2024) "Liquid chromatography methods as a solution to inaccuracies associated with purity assessment of citric acid-based carbon dots". *Microchemical journal*, 205, 111240. DOI 10.1016/j.microc.2024.111240

Photopolymer-Based Colorimetric Sensors Incorporating Natural Dyes for Detection of Toxic Substances

Chiara Olla,[1,*] Matteosalvatore Uccheddu,[2] Francesco Secci,[2] Pier Carlo Ricci,[1] and Annalisa Chiappone[2]

[1]Department of Physics, University of Cagliari, Cittadella Universitaria di Monserrato, Italy, chiara.olla@dsf.unica.it
[2]Department of Chemistry and Geological Science, University of Cagliari, Cittadella Universitaria di Monserrato, Italy

The increasing demand for sustainable and eco-friendly materials has gained considerable interest in natural dyes as alternatives to synthetic counterparts, which often present environmental and health risks.[1,2] Natural pigments such as anthocyanin and phycocyanin are biodegradable, non-toxic, and renewable, making them highly suitable for innovative applications beyond traditional dyeing. Notably, their colorimetric response to environmental factors such as pH changes and pollutant exposure allows them to work as chemical sensors.[3,4] This study investigates the incorporation of anthocyanin and phycocyanin into photopolymerizable resins for 3D printing to develop functional colorimetric chemosensors. By employing Digital Light Processing (DLP) 3D printing, we developed optimized formulations to ensure both printability and sensing effectiveness. The optical responses of the printed materials were characterized using optical spectroscopy, while photorheology was employed to evaluate their printing suitability. Our results demonstrate that these bio-based dyes enable the production of 3D-printed objects capable of detecting contaminants in both liquid and vapor phases through visible color changes, highlighting the potential of natural dye-based materials in the development of sustainable sensing technologies for environmental safety.

Figure 5 – 3D printed items containing anthocyanin.

REFERENCES

[1] Tkaczyk A., Mitrowska K., Posyniak A., (2020) "Synthetic organic dyes as contaminants of the aquatic environment and their implications for ecosystems: A review". *Science of The Total Environment*, 717 137222. https://doi.org/10.1016/j.scitotenv.2020.137222
[2] Ali H., (2010) "Biodegradation of Synthetic Dyes—A Review". *Water, Air, & Soil Pollution*, 213, 251-273. https://doi.org/10.1007/s11270-010-0382-4
[3] Wrolstad R.E., (2006) "Anthocyanin Pigments—Bioactivity and Coloring Properties". *Journal of Food Science*, 69 C419-C425. https://doi.org/10.1111/j.1365-2621.2004.tb10709.x
[4] Roy S. and Rhim J., (2021) "Anthocyanin food colorant and its application in pH-responsive color change indicator films". *Critical Reviews in Food Science and Nutrition*, 61, 2297-2325. https://doi.org/10.1080/10408398.2020.1776211

Inkjet Printing in Electrochemical Biosensing

Michal Otyepka[1,2]

[1]Czech Advanced Technology and Research Institute (CATRIN), Regional Centre of Advanced Technologies and Materials, Palacký University Olomouc, Šlechtitelů 27, Olomouc, 77900 Czech Republic, Michal.Otyepka@upol.cz
[2]IT4Innovation, VSB – Technical University of Ostrava, 17. listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic

Inkjet printing technology represents an innovative and versatile method for fabricating and modifying electrodes tailored specifically for advanced biosensing applications. Nevertheless, formulating suitable inks that satisfy the rigorous technological demands of inkjet printing while maintaining reliable and reproducible electrochemical performance poses significant challenges.

In addressing this complexity, graphene derivatives synthesized via fluorographene (FG) chemistry have demonstrated substantial promise. FG chemistry allows the selective and controlled chemical modification of the inherently inert graphene lattice under mild conditions. This approach produces single- and double-sided functionalized graphene derivatives with precisely tunable functionalization levels and uniform chemical groups distributed throughout the graphene framework [1,2]. Crucially, these tailored modifications maintain the essential conductivity of graphene while simultaneously introducing functional groups that significantly enhance the compatibility and interaction with bio-recognition elements [3,4].

The controlled synthesis of these graphene derivatives yields flakes with well-defined dimensions and properties optimal for inkjet printing applications. Key ink parameters such as stability, viscosity, and dispersion, essential for high-quality inkjet printing, are readily achievable with these FG-based inks. Recent developments in fully inkjet-printed electrodes employing FG-derived inks have confirmed their robust electrochemical performance, demonstrating accurate and sensitive biosensing capabilities [5,6].

This integration of chemical functionalization strategies and printing technologies exemplifies the interdisciplinary nature essential to understanding and characterizing complex material systems. Ultimately, these advances provide a scalable and economically viable route for constructing biosensors, contributing significantly to practical solutions in materials science, biotechnology, and sustainable analytical technologies [7].

REFERENCES

[1] Chronopoulos D. et al., (2017) Appl. Mater Today 9, 60
[2] Hruby V. et al., (2022) Nanoscale 14, 13490
[3] Vermisoglou E. et al., (2019) Chem. Mater 31, 4698
[4] Sedajova V. et al., (2024) Adv. Mater. Int.
[5] Flauzino J. M. R. et al., (2022) Biosens. Bioel. 195, 113628
[6] Flauzino J. M. R. et al., (2023) Small 19, 2207216
[7] Nalepa M.-A. et al., (2024) Biosens. Bioel. 256, 116277

Inverse Gas Chromatography in the Study of Surface Properties of Materials

Eva Otyepková [1], Michal Otyepka [2]

[1] Department of Physical Chemistry, Palacký University Olomouc, Czech Republic, eva.otyepkova@upol.cz
[2] CATRIN - RCPTM, Palacký University Olomouc, Czech Republic

Inverse gas chromatography (iGC) is a powerful and versatile technique for the characterization of surface and interfacial properties of solid materials, especially powders, fibers, films and nanostructured systems. This lecture provides a comprehensive overview of the principles, methodology, and applications of iGC .
In contrast to conventional gas chromatography, iGC uses the sample as a stationary phase and allows gas-phase probe molecules to interact with the material's surface. These interactions are then evaluated through retention volumes, enabling the determination of dispersive and specific (acid-base) surface energy components (Eq. 1), surface heterogeneity, thermodynamic parameters (such as the work of adhesion and cohesion), and BET surface area.

$$\gamma_S^T = \gamma_S^d + \gamma_S^{ab} \qquad (1)$$

The iGC method is described in detail, including sample preparation, measurement protocol, and the calculation of key parameters such as net retention volume and distribution coefficient. The lecture covers the determination of both dispersive and acid-base components of surface energy (Eq. 1), using Dorris-Gray and Schultz methods, and discusses the interpretation of heterogeneity profiles.
Practical examples are presented, including the effect of sieving on the surface properties of active pharmaceutical ingredients (APIs) (Figure 1) and the impact of different crystallization techniques on the surface energy of API. These case studies demonstrate how iGC can reveal subtle differences in surface characteristics that are critical for material performance and processing.

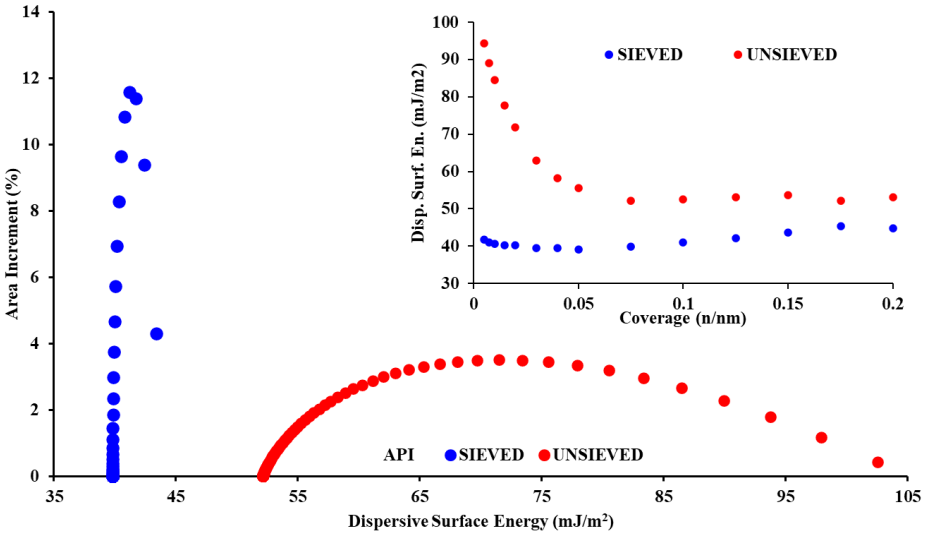


Figure 6 – Dispersive surface energy (profile – small; and distribution – bigger graph) of sieved and unsieved sample

In summary iGC is a sensitive, reproducible, and flexible tool for surface science, offering in-depth information about surface chemistry that is often inaccessible through other methods.

REFERENCES

[1] Bartova, A; et.al., (2022) "Controlled nucleation of crystallization process as an efficient tool to tune the properties of corticosteroid API". *POWDER TECHNOLOGY*, 402, 117334. DOI: https://doi.org/10.1016/j.powtec.2022.117334
[2] Saini, H; Otyepkova, E; et. al., (2022) "Hierarchical porous metal-organic framework materials for efficient oil-water separation." *J. MATER. CHEM. A*, 10 (6), 2751-2785. DOI: https://doi.org/10.1039/D1TA10008D
[3] Lazar, P; et.al., (2013) "Adsorption of Small Organic Molecules on Graphene". *J. Am. Chem. Soc.*, 135 (16): 6372-6377. DOI https://doi.org/10.1021/ja403162r
[4] Karlický, F; Otyepková, E; et.al., (2015) "Interplay between Ethanol Adsorption to High-Energy Sites and Clustering on Graphene and Graphite Alters the Measured Isosteric Adsorption Enthalpies". *J. Phys. Chem. C*, 119 (35), 20535 20543. DOI https://doi.org/10.1021/acs.jpcc.5b06755
[5] Lazar, P; Otyepkova, E; et.al., (2014) "The Nature of High Surface Energy Sites in Graphene and Graphite". *Carbon*, 73: 448 – 453. DOI https://doi.org/10.1016/j.carbon.2014.03.010
[6] Dorris, G.M.; Gray, D.G.; (1980) "Adsorption of n-alkanes at zero surface coverage on cellulose paper and wood fibers". *J. Colloid Interface Sci*, 77, 353–362. DOI https://doi.org/10.1016/0021-9797(80)90304-5
[7] Della Volpe, C; Siboni, S; (1997) "Some reflections on acid-base solid surface free energy theory". *J. Colloid Interface Sci.*, **195**, 121–136. DOI https://doi.org/10.1006/jcis.1997.5124
[8] Schultz, J; Lavielle, L; Martin, C; (1987) "The role of the interface in carbon fibre-epoxy composites". *J. Adhes.*, 23, 45–60. DOI https://doi.org/10.1080/00218468708080469

Simulation Insight into Bio-Nano Interface

Markéta Paloncýová[1]

[1]Czech Advanced Technology and Research Institute (CATRIN), Regional Centre of Advanced Technologies and Materials, Palacký University Olomouc, Šlechtitelů 27, Olomouc, 77900 Czech Republic, marketa.paloncyova@upol.cz

Carbon nanomaterials have revolutionized the field of biomedicine, offering opportunities for their diverse applications. Their unique tunable physicochemical, optical, mechanical and electronic properties make them ideal candidates for a wide range of biomedical applications. Carbon nanomaterials, including carbon nanotubes, graphene, and carbon dots, have shown remarkable promise in areas such as drug delivery, tissue engineering, biosensing, and imaging. However, to harness their full potential and ensure their safe and efficient use, it is crucial to gain a comprehensive understanding of their interactions with biomaterials at the molecular level, which is currently unavailable by experimental techniques. On the other hand, molecular dynamics simulations of complex bio-nano hybrid systems require a very careful setup and analyses, using mutually compatible force fields for individual system parts, analyses of both bio- and nano- materials and their mutual interactions, which is far from trivial.

Here we focus on the modeling of the interactions of carbon dots (CDs) and graphene derivatives with biomolecules. We investigated the interactions of CDs with simple canonical models of nucleic acids and identified preferential interaction modes and extended the model from simple duplexes up to nucleosomes. Further, we focused on understanding of the behaviour of graphene derivatives on complex lipid membranes both in atomistic resolution and in larger scales in coarse-grained resolution. Through these simulations, we elucidated the nature of interactions between graphene derivatives and lipid membranes, from tiny nanometer-scale flakes up to large experimentally relevant graphene models.

The simulations of bio-nano interface bring new challenges in their setup, requiring application of novel analysis techniques. We present here a complex approach to simulations of the bio-nano interface in multiscale resolution, necessary for capturing the required level of details. These simulations can be a start of in-silico studies on nanotoxicity of the nanomaterials or used for targeted design increasing their biocompatibility.

REFERENCES

[1] Paloncýová M., Langer, M., Otyepka, M., (2018), J. Chem. Theory Comput., 14, 2076-2083
[2] Langer M., Paloncýová, M., Medved', M., Otyepka, M., (2020), J. Phys. Chem. Lett., 11, 8252-8258
[3] Paloncýová M., Pykal, M., Kührová, P., Banáš, P., Šponer, J., Otyepka, M., (2022), Small, 18,

Sustainable Carbon Quantum Dots: From Fluorescent pH Sensors to Performance Enhancement in Solar Cells

Davide Tocco[1], Lorenzo Squillantini[2], Marco Natali[2], Francesca De Giorgio[2], Emiliano Fratini[1].

[1] Dipartimento di Chimica "Ugo Schiff" and Center for Colloid and Surface Science (CSGI), University of Florence, Via della Lastruccia 3, Sesto Fiorentino, Florence, 50019, Italy. davide.tocco93@gmail.com
[2] Consiglio Nazionale delle Ricerche, Istituto per lo Studio dei Materiali Nanostrutturati (CNR-ISMN) Via Piero Gobetti 101, 40129 Bologna, Italy.

Carbon Quantum Dots (CQDs) are an emerging class of carbon-based fluorescent nanomaterials with dimensions below 10 nm [1]. Compared to traditional semiconductor quantum dots, CQDs can be synthesized through sustainable approaches using cost-effective precursors such as citric acid (CA) [2]; moreover, CQDs exhibit lower toxicity and higher aqueous solubility [3]. These aspects make CQDs suitable for a wide range of applications including environmental monitoring, biomedicine [4], and optoelectronics [5]. In this work, CQDs were synthetized following a bottom-up approach via a thermal cracking method (200 °C, neat, in 45 min) starting from cheap and readily available precursors: citric acid and L-tryptophan. The use of tryptophan not only acts as a carbon source but also provides nitrogen doping, which enhances the fluorescence quantum yield and introduces functional groups that improve surface reactivity [6]. Various CA:Trp weight ratios were investigated (100:0, 95:5, 85:15, 80:20,75:25 and 70:30 w/w%) to evaluate their influence on optical and structural properties. CQDs emission fluorescence was studied across a wide pH range (2–14) and as a function of precursor composition. The physico-chemical characterization was carried out using UV-Vis and fluorescence spectroscopy, FT-IR, X-ray photoelectron spectroscopy (XPS), thermogravimetric analysis (TGA), wide-angle X-ray scattering (WAXS), and transmission electron microscopy (TEM), to investigate structure–property relationships, chemical composition, thermal stability, and morphological features. Moreover, the so-prepared CQDs were investigated for two different applications:

i) as pH-sensitive fluorescent sensors in a CO_2-responsive device,
ii) as additives in methylammonium lead iodide (MAPI)-based perovskite solar cells (PSCs).

A prototype pH-sensitive sensor was developed to detect CO_2 in a model culture medium simulating bacterial growth. CO_2 generated by bacterial metabolism diffused through a silicone-based membrane, acidifying the CQD solution (pH 6) and inducing a measurable fluorescence shift, demonstrating the feasibility of CQD-based, non-invasive CO_2 sensing. Among the synthesized materials, the CQDs obtained from the 85:15 Trp:CA ratio exhibited the best fluorescence performance for pH sensing, with a relative quantum yield of 15.5% at pH 3 and 3.5% at pH 10, confirming their suitability as effective fluorescent probes in variable pH environments.

For the photovoltaic application, CQDs (CA:Trp compositions 100:0, 80:20, 75:25, and 70:30 w/w%) were tested as additives in an inverted-architecture MAPI-based PSCs. Their surface functional groups (e.g., –COOH, $–NH_2$) facilitated passivation of grain boundaries and defects, improving film morphology and device stability. Among the tested formulations, the 70:30 composition led to a significant increase in power conversion efficiency (PCE), from 8.2% (reference) to 10.0%, along with an improved fill factor (FF).

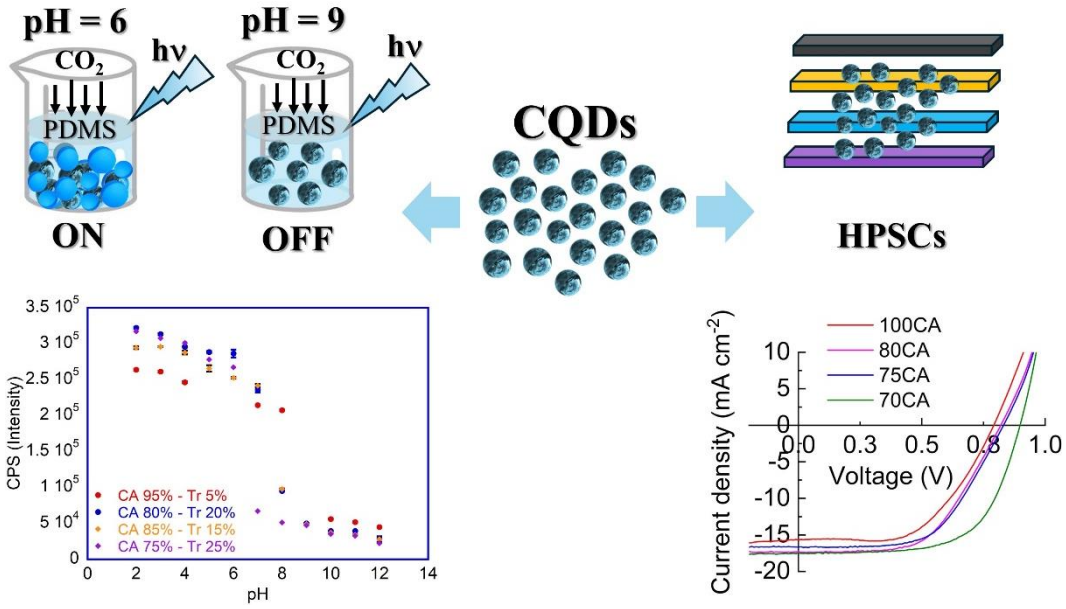


Figure 1 Schematic illustration of CQDs as: left panel, pH-sensitive fluorescent sensors in a CO_2-responsive device; right panel, additives in MAPI-based perovskite solar cells (PSCs).

REFERENCES

[1] X. Xu, R. Ray, Y. Gu, H. J. Ploehn, L. Gearheart, K. Raker, W. A. Scrivens, (2004) *J. Am. Chem. Soc.*, 126, 12736–12737.

[2] C. Olla, A. Cappai, S. Porcu, L. Stagi, M. Fantauzzi, M. F. Casula, F. Mocci, R. Corpino, D. Chiriu, P. C. Ricci, C. M. Carbonaro, (2023) *Nanomaterials*, 13, 1344.

[3] S. Chahal, J.-R. Macairan, H.-N. N. Bui, A. Smith, H. C. E. Larsson, R. Naccache, N. Tufenkji, (2024) *Environ. Sci. Adv.*, 3, 912–924.

[4] B. Wang, H. Cai, G. I. N. Waterhouse, X. Qu, B. Yang, S. Lu, (2022) *Small Sci.*, 2, 2200012.

[5] C. Ji, Y. Zhou, R. M. Leblanc, Z. Peng, (2020) *ACS Sensors*, 5, 2724–2741.

[6] X. Zhang, W. Zhang, S. Tang, (2019) *J. Photochem. Photobiol. A Chem.*, 372, 71–77.

Poster Presentations

Active Materials for On-Chip Integrated Quantum Light Sources Based on Metal complexes

Alcibiade Marco, Andrea Cocco, Maria Francesca Casula, Luca Pilia

Università degli Studi di Cagliari, m.alcibiade@studenti.unica.it

Materials showing nonlinear optical (NLO) properties are suitable for entangled photons generation by spontaneous parametric down-conversion (SPDC) mechanism. SPDC is an NLO process where a single photon splits into two or more entangled photons, a mechanism crucial for quantum optics and secure communication technologies.[1] Among the most promising NLO materials are push–pull metal complexes, characterized by a strong electron-donating (PUSH) group and an electron-withdrawing (PULL) group connected through a metal. This electronic asymmetry facilitates intramolecular charge transfer.[2] In the case of SPDC and second harmonic generation (SHG), such push and pull architectures enable efficient frequency conversion and polarization control of the emitted light. Transition metal centers like Ni(II), Pd(II), and Pt(II) further enhance NLO performance by promoting charge delocalization through metal–ligand backbonding and planar π-delocalized frameworks.

This study focuses on the synthesis and characterization of heteroleptic Pt(II) complexes containing a bipyridine ligand (PULL) and either benzene-1,2-dithiolate or 1,3-dithiol-2-thione-4,5-dithiolate (PUSH). The synthesized complexes were characterized using UV-Vis, IR, NMR spectroscopies, electrochemical methods and DFT calculations, to elucidate their structural and electronic properties.

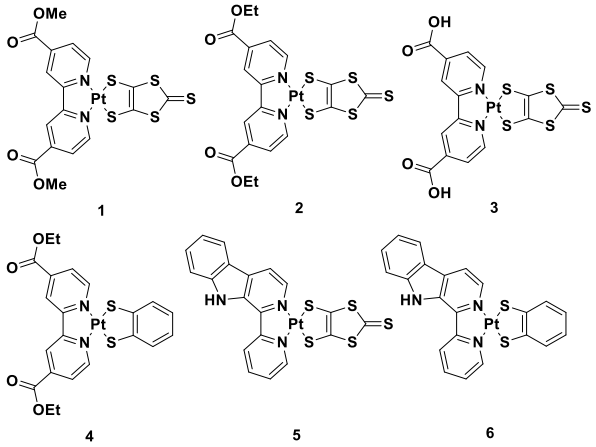
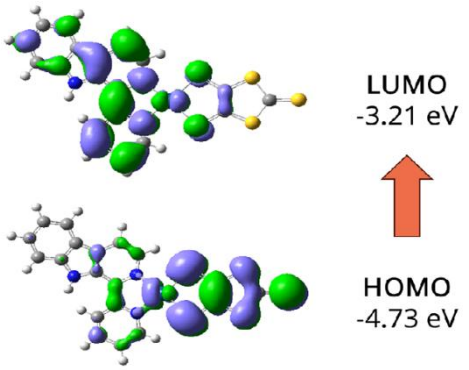


Figure 1 - Scheme of the synthesized complex

The synthesized Pt(II) complexes shown above (Figure 1) were subjected to spectrophotometric analysis to both confirm successful synthesis and characterize their electronic properties. UV-Vis absorption spectroscopy was employed to identify the characteristic absorption bands associated with mixed metal-ligand-to-ligand charge transfer (MLCT) and intreligand π–π* transitions. Measurements were carried out in solvents of varying polarity to assess the solvatochromic behavior of the complexes a key indicator of polarizable electronic structures and an essential requirement for materials exhibiting NLO. The observed shifts in absorption maxima across different solvents confirm the presence of significant solvatochromism, supporting the push–pull nature of the molecular design and their potential suitability for NLO applications such as SHG and SPDC. In addition, density functional theory (DFT) calculations were performed at the B3LYP level of theory to gain preliminary insight

into the electronic structure of the most promising compounds (Figure 2). [3] These computations allowed us to determine the frontier molecular orbitals (HOMO and LUMO) along with their respective energy levels and spatial distributions, as well as the static polarizability (α) and first hyperpolarizability (β) values. The resulting data provide a theoretical foundation for evaluating the charge-transfer character and the NLO potential of the synthesized complexes. The relatively high values of α and β obtained from the calculations further highlight the promising nonlinear optical properties of these systems.



	α_{iso} (10^{-24} esu)	β_{eff} (10^{-30} esu)
DMSO	112.93	507.18

Figure 2 - The frontier molecular orbitals of complex 5 with their Energy and the β value calculated using DFT.

This research was supported by European Innovation Council (EIC Pathfinder project "ARTEMIS" G. A. n. 101115149. We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 1409 published on 14.9.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title "Molecular Quantum Light Sources" (QuantaMol)– CUP F53D23008550001- Grant Assignment Decree No. 1380 adopted on 01/09/23 by the Italian Ministry of Ministry of University and Research (MUR).

REFERENCES

[1] M. Scalora, M. A. Vincenti, D. de Ceglia, V. Roppo, M. Centini, N. Akozbek, and M. J. Bloemer, (2010) "Second- and third-harmonic generation in metal-based structures". *Physical review,* 82, 043828. https://doi.org/10.1103/PhysRevA.82.043828

[2] Flavia Artizzu, Davide Espa, Luciano Marchiò, Luca Pilia, Angela Serpe, Paola Deplano, (2022) "Progress and perspectives on strategies to control photochemical properties in Metallo-Dithiolene Donor-Acceptor systems". *Inorganica Chimica Acta,* 531, 120731. https://doi.org/10.1016/j.ica.2021.120731

[3] Merve Simsek, Omer Tamer, Necmi Dege, Davut Avcı, Hayatullah Mahmoody, Yusuf Atalay, (2024) "A new mixed-ligand zinc(II) complex of 3-hydroxy and 4-chloro substituted pyridine-2-carboxylic acid: Synthesis, characterization, NLO properties and DFT calculation". *Materials Today Communications,* 38, 108021. https://doi.org/10.1016/j.mtcomm.2024.108021

Adsorption-derived Visible Light Photocatalytic Degradation Of Dyes Using Phenyl-modified graphitic carbon nitride/Strontium titanate composite(PhCN/$SrTiO_3$)

S. Bagchi [1, 2],*, P.C. Ricci [2,] M. Altomare[3]

[1] University of Perugia, Italy, saswatibagchi5498@gmail.com (S.Bagchi)
[2] University of Cagliari,Italy
[3] University of Twente, Enschede, The Netherlands

Photocatalytic oxidation has emerged as a promising technique for the efficient removal of low-concentration organic pollutants under ambient conditions, providing an energy-efficient and sustainable alternative to conventional treatments.[1][2] However, practical implementation is often hindered by intrinsic limitations such as catalyst deactivation, slow charge transport, and the formation of incomplete degradation products. Addressing these challenges, recent research has focused on engineering hybrid organic–inorganic photocatalysts with strong visible-light absorption and stable performance profiles.[3]

Graphitic carbon nitride (g-C_3N_4), particularly in its phenyl-modified form (PhCN), has shown significant potential due to its visible-light activity, non-toxicity, and structural tunability. The introduction of phenyl groups enhances π-conjugation and narrows the band gap (~2.0 eV), enabling more efficient light harvesting. Complementarily, strontium titanate ($SrTiO_3$), a perovskite oxide, offers high stability and electron mobility, though its wide band gap (~3.2 eV) limits its independent activation to UV light[4]. To harness the benefits of both components, a PhCN/$SrTiO_3$ hybrid was developed using a two-step process involving wet impregnation and a subsequent hydrothermal treatment in methanol.

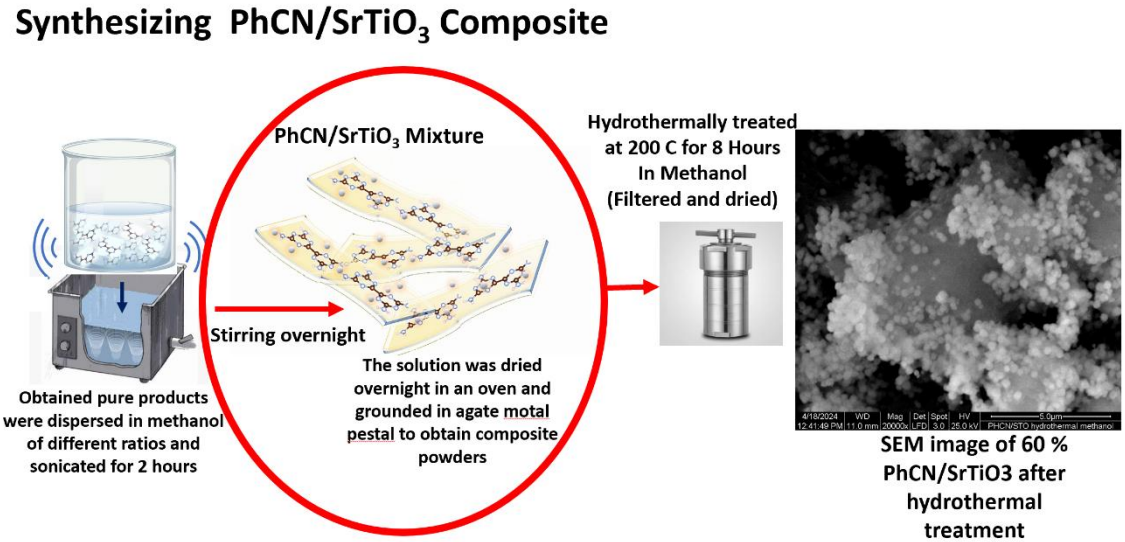


Figure 7 - Synthesis scheme of PhCN /$SrTiO_3$ wet impregnation followed by hydrothermal, showing the FESEM image of the final composite obtained

The PhCN precursor was synthesised by the thermal condensation of 6-phenyl-1,3,5-triazine-2,4-diamine at 400 °C [5], while $SrTiO_3$ nanoparticles were obtained via sol-precipitation using strontium nitrate and tetra-isopropyl titanate under basic conditions at 95 °C [6]. After thorough washing and drying, both materials were ultrasonically mixed in methanol in various ratios, followed by overnight stirring to ensure uniform dispersion. Among the various formulations, a 60:40 weight ratio (PhCN: $SrTiO_3$) was found to be optimal for adsorption.

This mixture was further subjected to hydrothermal treatment in methanol at 200 °C for 8 hours, resulting in a notable transformation in both photocatalytic and adsorption performance. Shown in **Figure 1.**

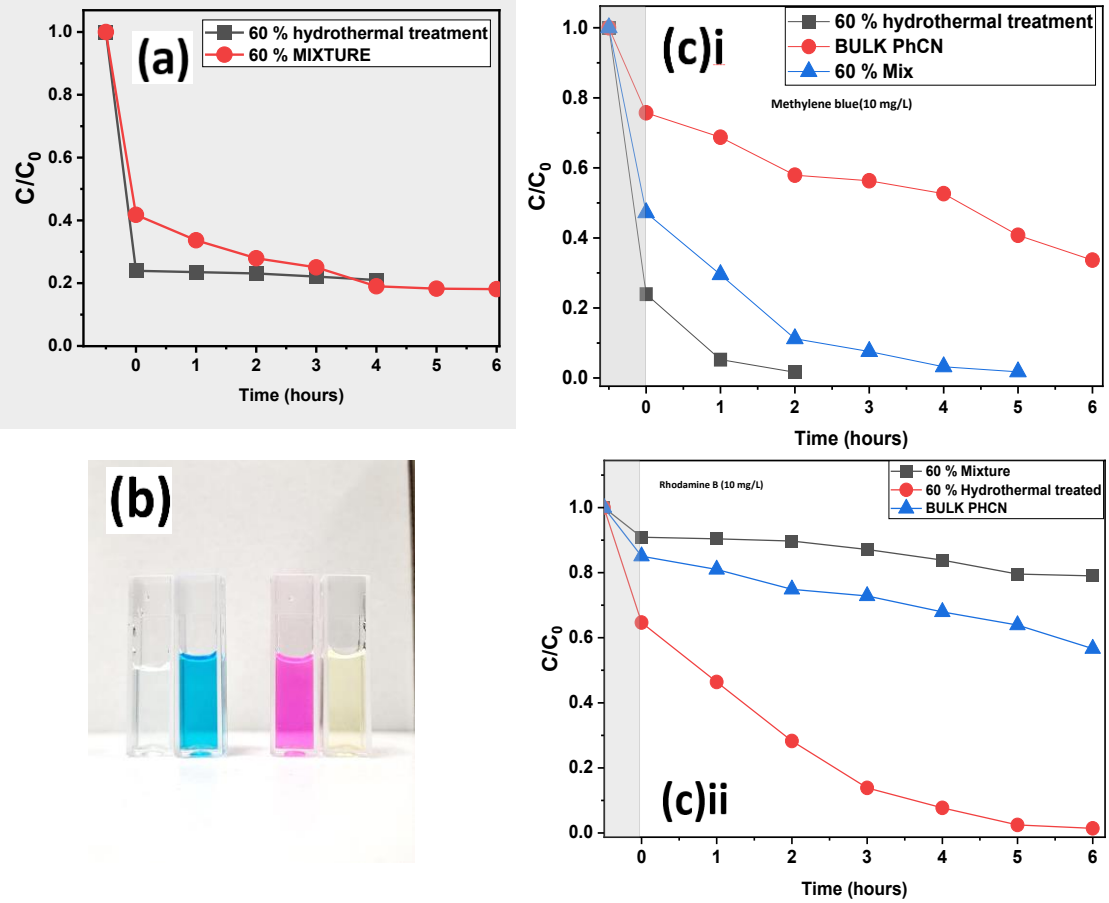


Figure 2 - The figure (a) shows the dark test in methylene blue dye (10mg/L) pre and post hydrothermal treatement, (c)i and (c)ii are the visible light dye degradation performance in methylene blue(10mg/L) and rhodamine B, respectively(10mg/L) and (b) shows the complete degradation of these dyes after 6 hours.

Photocatalytic activity was assessed under visible light using standard model pollutants: methylene blue (MB) and rhodamine B (RhB). Prior to hydrothermal treatment, the composite exhibited moderate MB adsorption (80% in 7 hours) but limited photocatalytic performance, especially against RhB. Following hydrothermal modification, the system demonstrated a dramatic enhancement: MB was adsorbed up to 80% within 30 minutes, even in the dark, and completely degraded in under 2 hours under visible light. Most notably, RhB, previously unaffected, was fully degraded within 6 hours, along with the hydrogen production evaluation reaction, which was performed in a monochromatic light source at 470 nm. An increase in production of approximately 1.8 times was observed compared to pre-hydrothermal treatment and bulk PhCN, with platinum and TEOA serving as cocatalysts and sacrificial agents, respectively. Reaching up to 1.35 mmol h^{-1} g-1, shown in **Figure 3**. These results indicate significant changes in surface properties, electronic structure, and light-responsiveness after treatment. Reactive species quenching experiments in rhodamine B degradation further revealed that the post-treated composite operated via a different dominant pathway under visible light, where enhanced electron mobility likely contributed to the increased degradation efficiency.

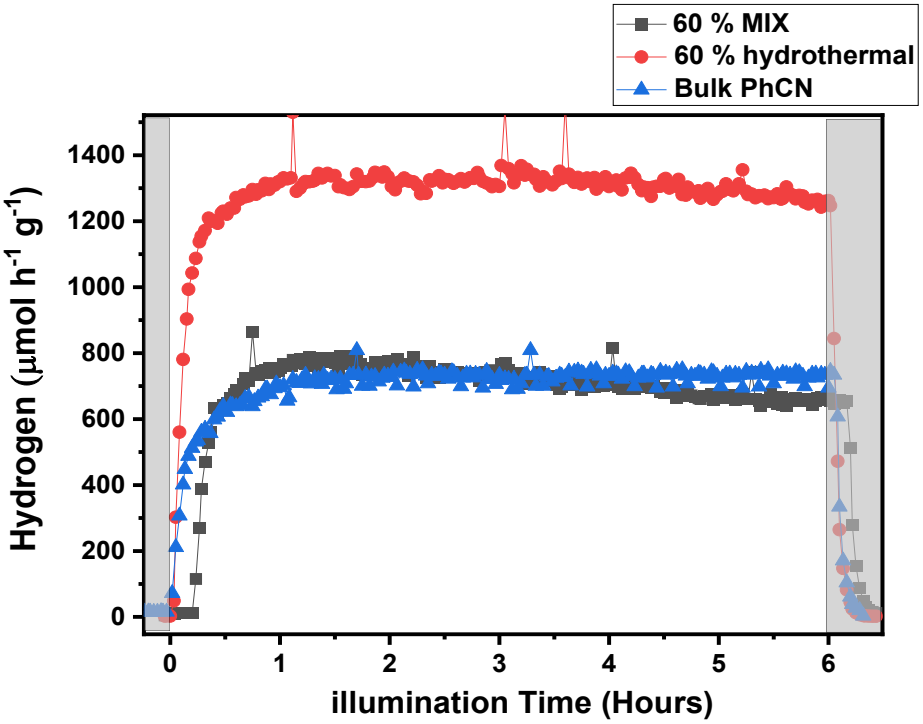


Figure 3 - Hydrogen evolution reaction of composite PhCN/$SrTiO_3$ pre and post hydrothermal treatement along with bulk PhCN in Monochromatic light source: 470 nm (50 mW/cm^2) with 12 % TEOA

This shift suggests a reconfiguration of internal charge dynamics, potentially through altered band alignment or interfacial electronic distribution, though detailed mechanistic analysis remains ongoing. A suite of morphological and structural characterisations confirmed substantial changes in material architecture after treatment. Improved dispersion of $SrTiO_3$ on PhCN surfaces, reduced aggregation, and increased porosity were observed, accompanied by shifts in optical absorption and surface charge behaviour. These transformations are attributed to the methanol-assisted hydrothermal process, which acts not only as a thermal restructuring step but also as a chemical environment that promotes better material integration and surface activation.

In conclusion, this work presents a robust hybrid photocatalyst engineered through a scalable synthesis and post-treatment strategy, achieving significantly enhanced adsorption and visible-light-driven degradation of multiple organic dyes. The results underscore the potential of interface engineering through hydrothermal processing in alcoholic media as a means to unlock synergistic behaviour in organic-inorganic photocatalyst systems. Future studies will delve deeper into the mechanistic underpinnings and explore the material's utility in hydrogen evolution and broader environmental remediation contexts.

REFERENCES

[1] Fujishima A., Honda K., (1972) "Electrochemical Photolysis of Water at a Semiconductor Electrode". *Nature*, 238, 37–38. https://doi.org/10.1038/238037a0

[2] Herrmann J.M., (1999) "Heterogeneous photocatalysis: fundamentals and applications to the removal of various types of aqueous pollutants". *Catalysis Today*, 53(1), 115–129. https://doi.org/10.1016/S0920-5861(99)00107-8

[3] Ong W.J., Tan L.L., Ng Y.H., Yong S.T., Chai S.P., (2016) "Graphitic Carbon Nitride (g-C_3N_4)-Based Photocatalysts for Artificial Photosynthesis and Environmental Remediation: Are We a Step Closer to Achieving Sustainability?". *Chemical Reviews*, 116(12), 7159–7329. https://doi.org/10.1021/acs.chemrev.6b00075

[4] Kudo A., Miseki Y., (2009) "Heterogeneous photocatalyst materials for water splitting". *Chemical Society Reviews*, 38(1), 253–278. https://doi.org/10.1039/B800489G

[5]Porcu S, Roppolo I, Salaun M, Sarais G, Barbarossa S, Casula MF, Carbonaro CM, Ricci PC (2020) "Come to light: Detailed analysis of thermally treated Phenyl modified Carbon Nitride Polymorphs for bright phosphors in lighting applications." *Applied Surface Science*, 504:144330. https://doi.org/10.1016/j.apsusc.2019.144330
[6]Zheng H., Liu X., Meng G., et al. (2001) "Fine $SrTiO_3$ and $Sr(Mg_{0.4}Ti_{0.6})O_3$–δ perovskite ceramic powders prepared by a sol-precipitation process." *Journal of Materials Science: Materials in Electronics*, **12**, 629–635. https://doi.org/10.1023/A:1012841816099

Relationship Between Optical and Structural Properties of Nitrogen-doped Carbon Dots.

Zaira Carboni[1], Chiara Olla[1], Carlo Maria Carbonaro[1], Markéta Paloncýová[2]

[1]Department of Physics, University of Cagliari, S.p. no. 8 Km 0700, 09042, Monserrato, CA, Italy, z.carboni2@studenti.unica.it
[2]Regional Centre of Advanced Technologies and Materials, Department of Physical Chemistry, Faculty of Science, Palacký University, 17. listopadu 1192/12, 771 46 Olomouc, Czech Republic

Carbon Dots (CDs) are a novel class of luminescent carbon-based nanomaterials that have attracted increasing attention due to their unique photoluminescent properties, low toxicity, chemical stability, and biocompatibility. Typically quasi-zero-dimensional, these nanoparticles exhibit a hybrid sp^2/sp^3 carbon core and a surface enriched with oxygen- or nitrogen-containing functional groups, offering great potential for applications ranging from bioimaging to optoelectronics.

In this study, we present a combined experimental and theoretical investigation of nitrogen-doped CDs synthesized from citric acid and urea in a 1:1 molar ratio.
The optical properties were characterized via UV-Vis absorption, steady-state photoluminescence, and time-resolved photoluminescence measurements.

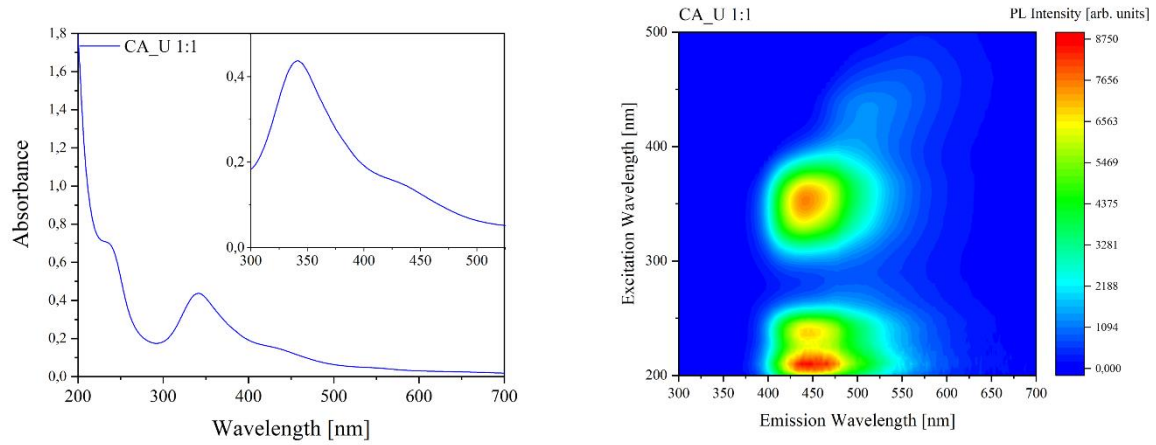


Figure 8 - UV-Vis optical characterization of the CDs obtained from citric acid and urea precursors with a 1:1 molar ratio**.**

To complement the experimental findings, molecular dynamics simulations were performed using GROMACS 2023.4 on the LUMI supercomputer. Two representative CD models were constructed: a pure CD functionalized with hydroxyl groups, and a nitrogen-doped CD featuring surface amine groups and graphitic nitrogen, simulating the 1:1 synthesis ratio. Structural characterization was carried out by analyzing the density distribution and the radius of gyration. The layer density distribution was measured to determine the distance between layers, and the radius of gyration was used to study the evolution of the system's compactness.
We further explored the interaction between these CD models and key fluorophores such as citrazinic acid, citrazinic acid amine and citrazinic acid amine amide. This multiscale approach offers insights into the structural and photophysical behavior of CDs, shedding light on the role of nitrogen doping and functional surface groups in tuning their emission properties.

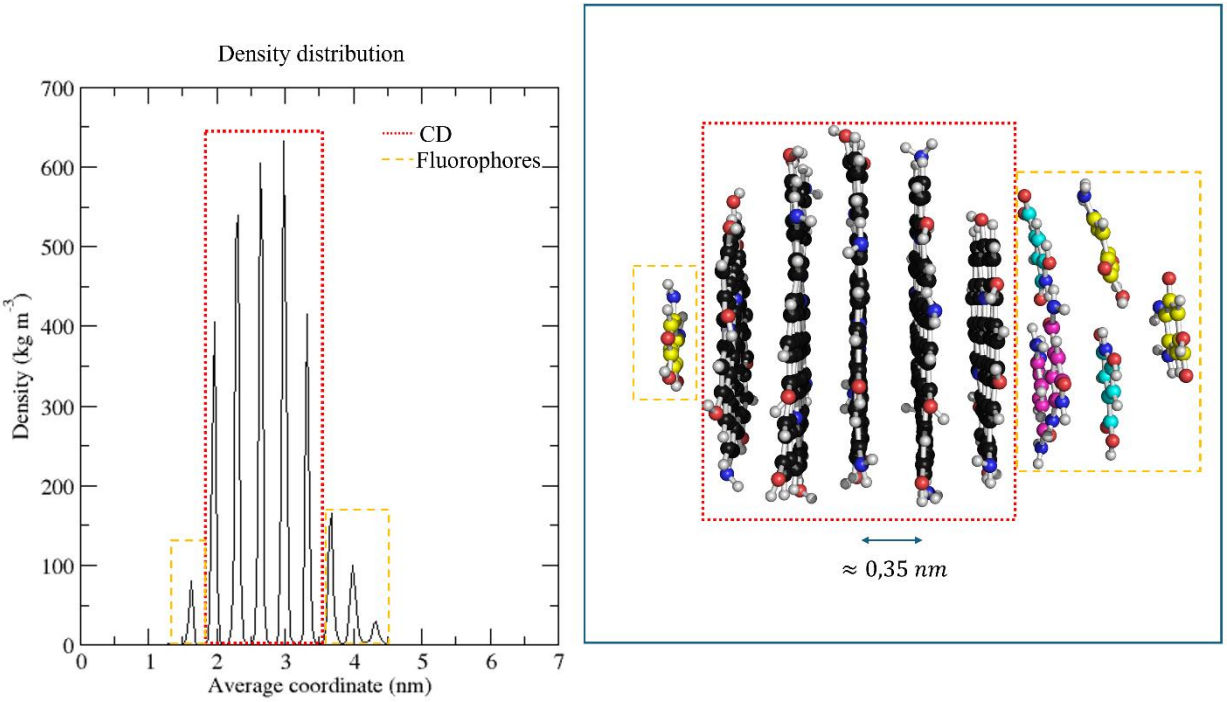


Figure 9 - Plot of the layer density distribution of the nitrogen-doped CD with amine groups on the surface along with the fluorophores citrazinic acid-like

Design and synthesis of Platinum(II) Donor–Acceptor Complexes for Second-Order Nonlinear Optics

A. Cocco,[1] M. Alcibiade,[1] M.F. Casula,[1] L. Pilia[1]

[1]Department of Mechanical, Chemical and Materials Engineering, University of Cagliari, Italy
andrea.cocco90@unica.it

The development of molecular materials for second-order nonlinear optics (NLO) greatly benefits from computational approaches that support and guide experimental design. In this study, we present a new series of heteroleptic Pt(II) donor–acceptor complexes, developed with the aim of enhancing intramolecular charge transfer (ICT) and, consequently, improving their second-order NLO response.[1]

Ground-state DFT calculations were performed to determine the energies and spatial distributions of the frontier molecular orbitals, with particular attention to the degree of HOMO–LUMO separation an essential parameter to promote efficient ICT upon excitation.[2] Furthermore, Time-dependent density functional theory (TD-DFT) simulations of UV-Vis spectra were conducted, showing excellent agreement with the experimental absorption data and confirming the charge-transfer nature of the electronic transitions, as shown in Figure 2. Theoretical hyperpolarizability (β) values were also estimated, indicating that the designed complexes possess good potential for NLO applications.

In this work, the Pt(II) complexes were synthesized through straightforward coordination reactions carried out under an inert atmosphere, by combining platinum precursors with acceptor ligands mainly quinoline or bipyridine derivatives and donor units such as dmit, dithiobenzene, or coumarin-based fragments. The reactions were conducted under mild conditions, and the products were obtained as solids, then purified and characterized. The synthetic strategy was optimized to ensure good yields and high product purity. Experimental characterization by NMR, elemental analysis, and X-ray diffraction confirmed the expected structural features, while SHG measurements for the experimental determination of β are currently underway.

These Pt(II) complexes also exhibited pronounced solvatochromic behavior, evidenced by significant shifts in their absorption maxima depending on solvent polarity, as can be seen in Figure 1. This phenomenon, monitored by UV-Vis spectroscopy in solvents with varying polarity, further supports the ICT nature of the electronic transitions. The observed negative solvatochromism is consistent with an increase in dipole moment upon excitation, in line with the donor–acceptor design of the complexes. These findings not only provide deeper insight into the electronic structure, but also highlight the potential tunability of their photophysical properties in different environments an especially relevant aspect for device integration.
As an exploratory extension, preliminary biological activity assays have been initiated to evaluate the potential anticancer properties of these complexes. Although still at an early stage, these studies could open promising interdisciplinary perspectives at the interface between photonics and bioinorganic chemistry.

This research demonstrates how computational calculations and modeling can effectively guide the synthesis of functional organometallic systems, accelerating the identification of promising candidates for nonlinear optical technologies.

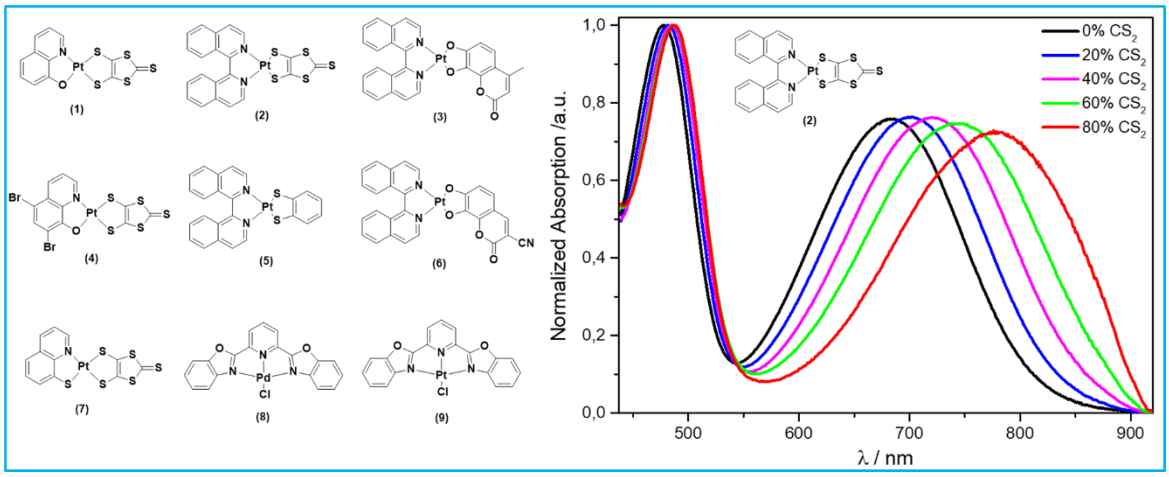


Figure 1 – Formulas of the synthesized complexes and absorption spectra of (2) in DMF at various carbon disulfide concentrations."

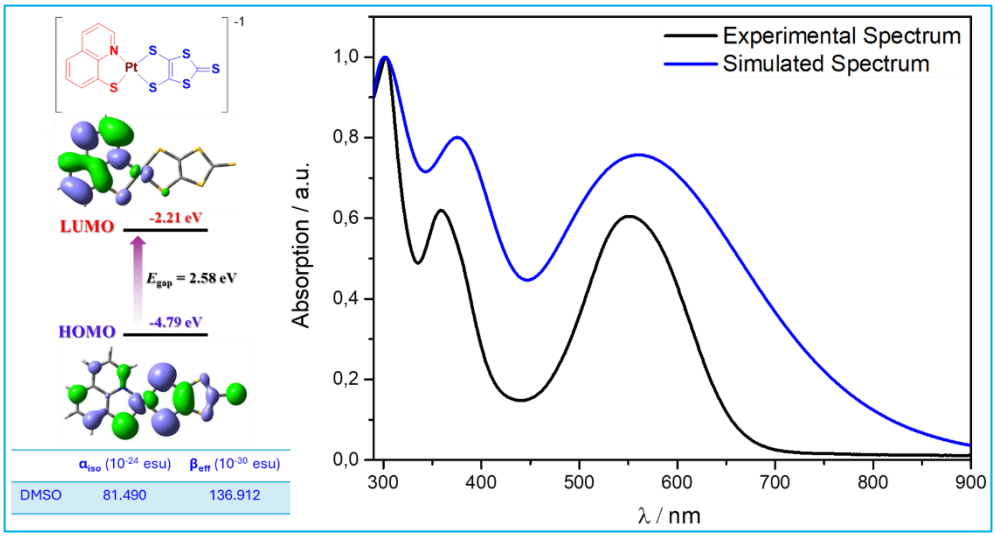


Figure 2 – Experimental and simulated UV-Vis absorption spectrum of (7) in DMSO solution, along with HOMO and LUMO molecular orbital diagrams and polarizability/hyperpolarizability parameters.

This research was supported by European Innovation Council (EIC Pathfinder project "ARTEMIS" G. A. n. 101115149. We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 1409 published on 14.9.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title "Molecular Quantum Light Sources" (QuantaMol)– CUP F53D23008550001- Grant Assignment Decree No. 1380 adopted on 01/09/23 by the Italian Ministry of Ministry of University and Research (MUR).

REFERENCES

[1] F. Artizzu, D. Espa, L. Marchiò, L. Pilia, A. Serpe, P. Deplano, (2022) Progress and Perspectives on strategies to control photochemical properties in Metallo-Dithiolene Donor-Acceptor systems. Inorg. Chim. Acta, 531, 120731. https://doi.org/10.1016/j.ica.2021.120731

[2] S. S. Attar, F. Artizzu, L. Marchiò, D. Espa, L. Pilia, M. F. Casula, A. Serpe, M. Pizzotti, A. Orbelli-Biroli, P. Deplano, (2018) Uncommon Optical Properties and Silver-Responsive Turn-Off/On Luminescence in a PtII Heteroleptic Dithiolene Complex. Chem. Eur. J., 24, 10503–10512. https://doi.org/10.1002/chem.201801697

Effect of Processing Parameters and Recipe Composition on Dough Rheology in *Carasau* Bread Production

Francesco Desogus[1], Nicola Melis[1], Fabio Fanari[2], Massimiliano Grosso[1]

[1]University of Cagliari – Department of Mechanical, Chemical and Materials Engineering – Via Marengo 2, 09123 Cagliari – e-mail: francesco.desogus2@unica.it
[2]Food Safety and Functionality Programme, Institute of Agriculture and Food Research and Technology (IRTA) – 17121 Monells, Spain

Carasau bread is a traditional Sardinian flatbread made from re-milled durum wheat semolina, water, yeast, and salt. It is characterized by its extreme thinness (less than 1 mm), crisp texture, and exceptionally long shelf life, due to its low moisture content. These features give it significant commercial appeal, with growing demand in Italy and internationally. Despite this market potential, production remains primarily at a small or medium scale, where empirical knowledge and manual expertise dominate the process. This hinders industrial scalability, which requires high levels of automation and real-time process control to ensure consistent product quality.
The dough's microstructure and mechanical properties – closely linked to gluten network development – are strongly influenced by both formulation and processing parameters [1]. Ingredients such as water, salt, and yeast play fundamental roles. Water often dominates interactions by competing for binding sites [2], while salt affects water distribution [9], delays gluten hydration, increases mixing resistance, reduces stickiness, stabilizes fermentation, and inhibits microbial growth [3-5]. Yeast mainly drives leavening through CO_2 production, but also releases fermentation by-products, such as ethanol, acetic acid, and succinic acid, that impact both dough structure and sensory properties [6].
Dough exhibits a non-linear viscoelastic behavior, where stress depends on both strain and strain rate. This complex response is typically assessed through rheological measurements, specifically dynamic oscillatory tests like Small Amplitude Oscillatory Shear (SAOS), which operate within the linear viscoelastic regime [7]. The frequency-dependent viscoelastic behavior of semolina-based doughs aligns well with the "weak gel model" [8]. At low stress, this structure behaves like a solid ("strong gel"), but transitions toward fluid-like behavior when weak intramolecular interactions are disrupted under high stress.
The dependence of storage (G') and loss (G") moduli on frequency can be described using power-law relationships:

$$G'(\omega) = K_0' \cdot \omega^{n'} \quad (1)$$

$$G''(\omega) = K_0'' \cdot \omega^{n''} \quad (2)$$

In addition to their frequency-dependent response, doughs exhibit time-dependent recovery behavior under constant stress, typically characterized through creep tests. Here, the compliance J (ratio between the strain and the constant stress) quantifies deformation and is commonly modeled using the Burgers model:

$$J(t) = J_0 + J_m \cdot \left(1 - e^{-\frac{t}{\tau}}\right) + \frac{t}{\eta_0} \quad (3)$$

This equation incorporates instantaneous compliance (J_0), retarded compliance (J_m), relaxation time (τ), and steady-state viscosity (η_0), offering a comprehensive description of dough's viscoelastic profile.
Furthermore, mechanical properties can be investigated via Texture Profile Analysis (TPA), which involves axial compression at constant speed and records force response. From this, key parameters such as hardness (Ha), cohesiveness (Co), elasticity (El), gumminess (Gu), and toughness (To) are derived [9].
Dough samples were prepared using commercial re-milled semolina (Brundu, with 71.0 wt% carbohydrates, 13.0 wt% proteins, 1.5 wt% fat), fresh brewer's yeast (*Saccharomyces cerevisiae*), sea salt, and distilled water. Each batch consisted of 500 g of semolina and 260 g of water (52 wt%), mixed using a bench-top kneader. Five process parameters were selected for investigation: salt amount (m_s), yeast amount (m_y), water temperature (T_w), mixing time (t_{mix}), and leavening time (t_{leav}).

To efficiently explore their effects, a fractional factorial Design of Experiments (DOE) was employed – specifically, a 2^{5-1} design of resolution V – resulting in 35 experimental runs, including three center points to assess model linearity. The design generator E = ABCD was used, allowing clear resolution of main effects and two-way interactions.
Rheological testing was conducted on an MCR 102 rheometer (Anton Paar GmbH, Austria) with 25 mm parallel plates and a 2 mm gap, maintaining a constant temperature of 25°C via Peltier control. Measurements were taken both before and after leavening. Frequency sweep tests were performed over a range of 1–100 rad·s^{-1} at 0.1% strain, within the linear viscoelastic region (LVE), as determined by preliminary amplitude sweeps. Storage modulus (G′), loss modulus (G″), and complex modulus (G*) were modeled using power-law equations to derive parameters K_0 and n. Creep tests involved applying a constant stress of 50 Pa for 120 s. Compliance data were analyzed using the Burgers model to extract J_0, J_m, τ, and η_0. TPA was also carried out using a custom-designed 3D-printed PLA fixture mounted on the same rheometer. A cylindrical probe (3.5 cm diameter) compressed dough samples (2.6 cm high) twice to a depth of 7 mm at a speed of 1 mm·s^{-1}.
For the dough samples analyzed prior to leavening, the influence of processing variables on rheological parameters was assessed using linear models. A backward elimination method with a p-value threshold of 0.05 was applied to identify statistically significant effects. Table 1 summarizes the results as positive (+) or negative (-) interactions.

	K_0*	*n**	K_0'	*n'*	K_0"	*n"*	J_0	J_m	τ	η_0	Ha	Co	El	Gu	To
m_s						+			+	-					
m_y	-		-			-				-	+	+		+	
T_W									-	-		+		+	+
t_{mix}	-	+	-	+						-	+		+		+
m_s * m_y										+					
m_s * T_W									+						
m_s * t_{mix}															
m_y * T_W												-		-	
m_y * t_{mix}	+		+								+				
T_W * t_{mix}															

Table 10 – Effect of processing parameters – salt content (m_s), yeast content (m_y), water temperature (T_w), and mixing time (t_{mix}) – on the rheological properties of unleavened dough samples

REFERENCES

[1] Fanari F., Carboni G., Desogus F., Grosso M., Wilhelm M., (2022) "A chemometric approach to assess the rheological properties of durum wheat dough by indirect FTIR measurements", *Food and Bioprocess Technology*, 15(5), 1040–1054, doi.org/10.1007/s11947-022-02799-z.
[2] Mani K., Trägårdh C., Eliasson A.-C., Lindahl L., (1992) "Water content, water soluble fraction, and mixing affect fundamental rheological properties of wheat flour doughs", *Journal of Food Science*, 57(5), 1198–1209, doi.org/10.1111/j.1365-2621.1992.tb11298.x.
[3] McCann T.H., Day L., (2013) "Effect of sodium chloride on gluten network formation, dough microstructure and rheology in relation to breadmaking", *Journal of Cereal Science*, 57(3), 444–452, doi.org/10.1016/j.jcs.2013.01.011.
[4] Bloksma A.H., (1990) "Rheology of the breadmaking process", *Cereal Foods World*, 35, 228–236.
[5] Chen G., Ehmke L., Sharma C., Miller R., Faa P., Smith G., Li Y., (2019) "Physicochemical properties and gluten structures of hard wheat flour doughs as affected by salt", *Food Chemistry*, 275, 569–576, doi.org/10.1016/j.foodchem.2018.07.157.
[6] Meerts M., Ramirez Cervera A., Struyf N., Cardinaels R., Courtin C.M., Moldenaers P., (2018) "The effects of yeast metabolites on the rheological behaviour of the dough matrix in fermented wheat flour dough", *Journal of Cereal Science*, 82, 183–189, doi.org/10.1016/j.jcs.2018.06.006.
[7] Morrison F.A., (2001), Understanding Rheology (Topics in Chemical Engineering), Oxford University Press, USA.
[8] Gabriele D., de Cindio B., D'Antona P., (2001) "A weak gel model for foods", *Rheologica Acta*, 40(2), 120–127, doi.org/10.1007/s003970000139.
[9] Peleg M., (2019) "The instrumental texture profile analysis revisited", *Journal of Texture Studies*, 50(5), 362–368, https://doi.org/10.1111/jtxs.12392.

Enhanced PhCN Nanosheet Stacking via WS_2 Nano-Linkers: A Metal Co-Catalyst Free 2D-2D Hybrid for Broad-Spectrum H_2 Production

M.Hazra[1], M. Hofer[2], B. Fickl[2], A. Ertl[2], S. Myakala[2], D. Eder[2], B. Bayer[2], A. Cherevan[2], P. Ricci[1]

[1]University of Cagliari – Cagliari (Italy), moulika.hazra@unica.it
[2]TU Wien -Vienna (Austria)

Photocatalysis has emerged as a sustainable technology to address decarbonization concerns through photocatalytic hydrogen evolution reaction (HER). Recent years have experienced a surge in the reports of novel photocatalysts which showed remarkable advancements in photocatalytic HER technology. A wide range of materials, from inorganic oxides like ZnO and TiO_2, to metal chalcogenides such as CdS, MoS_2, and WS_2, as well as emerging organic and polymeric semiconductors like graphitic carbon nitride (g-C_3N_4) and covalent organic frameworks (COFs), have been extensively investigated for photocatalytic hydrogen evolution.[1] These materials are chosen based on their suitable band gaps, chemical stability, and ability to generate and separate charge carriers efficiently under solar irradiation. Recent advances also include heterostructures, doped systems, and single-atom catalysts designed to improve visible-light absorption and enhance hydrogen evolution kinetics.

The following are the biggest challenges possessed by the above-mentioned systems: i) Achieving broad light spectrum activity- as it is essential for the efficient use of the solar spectrum and some photocatalysts are only active under UV radiation, ii) Using earth abundant materials- because of economic constraints and sustainability goals where the use of effective but expensive materials would not be scalable, iii) Synthesis through green methods- to prevent use of hazardous chemicals during processing and maintain ecological goals, iv) Elimination of noble metal co-catalysts- to reduce the cost of the HER process and eliminate the probability of metal ions entering the aquatic/marine food chain.

In our work- we address these challenges by utilizing a phenyl-doped carbon-nitride PhCN system with WS_2 to create 2D-2D nanohybrids. Phenyl groups provide electron-rich aromatic rings that promote efficient charge transfer and reduce the recombination rate of electron-hole pairs.[2] While, WS_2 has lower Tafel slope and an earlier overpotential which makes it more suitable for photocatalytic HER in addition to being less toxic and cheaper as compared to other TMDCs for co-catalytic purposes.[3] Since PhCN and WS_2 are both van- der Walls 2D materials, they could be exfoliated into low dimensional nanosheets to increase the surface-to -volume ratio and intuitively increase the interaction with the neighboring atoms. Liquid phase exfoliation (LPE) is a simple yet effective technique which does not require energy-high or costly apparatus and has been proven to be a successful method for the exfoliation of TMDCs and carbon nitrides.[4] [5]

As the extent of exfoliation depends upon the choice of the exfoliation medium, different solvents were tested to identify the best exfoliant for PhCN and WS_2 for high H_2 production. Isopropyl alcohol (IPA) showed the highest yield for exfoliation for PhCN and WS_2. Liquid-phase exfoliation enhanced H_2 production from PhCN and was successful in producing few-layered 2H WS_2 with a direct bandgap. WS_2 nanoflakes of two sizes, obtained via liquid-centrifuge cascading, were hybridized separately with exfoliated PhCN through electrostatic self-assembly to obtain two hybrid system. This was done to characterize the effect of flake size of WS_2 on its co-catalytic prowess. Structural characterizations (XRD, HRTEM, STEM, EDS, XPS) confirmed successful integration of WS_2 into the PhCN matrix, increasing its stacking order. HER tests were performed with 1–5 wt% WS_2 doping to optimize the hybrid's activity. The scalable synthesis reported avoids heat treatments and costly steps, making it suitable for practical applications. The integration of WS_2 with PhCN increased its HER activity by 42x while showing ~20% activity (μmol $g^{-1}h^{-1}$) of Pt metal co-catalyst. We conclude that longer and heavier WS_2 nanoflakes acted as better linkers of PhCN nanosheets and resulted in higher HER activity. Through optical characterization techniques like absorption, steady-state luminescence and time-resolved photoluminescence studies, an enhanced charge-carrier migration to WS_2 was observed which was aided by the WS_2 linking in between the PhCN nanosheets.

We report a 2D-2D hybrid photocatalyst which produces H_2 without the use of a metal co-catalyst ideal for utilizing the solar spectrum. The importance of the lesser studied 2H phase of WS_2 for co-catalyst usage is established and the first study of exfoliated PhCN for HER is carried out.

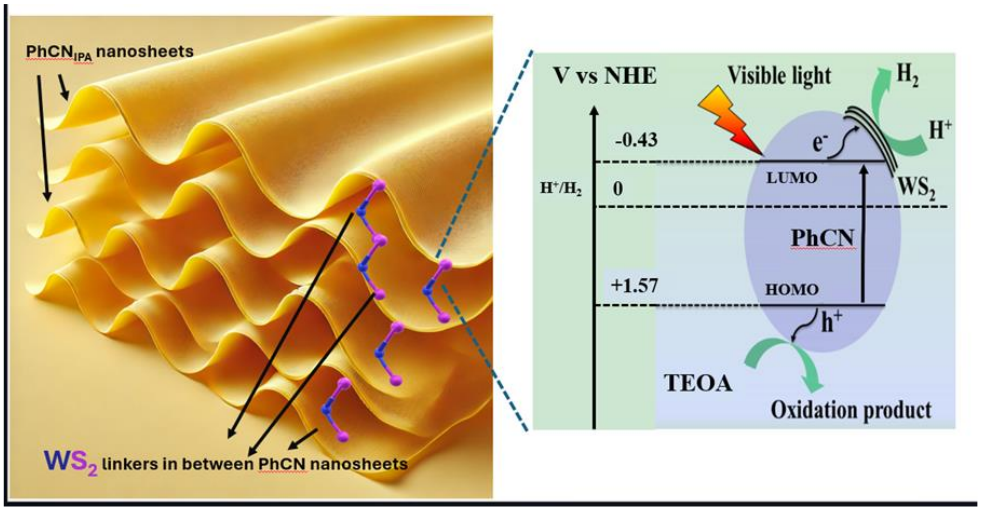


Figure 11 – Mechanism of working of PhCN/WS_2 hybrid system under 445nm irradiation.

REFERENCES

[1] Sadeq, A. M. et al. (2024) Hydrogen energy systems: Technologies, trends, and future prospects. Science of the Total Environment vol. 939 Preprint at https://doi.org/10.1016/j.scitotenv.2024.173622

[2] Hazra, M. et al. (2025) Elucidation of a Core–Shell Structure in Phenyl-Grafted Carbon Nitride/TiO2 Nanohybrids for Visible-Light-Mediated H_2 Production with Simultaneous Rhodamine B Degradation. ACS Appl Nano Mater doi:10.1021/acsanm.4c05592.

[3] Koyyada, G. et al. (2019) Enhanced solar light-driven photocatalytic degradation of pollutants and hydrogen evolution over exfoliated hexagonal WS_2 platelets. Mater Res Bull 109, 246–254.

[4] Sharma, R. et al. (2023) Liquid Phase Exfoliation and Characterization of Few Layer MoS_2 and WS_2 Nanosheets as Channel Material in Field Effect Transistor. Transactions on Electrical and Electronic Materials 24, 140–148.

[5] Backes, C. et al. (2016) Preparation of liquid-exfoliated transition metal dichalcogenide nanosheets with controlled size and thickness: A state of the art protocol. Journal of Visualized Experiments 2016.

Compact LIBS & Raman Detection System for Raw Material Exploration

Riccardo Lodo[1], Moulika Hazra[1], Stefania Porcu[1], Riccardo Corpino[1] Pier Carlo Ricci[1]

[1]Department of Physics, University of Cagliari, S.P. No. 8 Km 0.700, 09042 Monserrato, Italy

The exploration of critical raw materials (CRMs) in deep-seated deposits is essential for achieving sustainable resource management and reducing Europe's dependency on external supplies. As part of the DEXPLORE project (Grant Agreement No. 101178897, funded under Horizon Europe Call HORIZON-CL4-2024-RESILIENCE-01), a compact detection system integrating Laser-Induced Breakdown Spectroscopy (LIBS) and Raman spectroscopy was developed.

The system utilized the second harmonic of a Nd:YAG laser operating at 532 nm with a temporal pulse width of less than 10 ns. For LIBS measurements, the spectral acquisition window was set to 10 ns, and individual spectra were collected within a few seconds, ensuring rapid data acquisition. Raman spectroscopy, achieved spectral acquisition times under one minute, balancing speed and high-resolution data capture.

Optimization measurements were performed on a set of minerals to optimize the system and validate its capabilities to identify sample's composition through the combined analysis of LIBS and Raman spectra. The system showed stable performance across different spectral regions and a good signal-to-noise ratio.

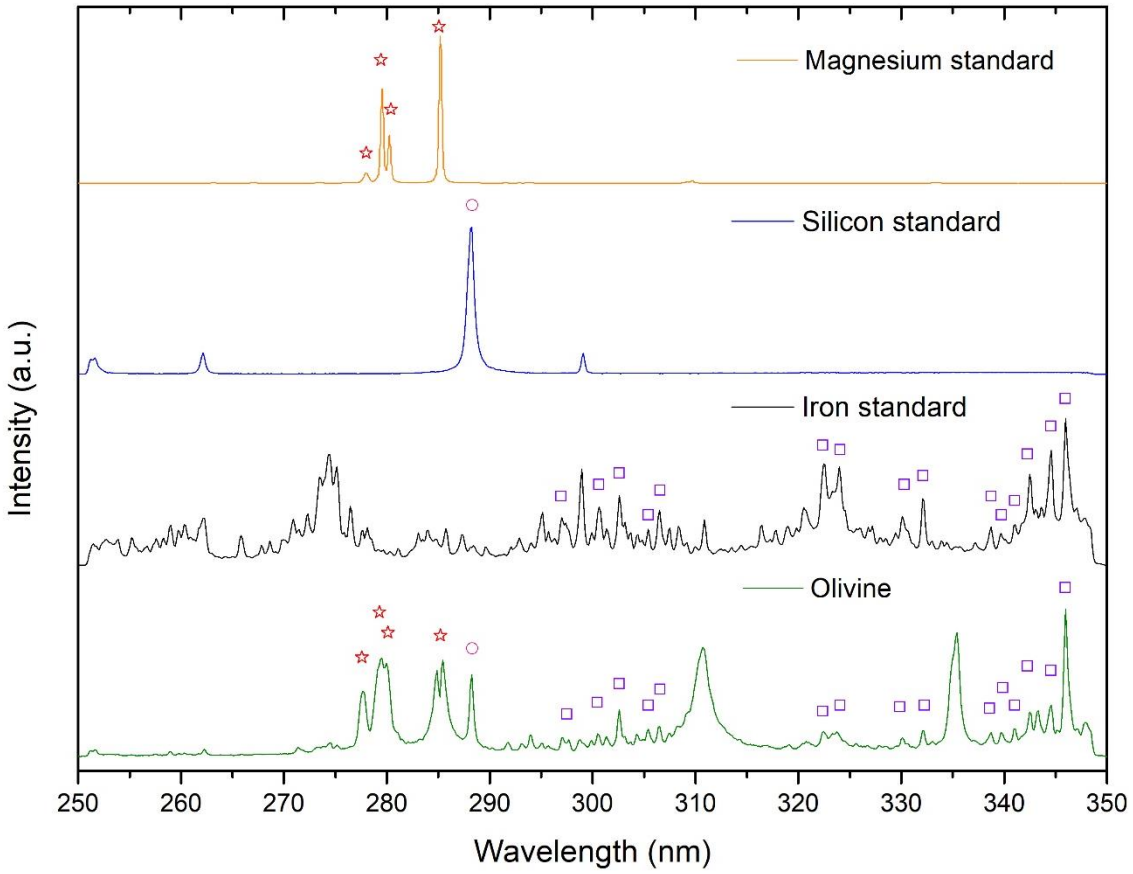


Figure 1 – LIBS spectrum of Olivine compared with Standard LIBS spectra of Iron, Silicon and Magnesium.

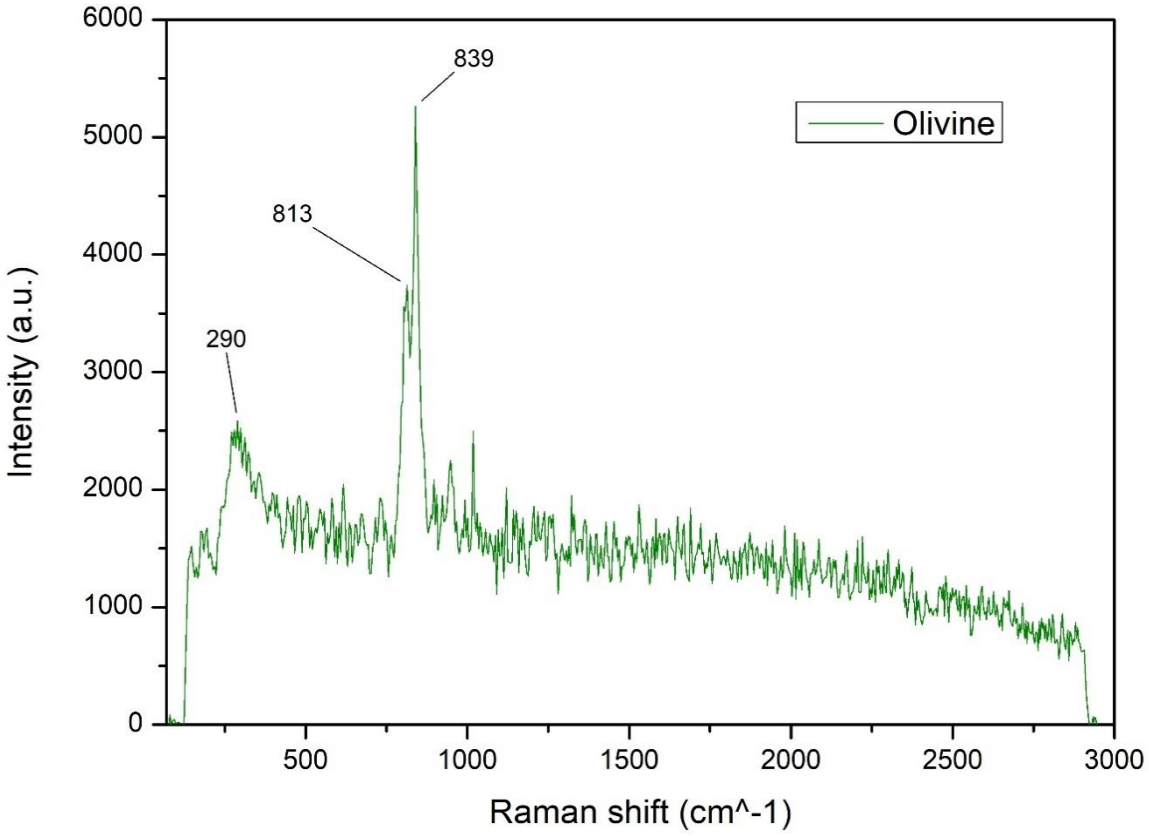


Figure 2- Raman spectrum of Olivine

Antimicrobial Peptides Histatin 5/6: Extraction, Purification and Adsorption on Mesoporous Silica Nanoparticles

Gaia Maria Meloni[1], Cristina Carucci[1], Cristina Contini[2], Giulia Guadalupi[2], Alessandra Olianas[2], Andrea Salis[1]

[1]Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, 09042, Monserrato, Italy
[2]Dipartimento di Scienze della Vita e dell'Ambiente, Università degli Studi di Cagliari, 09042, Monserrato, Italy
g.meloni87@studenti.unica.it

Histatin 5 and 6 (H5/H6) are histidine-rich, cationic peptides secreted into human saliva by salivary glands. H5/H6 are well known for their fungicidal activity against the pathogenic yeast *C.Albicans*. [1] Mesoporous silica nanoparticles (MSN) are silica-based nanostructured materials characterized by an ordered arrangement of mesopores, a high superficial area and a narrow pore size distribution (between 2 and 50 nm). In this study H5/H6 adsorption on bare and amino functionalized mesoporous silica nanoparticles (MSN and MSN-NH_2) were investigated. [2] Firstly, the peptides were extracted from human saliva and purified by means of the protocol proposed by Flona et al. [3] which includes the use of RP - HPLC. MSN and amino functionalized MSN (MSN-NH_2) samples were synthesized and fully characterized through physico-chemical techniques such as Small Angle X-Ray Scattering (SAXS), Transmission Electron Microscopy (TEM) and Fourier Transform Infrared Spectroscopy (FTIR) (Figure 1). H5/H6 peptides were dissolved in a 10 mM Tris-HCl buffer solution at pH 7 and adsorbed on MSN and MSN-NH_2. H5/H6 absorbed amount was quantified with bicinchoninic acid assay. The highest adsorbed amount was obtained for the bare MSN compared to MSN-NH_2 (8.49 ± 0.08 mg g^{-1} vs. 4.22 ± 0.08 mg g^{-1}, respectively). For bare MSN silanol groups, at pH 7, will be negatively charged, while the peptide will be positively charged (IEP ~ 10) favoring electrostatic interactions. On the other hand, due to the presence of the amino groups, protonated at pH 7, similarly to H5/H6 MSN-NH_2 will be positively charged. In this case, repulsive electrostatic interactions, together with attractive van der Waals forces, take place.

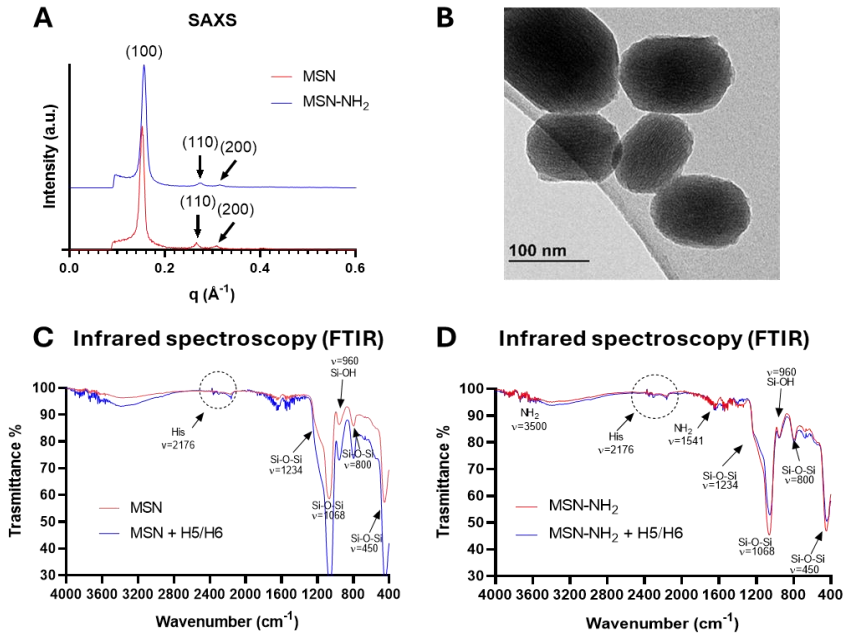


Figure 1 – **A.** SAXS pattern of bare and amino functionalized MSN; **B.** TEM image of MSN; **C.** FTIR spectra of MSN before and after adsorption; **D.** FTIR spectra of MSN-NH_2 before and after adsorption

REFERENCES

[1] Norris HL, Kumar R, Ong CY, Xu D, Edgerton M., *J. Fungi*, 2020, **6 (3)**, 124. DOI: 10.3390/jof6030124

[2] Carucci C., Pablos J.L., Romero Antolìn A., González, B.; Colilla, M.; Izquierdo Barba, I.; Salis, A.; Monduzzi, M.; Vallet-Regí, *Micropor Mesopor Mater*, 2024, **363**, 112810. DOI: 10.1016/j.micromeso.2023.112810
[3] Flora B, Gusman H, Helmerhorst EJ, Troxler RF, Oppenheim, F. G., *Protein Expr and Purif*, **23(1)**, 198-206, DOI: 10.1006/prep.2001.1493.

Comparative Molecular Dynamics Simulations of Human Telomeric G-Quadruplexes: Evaluating Ligand-Induced Stabilization of Parallel and hybrid Topologies

Olla G.[1], Satta G.[2], Carraro M.[2], Pisano L.[2], Carucci C.[1], Salis A.[1], Mura M.[1], Marincola Cesare F.[1], Mocci F.[1]

[1]Department of Chemical and Geological Sciences, University of Cagliari, Monserrato, Italy. g.olla14@studenti.unica.it
[2]Department of Chemistry and Pharmacy, University of Sassari, Sassari, Italy.

This template provides an example of the layout and style required for the preparation of two-page-extended DNA in the cell nucleus is mostly found in a double helix shape. However, there are also other secondary structures, like G-quadruplexes, which are very important for biological functions. G-quadruplexes (G4s) are involved in controlling gene activity and in DNA replication. One way to stabilize the formation of G-quadruplexes is by introducing ligands that can bind to G4s and help keep their structure stable.

In a previous study, we investigated the effect of a porphyrin-based ligand 4-[2-[10,15,20-tris[1-(2-amino-2-oxoethyl)pyridin-1-ium-4-yl]-21,24-dihydroporphyrin-5-yl] pyridin-1-ium-1-yl]acetamide (p11b), on the stability of the human telomeric G4 structure with parallel topology (PDB: 1KF1, sequence: 5(AGGGTTAGGGTTAGGGTTAGGG)-3), using molecular dynamics (MD) simulations. The results from the simulations with 1KF1 showed that the G-quadruplex without the ligand has a greater tendency to unfold compared to the system in the presence of the ligand [1].

In this study, we extend our analysis to another topology of the human telomeric G-quadruplex structure, focusing on the hybrid topology adopted in the PDB structure 143D, which has the same sequence of 1KF1. The objective is to verify whether the system is stabilized or destabilized in the presence of the ligand. MD simulations were performed using the OL15 [2] force field for the DNA and GAFF [3] for the ligand, with solvation modeled using the SPCE water model.

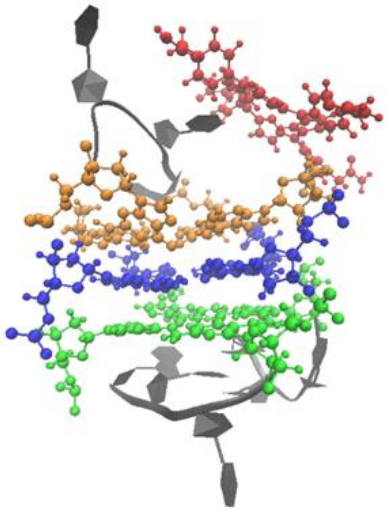


Figure 12 – Graphical representation of 143D with ligand using a different color for each loop and tetrad (Color code: first quartet, orange; second quartet, blue; third quartet, green; loops, grey.)

Simulations were conducted at both room temperature (300 K) and elevated temperatures (500 K, 525 K, and 550 K), maintaining constant pressure and temperature (NPT ensemble) at room temperature and constant volume and temperature (NVT ensemble) at high temperatures. The purpose of the high-temperature simulations was to determine the stabilizing or destabilizing effects of the ligand: if the complex's denaturation temperature is higher than that of the G4 alone, the ligand is considered to stabilize the G4; if lower, it implies a destabilizing effect [4,5,6]. RMSD analyses over simulation time were used to monitor structural integrity and detect denaturation events.

Preliminary results suggest that the ligand stabilizes the parallel topology but not the hybrid topology. These findings partially align with experimental observations (manuscript in preparation), which indicate a destabilizing effect of this ligand on the hybrid G-quadruplex.

REFERENCES

[1] Satta G., Trajkovski M., Cantara A., Mura M., Meloni C., Olla G., Dobrovolná M., Pisano L., Gaspa S., Salis A., De Luca L., Mocci F., Brazda V., Plavec J. and Carraro M. (2024) "Complex Biophysical and Computational Analyses of G-Quadruplex Ligands: The Porphyrin Stacks Back". Chemistry – A European Journal, 30(69), e202402600. 10.1002/chem.202402600.

[2] Zgarbová M., Šponer J., Otyepka M., Cheatham T. E., Galindo-Murillo R. and Jurečka P. (2015) "Refinement of the Sugar-Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA". Journal of Chemical Theory and Computation, 11(5), 1487-1499. 10.1021/acs.jctc.5b00716.

[3] Wang J., Wolf R. M., Caldwell J. W., Kollman P. A. and Case D. A. (2004) "Development and testing of a general amber force field". Journal of Computational Chemistry, 25(9), 1157-1174. 10.1002/jcc.20035.

[4] Todde G., Hovmöller S., Laaksonen A. and Mocci F. (2014) "Glucose oxidase from Penicillium amagasakiense: characterization of the transition state of its denaturation from molecular dynamics simulations". *Proteins*, 82(10), 2353. 10.1002/prot.24596.

[5] R. Day, B. J Bennion, S. Ham, V. Daggett (2002) "Increasing temperature accelerates protein unfolding without changing the pathway of unfolding". *J Mol Biol*, 322, 189. 10.1016/s0022-2836(02)00672-1.

[6] Mulliri S., Laaksonen A., Spanu P., Farris R., Farci M., Mingoia F., Roviello G.N. and Mocci F. (2021) "Spectroscopic and In Silico Studies on the Interaction of Substituted Pyrazolo[1,2-a]benzo[1,2,3,4]tetrazine-3-one Derivatives with c-Myc G4-DNA". International Journal of Molecular Sciences, 22(11), 6028. https://doi.org/10.3390/ijms22116028

Computational Insights into G-Quadruplex Stability in Human Papilloma Virus: The Role of Different Counterions

Enrico Puddu, Francesca Mocci

University of Cagliari, Department of Chemical and Geological Sciences, Cittadella Universitaria, I-09042 Monserrato, Italy
e.puddu38@studenti.unica.it

Human Papillomaviruses' (HPVs) are among the most common sexually transmitted infections and are associated with the development of head and neck, skin and anogenital cancer, including cervical cancer, which remains one of the one of the most significant global health challenges [1].
In this study we investigate the stability of a G-Quadruplex present in HPV type 52, a strain frequently detected in patients with vaginal cancers and precancerous lesions [2]. The aim is to identify molecules capable of stabilizing this G-quadruplex conformation in viral DNA, thereby inhibiting replication and paving the way for novel antiviral therapeutic strategies.
G-quadruplex (G4) are DNA structures stabilized by eight Hoogsteen hydrogen bonds between G-quartet-forming base, by coordinated metal ions in the central cavity of the G-quadruplex structure and through the ordered stacking of coplanarly aligned aromatic moieties. They play a significant role in various cellular processes and show high potential for application. G-quadruplexes' formation in the promoters of several genes has been demonstrated to affect their expression and indicates that G-quadruplexes can act as transcriptional regulators [1] and for this reason, they are considered promising targets for drug development [3].

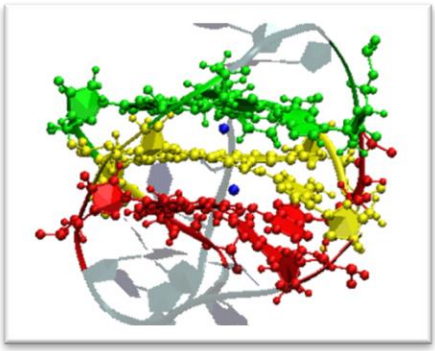


Figure 13 - HPV G-Quadruplex: quartets are in green, yellow and red. Ions are in blue. Same colors are used in graphs.

The three-dimensional G4 structure we use in this study was retrieved from RCSB Protein Data Bank (DNA PDB 5O4D). We have selected one of the 10 different conformations it contains proceeding to evaluate its stability through molecular dynamics methods.
At this stage of the study, we are focusing on comparing the results obtained from MD simulations performed using sodium ions with those from a previous study that employed potassium ions [4].
The simulated system comprises a G4 structure, modeled with the OL15 force field, immersed in a 150 mM NaCl aqueous solution, using the SPC/E water model and the Joung and Cheatham parameters for the ions. Two ions were manually added in the core channel of HPV G4 **(Figure 1)**. We plan to extend the study by also employing different force fields to compare the results obtained.
After the creation of the simulation box, the system was equilibrated with two energy minimization runs, followed by six runs of Molecular Dynamics (MD) of 10ns length, imposing restraints on the G4 and channel ions, of decreasing strength, until complete removal in the last run.

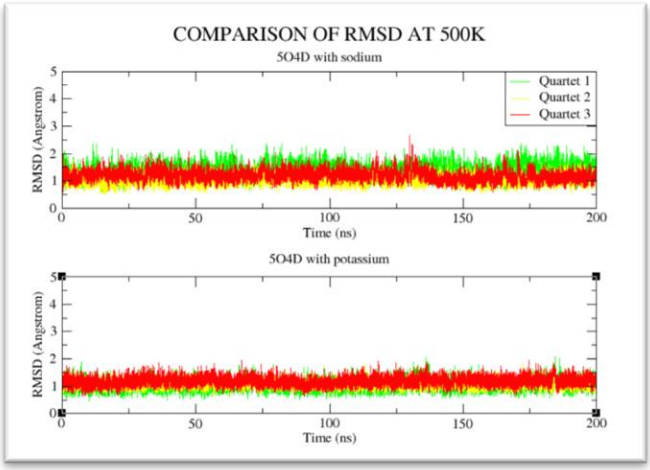


Figure 14 - Comparison of RMSDs at 500K.

The Production Phase was of 1 μs length at 300K (constant temperature) with no restraints and of 200ns at 500K (constant temperature) with no restraints. We analyzed the results by evaluating the Root Mean Square Deviation (RMSD) of the quadruplex during the MD trajectories and observed that the HPV G4 structure exhibits high stability at 300 K, reaching equilibrium under these conditions. Given that both ionic environments confer substantial structural stability, we extended our analysis to assess the behavior of the system at elevated temperatures.

At 500 K **(Figure 2)**, although both systems remain in an equilibrium state, the system employing potassium ions as counterions shows slightly lower RMSDs of the residues forming the quartets compared to the system with sodium ions.

As a future goal, we aim to run more MDs at higher temperatures to better evaluate G4 stability with and without a ligand. Employing temperatures higher than those typically used in experimental settings has proven effective in accelerating the denaturation process, allowing it to occur within the timescales accessible to MD simulations [3,4,5]. Previous research has shown that such temperature increases do not affect the overall denaturation pathway [5].

This study is part of the development of new strategies to target viruses, by the rational design of G-quadruplex targeting molecules capable of stabilizing the G4 structure.

REFERENCES

[1] Tlučková, K.; Marušič, M.; Tóthová, P.; Bauer, L.; Šket, P.; Plavec, J.; Viglasky, V. Human Papillomavirus G Quadruplexes. Biochemistry 2013, 52 (41), 7207–7216. https://doi.org/10.1021/bi400897g.

[2] Satta, G.; Trajkovski, M.; Cantara, A.; Mura, M.; Meloni, C.; Olla, G.; Dobrovolná, M.; Pisano, L.; Gaspa, S.; Salis, A.; De Luca, L.; Mocci, F.; Brazda, V.; Plavec, J.; Carraro, M. Complex Biophysical and Computational Analyses of G-Quadruplex Ligands: The Porphyrin Stacks Back. Chemistry – A European Journal 2024, 30 (69), e202402600. https://doi.org/10.1002/chem.202402600.

[3] Wang, M.; Liang, H.; Yan, Y.; Bian, R.; Huang, W.; Zhang, X.; Nie, J. Distribution of HPV Types among Women with HPV-Related Diseases and Exploration of Lineages and Variants of HPV 52 and 58 among HPV Infected Patients in China: A Systematic Literature Review. Human Vaccines & Immunotherapeutics 2024, 20 (1), 2343192. https://doi.org/10.1080/21645515.2024.2343192.

[4] Mulliri, S.; Laaksonen, A.; Spanu, P.; Farris, R.; Farci, M.; Mingoia, F.; Roviello, G. N.; Mocci, F. Spectroscopic and In Silico Studies on the Interaction of Substituted Pyrazolo[1,2-a]Benzo[1,2,3,4]Tetrazine-3 One Derivatives with c-Myc G4-DNA. International Journal of Molecular Sciences 2021, 22 (11), 6028. https://doi.org/10.3390/ijms22116028.

[5] Orrù M.; "Studio Computazionale Di Un G-Quadruplex Virale e Delle Sue Interazioni Con Potenziali Ligandi"; Bachelor Thesis; University of Cagliari, 2021/2022; Relator: Mocci F.

Photochromic Mechanism of Tungsten Oxide

Sofia Rocca[1,2], Andre Pinna[3]
Francesca Picciau[3], Daniele Chiriu[2], Stefania Porcu[2], Pier Carlo Ricci[2]

[1]Università degli Studi di Perugia, sofia.rocca@dottorandi.unipg.it
[2]Dipartimento di Fisica, Università degli Studi di Cagliari
[3]Active Label srl

Photochromic materials change color when exposed to electromagnetic radiation, typically shifting from a colorless or whitish state to a colored one. Depending on their composition, this transition can be either reversible or irreversible, and the persistence of the colored phase varies by material. Photochromic materials can be classified into three types based on their composition: organic, inorganic, or hybrid.
Among inorganic photochromic materials, tungsten trioxide (WO_3) is the most widely studied due to its exceptional stability and outstanding photochromic performance.

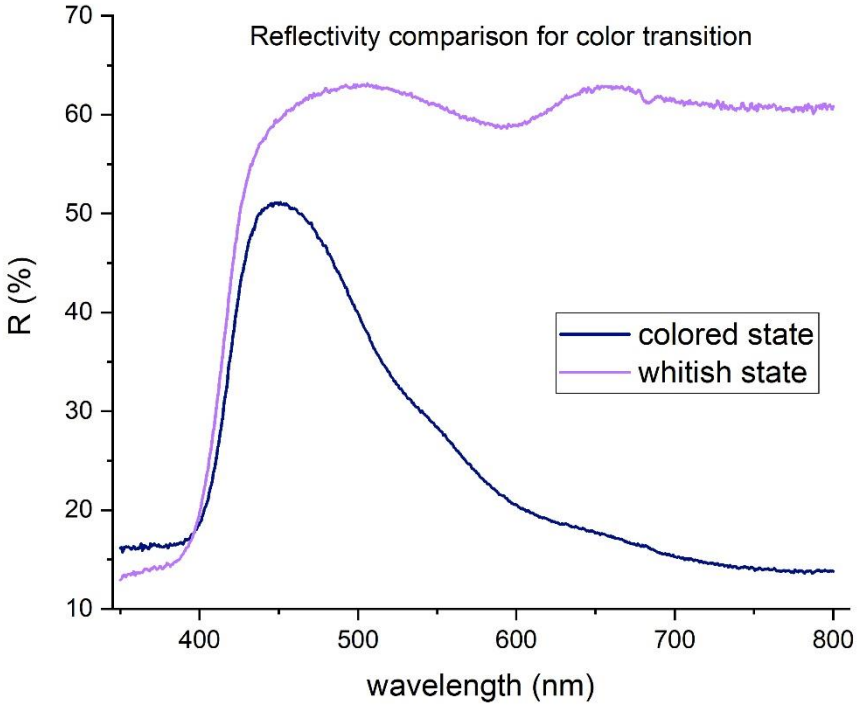


Figure 15- Reflectivity comparison for the color transition between the whitish state and the colored one.

This study examines the synthesis of photochromic WO_3 nanofibers and characterizes their colored state by investigating how their persistence changes under varying environmental conditions, particularly humidity. Controlled experiments reveal that maintaining constant temperature while increasing atmospheric humidity decreases colored state persistence, promoting faster recovery to the colorless phase.

REFERENCES

[1] Zhang, Y., & Wang, Q. (2024). Acceleration photochromic performance in tungsten oxide. *Optical Materials*, *157*, 116365.

[2] Ejeromedoghene, O., Zuo, X., Ogungbesan, S. O., Oderinde, O., Yao, F., Adewuyi, S., & Fu, G. (2022). Template synthesis and characterization of photochromic tungsten trioxide nanofibers. *Journal of Materials Science: Materials in Electronics*, *33*(10), 7371-7379.

Nanostructured Cerium Oxide-based catalysts for the direct synthesis of dimethyl carbonate from CO_2

Nicoletta Rusta[1], Valentina Mameli[1], Fausto Secci[1], Elisabetta Rombi[1],Carla Cannas[1]

[1] University of Cagliari, Department of Chemical and Geological Sciences, S.S: 554 bivio per Sestu, 09042, Monserrato (CA), n.rusta@studenti.unica.it.

Dimethyl carbonate (DMC) is a valuable eco-friendly compound, and its increasing demand is driven by the fast growth of its use in a wide range of applications (polycarbonates, solvent, pharmaceutical, fuel and the lithium-ion battery industries). There are several synthetic pathways that are used for the production of DMC, but most of them involve toxic and dangerous substances, as reagents, catalysts and by-products. For example, most of the industrial production of DMC still uses phosgene, a highly toxic chemical that can cause several health issues even in low concentration.

In recent decades, research has been focused on developing more sustainable synthetic approaches that can replace the phosgene method. Currently the attention has been paid on the direct synthesis from CO_2 and methanol in agreement with the principles of green chemistry. In addition, the use of low-cost CO_2 offers direct benefits to the environment by creating valuable products from unwanted CO_2, turning waste into fuel. However, this strategy still remains at laboratory level because of poor conversions and low yields of DMC, on account of the thermodynamic stability and kinetic inertness of CO_2. In order to overcome these drawbacks, new and efficient catalysts has to be developed. Among all the catalytic systems studied for this synthesis, Ce-based catalysts have attracted particular attention for their chemical stability, redox properties and high catalytic activity.

In this work, nanostructured CeO_2-bearing catalysts have been prepared following two green and easy chemical approaches based on sol-gel self-combustion or solvothermal processes. Nanostructured single-phase powders with different characteristics have been achieved thorough sol-gel self-combustion synthesis by varying the complexing agent (citric acid, glycine), the metal nitrate to complexing agent ratio and the ignition temperature. A sol-gel self-combustion strategy combined with an impregnation approach has been also proposed to incorporate CeO_2 in form of very small nanoparticles into the mesochannels of SBA-15 and MCM-41. Colloidal dispersions of CeO_2-based nanoparticles with different size and morphology have been obtained by solvothermal strategy using a proper capping agent together with the metal precursor to control the nucleation and growth kinetics of the nanoparticles. Synthetic temperature, capping agent (oleic acid, oleylamine or a mixture), metal precursor to capping agent ratio have been modified and the effects on the nanoparticles have been studied. The green approach, the low cost precursors, the repeatability, and the possibility of scaling up the processes render these synthetic strategies promising pathways to obtained nanostructured CeO_2-based catalysts for industrial applications.

The as-obtained catalysts have been characterised by a multi-technique approach using powder X-Ray Diffraction (PXRD), Transmission Electron Microscopy (TEM), Fourier transform infrared spectroscopy (FTIR), Thermogravimetric analysis (TGA), N_2-physisorption.

Insights into Small Molecule Stabilization of Viral G-Quadruplexes via Molecular Dynamics and Docking Simulations

Aamir Saeed[1], Flaminia Cesare Marincola[2], Francesca Mocci[3]

[1,2,3]Department of Chemical and Geological Sciences, University of Cagliari, 09042 Monserrato, Italy
Email. Aamir.saeed@unica.it

G-quadruplexes (G4s) are noncanonical four-stranded nucleic acid secondary structures formed by guanine-rich sequences that stack into planar G-tetrads stabilized by Hoogsteen hydrogen bonding and monovalent cations [1]. Many regulatory genomic regions, including telomeres, promoters, and untranslated regions, contain sequences capable of forming G4s, often referred to as putative G-quadruplex sequences (PQs). G4s play essential roles in viral genome stability, transcription, and replication [2]. While their functions have been extensively studied in human genomes, their presence and regulatory significance in viral genomes, particularly in the RNA genome of Zika virus and the DNA genome of Monkeypox virus, remain largely unexplored. Understanding the structural stability and dynamics of viral G4s could reveal novel regulatory mechanisms and potential antiviral targets. Due to the absence of experimentally resolved three-dimensional structures of viral G4s, we investigated PQ motifs from Monkeypox (MPG4: GGTCTAGGATGAGGATCAGG) and Zika (ZRG4: GGUGGGGGACUGG) viruses using a comparative modeling approach. Structural templates were selected from the RCSB PDB based on sequence alignment and structural similarity to the human telomeric G-quadruplex (PDB: 1KF1) [3] and a GGA triplet motif (PDB: 1OZ8) [4]. Homology screening identified 1KF1 and 1OZ8 as the closest structural matches, which were modified using PyMOL mutagenesis and energy minimization to construct two-quartet G4 models for DNA (MPG4) and RNA (ZRG4).

Molecular dynamic simulations were performed to evaluate the structural dynamics and ion stability of the modeled G4s. Amber OL15 [5] and OL3 [6] force fields were used in 1 μs simulations under both Langevin and Berendsen thermostats. Under Langevin dynamics at 300 K [7], both G4s remained structurally stable, maintaining intact G-quartet (GQ) cores, with RMSD values of approximately 4 Å for MPG4 and 1.5 Å for ZRG4 (Figure 1A and 1B). Both systems exhibited stable RMSD oscillations averaging around 1.5 Å, indicating rigidity in the GQ framework (Figure 1A and 1B). The coordinated K^+ ion, essential for neutralizing the negative charge density and maintaining the Hoogsteen hydrogen bonding (HHB) network, remained stably positioned throughout the simulations. In MPG4, the K^+ ion exhibited slightly larger oscillations of about 0.7 Å, reflecting the intrinsic flexibility of the loop regions. In ZRG4, the K^+ ion remained consistently coordinated with only minor displacements of approximately 0.2 Å, suggesting strong interactions with O6 atoms. ZRG4 maintained RMSD values between 2.5 and 3 Å, further supporting stable ion coordination and HHB integrity. In contrast, simulations using the Berendsen thermostat [8] led to substantial RMSD increases and partial destabilization of both G4 models. The Berendsen thermostat's limitations in temperature and pressure coupling led to increased fluctuations and destabilization, whereas Langevin dynamics, with its additional friction and random noise, ensured better structural preservation.

These findings support the structural stability of G4s in the genomes of Monkeypox and Zika viruses, reinforcing their potential regulatory roles in viral gene expression. Additionally, the observed differences between Langevin and Berendsen thermostat simulations highlight the importance of choosing appropriate simulation parameters when modeling G4 structures over extended timescales. This work lays a computational foundation for future studies exploring viral G4s as potential antiviral

targets. Targeting G4s stability with small molecules could provide novel antiviral strategies, with their effect on G4 formation and stability validated through circular dichroism (CD) spectroscopy.

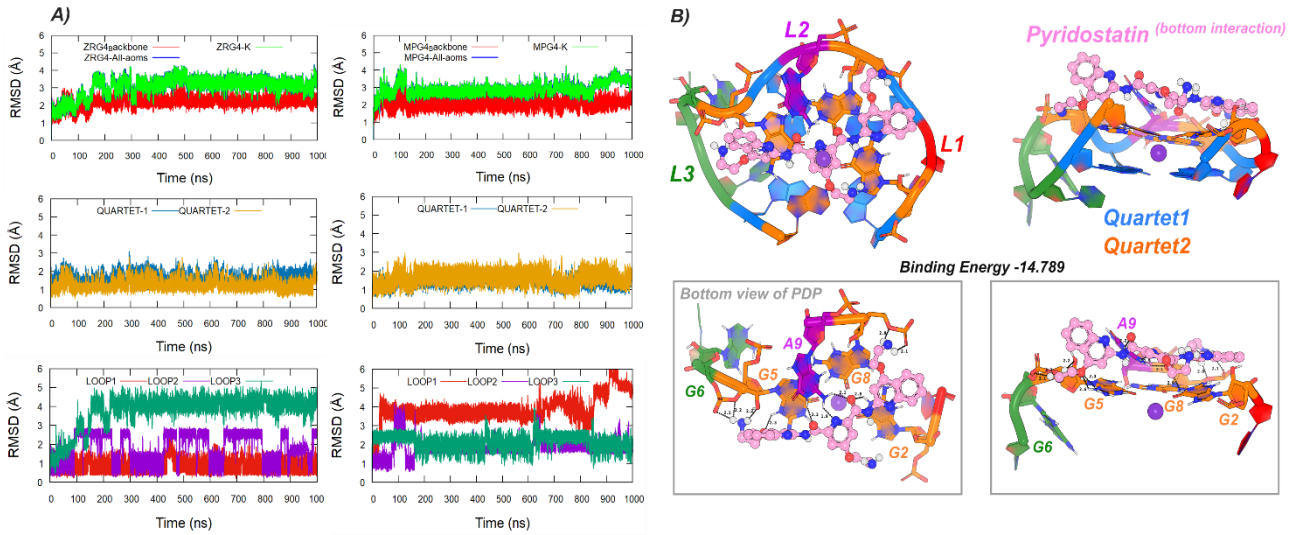


Figure 16 - **(A)** Molecular dynamics simulations of ZRG4 and MPG4 G-quadruplex structures were performed under a Berendsen thermostat at 300 K for 1000 ns. RMSD plots illustrate structural fluctuations over time, highlighting deviations in the backbone, all atoms, K^+-coordinated core, individual G-quartets, and loop regions. **(B)** Molecular docking of Pyridostatin with ZRG4 reveals the ligand bound at the base of the second G-quartet in a fully stacked conformation. The complex is stabilized through multiple hydrogen bonds with guanine bases, reinforcing the structural integrity of the G-quadruplex.

REFERENCES

[1] Pathak R, (2023) "G-quadruplexes in the viral genome: unlocking targets for therapeutic interventions and antiviral strategies". *Viruses*, *15*(11), 2216.doi.org/10.3390/v15112216

[2] Rhodes D, & Lipps H J, (2015) "G-quadruplexes and their regulatory roles in biology". *Nucleic acids research*, *43*(18), 8627-8637. doi.org/10.1093/nar/gkv862

[3] Parkinson G N, Lee M P, & Neidle S, (2002) "Crystal structure of parallel quadruplexes from human telomeric DNA". *Nature*, *417*(6891), 876-880. doi.org/10.1038/nature755

[4] Matsugami A, Okuizumi T, Uesugi S, & Katahira M, (2003) "Intramolecular higher-order packing of parallel quadruplexes comprising a G: G: G: G tetrad and a G (: A): G (: A): G (: A): G heptad of GGA triplet repeat DNA". *Journal of Biological Chemistry*, *278*(30), 28147-28153. doi.10.1074/jbc.M303694200

[5] Galindo-Murillo R, Robertson J C, Zgarbova M, Sponer J, Otyepka M, Jurecka P, & Cheatham III T E, (2016) "Assessing the current state of amber force field modifications for DNA". *Journal of chemical theory and computation*, *12*(8), 4114-4127.doi.org/10.1021/acs.jctc.6b00186

[6] Zgarbová M, Otyepka M, Sponer J, Mladek A, Banas P, Cheatham III T E, & Jurecka P., (2011) "Refinement of the Cornell et al. nucleic acids force field based on reference quantum chemical calculations of glycosidic torsion profiles". *Journal of chemical theory and computation*, *7*(9), 2886-2902. doi.org/10.1021/ct200162x

[7] Bussi G, Donadio D, & Parrinello M, (2007) "Canonical sampling through velocity rescaling". *The Journal of chemical physics*, *126*(1).doi.org/10.1063/1.2408420

[8] Huey R, Morris G. M, & Forli S., (2012) "Using AutoDock 4 and AutoDock vina with AutoDockTools: a tutorial". *The Scripps Research Institute Molecular Graphics Laboratory*, *10550* (92037), 1000.

Characterization of Nonlinear Optical Crystals

Manuela Schirru[1], Andrea Cocco[1], Marco Alcibiade[1], Anna Corrias[2], Maria Francesca Casula[1] and Luca Pilia[1]

[1]Department of Mechanical, Chemical and Material Engineering, University of Cagliari, Cagliari, Italy
[2]School of Chemistry and Forensic Science, University of Kent, Canterbury, UK
manuela.schirru@unica.it.

Nonlinear optical (NLO) crystals are pivotal for many electronic optical devices for laser technology, optical communication, defence and security because they can be used to convert the frequency of the laser light, making it possible to operate in specific regions of the electromagnetic spectrum that would typically be unreachable [1][2]. Herein, the studied materials are formed by metal ions (Pt, Cu, Zn, or Ni) coordinated by organic ligands such as 1,3-dithiolo-2-thione-4,5-dithiolato (dmit), giving birth to heteroleptic and homoleptic complexes.

Within the framework of the QUANTAMOL project funded by the European Union-Next Generation EU, and by taking advantage of the collaboration with the University of Kent under the MGR (Mobilità Giovani Ricercatori) mobility grant, the characterization of these synthesized molecules was performed to investigate their thermal and structural stability, by focusing on techniques such as thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) and X-ray diffraction (XRD). Among the investigated parameters, there were their range of temperature, the optimal atmosphere for the thermal cycle, and the environmental material conservation.

Thermal analysis was performed up to 1200 °C for most samples, while complexes with limited stability were handled under inert atmosphere and analysed up to 600 °C to verify the possibility of determining the different mass losses of the complexes and the relative heat flows associated with the thermal transitions.
The thermal analysis was supported by XRD characterization: where possible, the XRD investigation of the complexes was carried out before and after the thermal cycle. Furthermore, the XRD characterization in air (collected on all samples) was supported by measurements in an argon atmosphere for the air-sensitive samples to evaluate their stability and the operating conditions to be used subsequently for the thermal analyses (**Figure 1**). The comparison between the XRD patterns collected in air and in argon confirms differences that suggest changes in the crystalline structure.

Finally, the analysis of the samples after thermal analysis allowed us to identify the crystalline phases obtained after the combustion of the complexes, obtaining the metals or their oxides.

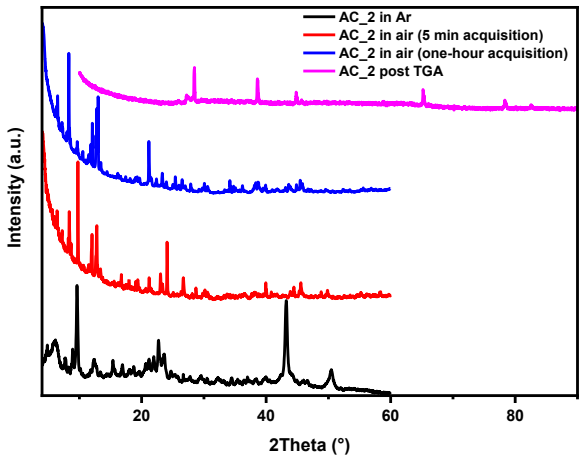


Figure 1 ─ XRD profiles of the NLO crystal Pt($COXBr_2$)dmit TBA in argon atmosphere; in air (5 min and 1 hour acquisition) and the residual crystalline phase obtained after TGA analysis under inert atmosphere (up to 600°C).

We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 1409 published on 14.9.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title "Molecular Quantum Light Sources" (QuantaMol)– CUP F53D23008550001- Grant Assignment Decree No. 1380 adopted on 01/09/23 by the Italian Ministry of Ministry of University and Research (MUR).

REFERENCES

[1] Bo Z., Mao-Yin R., Xin-Tao W., Hua L., Qi-Long Z., (2024). "Recent advances and future perspectives on rare-earth-based nonlinear optical materials with π-conjugated [XO_3] (X= B, C, N) units", Coordination Chemistry Reviews, Volume 517, 216053, https://doi.org/10.1016/j.ccr.2024.216053.

[2] Ahn N., Livache C., Pinchetti V., Klimov V.I., (2023). "Colloidal Semiconductor Nanocrystal Lasers and Laser Diodes", Chemical Reviews, Volume 123, 8251-8296, https://doi.org/10.1021/acs.chemrev.2c00865.

Preparation, characterization and biocompatibility evaluation of glycine betaine surfactant-based liposome (SBLs)

Michela Tozzi,[1] Franca Piras,[2] Antonella Rosa,[2] Angelo Frongia,[1] Marco Piludu,[2] Valeria Sogos,[2] Cristina Carucci,[1*] Andrea Salis,[1] Flaminia Cesare Marincola[1*]

[1]Department of Chemical and Geological Sciences and CSGI, University of Cagliari, Cittadella Universitaria, S.S. 554 bivio Sestu, Monserrato, 09042, CA, Italy
[2]Department of Biomedical Sciences, University of Cagliari, Cittadella Universitaria, SS 554 Bivio Sestu, 09042 Monserrato, CA, Italy
m.tozzi@studenti.unica.it

Liposomes containing surfactants are characterized by a peculiar deformability [1] that makes them ideal for transdermal drug delivery (TDD) as they can pass the stratum corneum with more ease compared to traditional liposomes.[2] In this study, 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) was combined with cleavable surfactants made of glycine betaine esters (GBCn) to prepare surfactant-based liposomes (SBLs). For this aim, two different betaine esters, namely dodecyl betainate (GBC12) and hexadecyl betainate (GBC16) were synthetized. SBLs were prepared using various percentages of surfactants: 10, 30 and 70%. These systems were dispersed in four different media: H_2O, NaCl 10 mM, NaCl 100 mM and PBS 150 mM (pH 7.4).
The hydrodynamic diameter (D_H) and the zeta potential (ζ) of SBLs were determined through dynamic light scattering (DLS) and electrophoretic light scattering (ELS) respectively. Measurements were repeated at 7, 14 and 30 days after preparation in order to assess the storage stability of these systems. For the sake of comparison, pure DOPC liposomes were used as reference.
Our findings show that both the surfactant molar percentage and media have a significant impact on ζ, changing from about 0 mV in DOPC liposomes up to +50 mV in SBL12 with 70% of surfactant in water and +80 mV in SBL16 with 70% of surfactant in NaCl 10 mM. Furthermore, while zeta potential decreased as a function of media ionic strength both in pure DOPC liposomes and SBLs, D_H of DOPC liposome was more strongly affected than SBLs. All prepared systems showed good storage stability after one month from preparation.
To assess the kinetic of the surfactants' hydrolysis, NMR spectra of free GBCn and SBLs were recorded at different time intervals and compared. Figure 1 shows the hydrolysis kinetic findings for the experiments conducted in PBS (pH 7.4). At physiological-like conditions, free GBC12 hydrolysed completely in 24 h, while both GBC12 and GBC16 within the SBLs show a much slower hydrolysis kinetic. In particular, SBL containing 10% of GBCn (SBL-10) showed no hydrolysis after 24 h from preparation; SBL with 30% of GBCn (SBL-30) showed about 10% of hydrolysis and SBL with 30% of GBCn (SBL-70) showed less than 50% of hydrolysis. These results indicate enhanced resistance of the surfactants to hydrolysis when they are combined with DOPC to form liposomes.
Lastly, the citotoxicity was assessed through HaCaT cell viability assay showing no decrease in cell viability for all SBL12, SBL16-10 and SBL16-30 when used at a concentration of 50 μg/ml. Additionally, SBL12-10 (SBL12 with 10% of GBC12) was not cytotoxic even at higher concentration (125 μg/mL). The overall results suggest possible use of SBLs, especially SBL12-10 as a drug delivery system. Future work will focus on encapsulation of a hydrophilic drug inside the best SBLs formulations (SBL12 and SBL16-10) to study the encapsulation efficiency and the release.

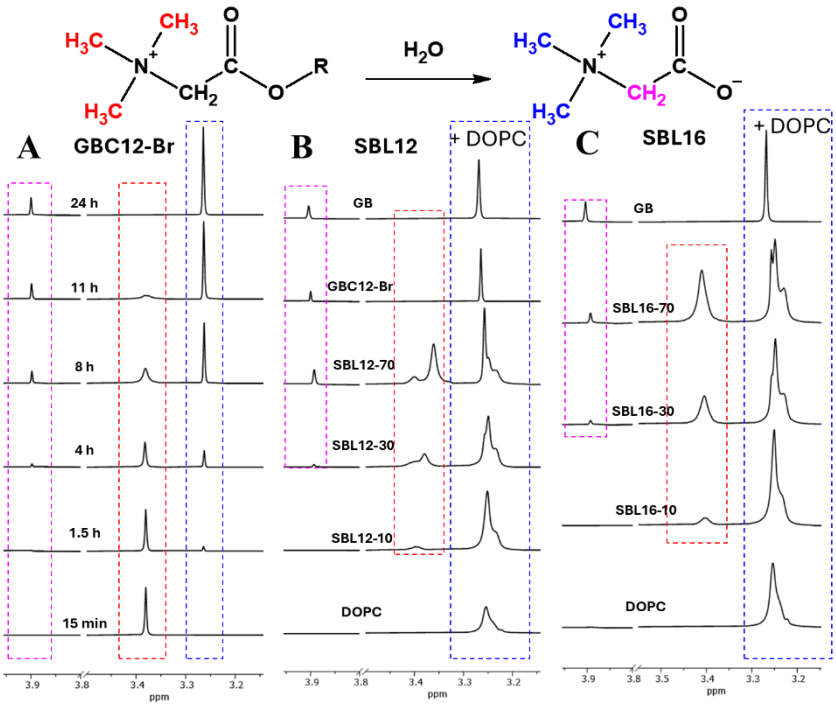


Figure 17 – Portions of the ^{1}H NMR spectra of: (A) free GBC12 during 24 h in PBS (pH 7.4); (B) SBL12 and (C) SBL16 after 24 h in PBS (pH 7.4). DOPC and GB are shown as references.

REFERENCES

[1] Matharoo N., Mohd H., Michniak-Kohn B. (2024) "Transferosomes as a transdermal drug delivery system: Dermal kinetics and recent developments" *WIREs Nanomedicine and Nanobiotechnology*, *16* (1). DOI:10.1002/wnan.1918

[2] Kuznetsova D. A., Vasilieva E. A., Kuznetsov D. M., Lenina O. A., Filippov S. K., Petrov K. A., Zakharova L. Ya., Sinyashin O. G., (2022) "Enhancement of the Transdermal Delivery of Nonsteroidal Anti-inflammatory Drugs using Liposomes Containing Cationic Surfactants" *ACS Omega*, 7, 25741−25750. DOI:10.1021/acsomega.2c03039

Invited Speakers and Contributors

A

Alcibiade Marco: Active Materials for On-Chip Integrated Quantum Light Sources Based on Metal Complexes (poster)

B

Bagchi Saswati: Adsorption-derived visible light photocatalytic degradation of dyes using phenyl-modified graphitic carbon nitride/Strontium titanate composite (poster)

C

Carboni Zaira: Relationship Between Optical and Structural Properties of Nitrogen-doped Carbon Dots (poster)

Carucci Cristina: Investigating protein corona formation; BSA interactions with bare and amino functionalized mesoporous silica nanoparticles (oral)

Chiappone Annalisa: Vat 3D printing of ionically conductive polymers for tactile sensors (oral)

Cocco Andrea: Design and synthesis of Platinum(II) Donor–Acceptor Complexes for Second-Order Nonlinear Optics (poster)

D

Desogus Francesco: Effect of processing parameters and recipe composition on dough rheology in carasau bread production (poster)

Dettori Riccardo: Linear Machine-Learning Approaches For Accurate Atomistic Simulations (oral)

H

Hazra Moulika: Enhanced PhCN Nanosheet Stacking via WS2 Nano-Linkers: A Metal Co-Catalyst Free 2D-2D Hybrid for Broad-Spectrum H2 Production (poster)

L

Lodo Riccardo: Compact LIBS & Raman Detection System for Raw Material Exploration (poster)

M

Malfatti Luca: Light-activated Carbon dots for functional applications (oral)

Mastrangelo Rosangela: Surface-modified agar microgels as food foams stabilizers (oral)

Melis Claudio: Engineering thermal transport in transition metal dichalcogenides: from molecular modifications to defect-engineered superlattices (oral)

Melis Nicola: Nanoporous Au in Dye-Contaminated Water: A Case Study with Methyl Orange (oral)

Meloni Gaia Maria: Antimicrobial Peptides Histatin 5/6: Extraction, Purification and Adsorption on Mesoporous Silica Nanoparticles (poster)

Medved' Miroslav: Computational Insights into Molecular Photochromism (oral)

Mussavi Rizi Seyed H.: Advances in Bioresorbable phospate glass optical fiber fabrication (oral)

N

Nociarová Jela: NMR Spectroscopy as a Tool for Characterization of Molecular Fluorophores in Carbon Dots: Challenges and Opportunities (oral)

O

Olla Chiara: Photopolymer-Based Colorimetric Sensors Incorporating Natural Dyes for Detection of Toxic Substances (oral)

Olla Giulia: Comparative Molecular Dynamics Simulations of Human Telomeric G-Quadruplexes: Evaluating Ligand-Induced Stabilization of Parallel and hybrid Topologies (poster)

Otyepka Michal: Inkjet Printing in Electrochemical Biosensing (oral)

Otyepková Eva: Inverse Gas Chromatography in the Study of Surface Properties of Materials (oral)

P

Paloncýová Markéta: Simulation Insight into Bio-Nano Interface (oral)

Puddu Enrico: Computational Insights into G-Quadruplex Stability in Human Papilloma Virus: The Role of Different Counterions (poster)

R

Rocca Sofia: Photochromic Mechanism of Tungsten Oxide (poster)

Rusta Nicoletta: Nanostructured Cerium Oxide-based catalysts for the direct synthesis of dimethyl carbonate from CO2 (poster)

S

Saeed Aamir: Insights into Small Molecule Stabilization of Viral G-Quadruplexes via Molecular Dynamics and Docking Simulations (poster)

Schirru Manuela: Characterization of Nonlinear Optical Crystals (poster)

T

Tocco Davide: Sustainable Carbon Quantum Dots: From Fluorescent pH Sensors to Performance Enhancement in Solar Cells (oral)

Tozzi Michela: Preparation, characterization and biocompatibility evaluation of glycine betaine surfactant-based liposome (SBLs) (poster)