



# **XXXV Congresso Annuale SISN**

Venezia, 16-18 settembre 2024

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## **Book of abstracts**



**Società Italiana di  
Scienze Neutroniche**  
Associazione di Promozione Sociale

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Immagine di copertina: Wolfgang Moroder.

# Programma

Auditorium "Danilo Mainardi"  
Edificio Alfa, Campus Scientifico  
Università Ca' Foscari Venezia  
Mestre (VE)

## Lunedì 16 settembre 2024

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14:00 **Registrazione**

14:30 **Apertura e saluti**

**M. Zanatta**, Presidente SISN APS

**E. Cattaruzza**, Prorettore Università Ca'Foscari Venezia

14:50 **Keynote Lecture: neutroni & beni culturali**

**F. Grazzi**, *Non-invasive characterization of ancient bronzes and of their manufacturing techniques through neutron advanced techniques: an overview and a peculiar case studio from ancient Japan*

15:30 **A. Venturi**, *Neutrons for painting conservation: addressing varnish blanching through scattering techniques and optical methods*

15:50 **A. Rodzinka**, *Application of neutron science in the study of ancient Iranian weaponry*

16:10 **F. Cantini**, *Preliminary results on an ongoing study of 28 fragments of equestrian gilded monumental-statuary complexes rediscovered near Parco dei Renai Signa, Firenze, Italy.*

16:30 **Coffee break**

17:00 **A. Pietropaolo**, *Update on the SORGENTINA Project.*

17:20 **L. Spagnuolo**, *The ENEA TRIGA RC-1 neutron source: from activation analyses to radioisotopes production.*

17:40 **G. Ottaviano**, *A multipurpose compact neutron generator for applications in nuclear medicine and nuclear.*

18:00 **SISNyoung**, sessione informale dedicata a soci Junior della SISN APS

## Martedì 17 settembre 2024

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09:00 **Keynote Lecture: neutroni & materiali per l'energia**

**F. Foglia**, *Neutrons: powering the future of green energy.*

09:40 **M. Laurati**, *Link between permanent shear-banding and local concentrate fluctuations in suspensions of compressible microgels.*

10:00 **B. Rosi**, *Structural and dynamical properties of PS-PNIPAM block copolymer micelles in concentrated samples.*

10:20 **A. Cangiano**, *SANS-driven insights into the self-assembly and optimization of metal-based superlattices.*

10:40 **N. Gallucci**, *CeO<sub>2</sub> nanoparticles coated with a dopamine-derivatized molecule: the role of surface functionalization on the structural organization.*

11:00 **Coffee break**

11:20 **V. Nigro**, *Small Angle Neutron Scattering investigation of ageing in CuCrZr alloy for fusion reactor technology.*

11:40 **A. Calamida**, *Determination of the fast and thermal neutron fields inside a shielding mock-up for fusion plants.*

12:00 **L. Silvi**, *Study of the effects of chronic neutron exposure on plants for agrospace-related activities.*

12:20 **M. Polo**, *Simulating the performance of a 3D silicon detector for neutron imaging.*

12:40 **Lunch break & poster session**

14:30 **Quali prospettive per la neutronica in europa?**

**Stefano Deledda**, vice-chair ENSA

15:30 **Assemblea dei soci SISN APS**

18:00 **Conclusione dei lavori**

20:00 **Cena Sociale**

Ristorante San Trovaso

Calle Larga Nanni

Venezia

## Mercoledì 18 settembre 2024

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### 09:00 Aggiornamenti sui progetti italiani nella neutronica

- A. Orecchini, T-REX@ESS.
- A. Perrichon, VESPA@ESS.
- F. Natali, IN13+@ILL.
- A. Scherillo, INES@ISIS.

### 10:30 Coffee Break

### 11:00 Keynote Lecture: Neutroni & scienze della vita

**S. Capaccioli**, *Cage dynamics revealed by EINS as a key quantities for pharmaceutical stability.*

11:40 **I. De Cristofaro**, *Design and physicochemical characterization of liposomes for enhanced intracellular delivery of therapeutics.*

12:00 **B. Barletti**, *Nanostructural characterisation of glycosylated protein biomarker interaction with lipid bilayer membranes: basis for biosensor development.*

12:20 **I. Mosca**, *Dynamic cluster formation, viscosity and diffusion in monoclonal antibody solutions.*

### 12:40 Conclusioni e saluti

# Keynote lecture

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## Neutroni & beni culturali

### **Non-invasive characterization of ancient bronzes and of their manufacturing techniques through neutron advanced techniques: an overview and a peculiar case studio from ancient Japan**

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Francesco Grazzi

*Consiglio Nazionale delle Ricerche, Istituto di Fisica Applicata, Sesto Fiorentino, Italy.  
Istituto Nazionale di Fisica Nucleare, Sez. Di Firenze, Sesto Fiorentino, Italy.*

The technology of solid bronze casting is one of the most ancient systems in history for the creation of specifically shaped metal artefacts, which can be used to produce specific tools or wonderful piece of art. Discriminating which casting method was used can be critical for understanding the technological process and reconstructing its historical context.

Those artefacts often are heavily corroded or artificially patinated and direct investigation of sound metal is difficult unless severe sampling is applied. Neutron techniques offer the possibility to characterize the metal applying a non-invasive approach, allowing to obtain morphological, microstructural, and compositional details by exploiting a combination of neutron diffraction and imaging methods. An overview of the neutron methods and their application to bronze artefacts will be presented.

I will also present the preliminary results of the neutron analysis performed on a large set of bronze arrowheads from archeological burial mounds of Okayama prefecture in Japan (Kofun and Yayoi periods), in the frame of a collaboration project between CNR, INFN, Università di Torino and Okayama University.

All results aim to identify the particular casting methods and distinguish the possible evolution of technology through time, revealing new details about bronze casting during the period of state formation in Japan.

## Neutroni & materiali per l'energia

### Neutrons: powering the future of green energy

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Fabrizia Foglia

*Department of Chemistry, University College London,  
Christopher Ingold Building, 20 Gordon Street, London, WC1H 0AJ, UK*

Despite the widespread use (e.g. in healthcare, energy and water treatment applications) and the continued development of new materials and solutions for their implementation in advanced devices, improving membrane performance and durability remains a non-trivial problem. In large part this is due to the lack of a detailed understanding of the dynamics of the permeant confined within the membrane structures, that are typically multi-scale in terms of correlation lengths and relaxation timescales for the different processes involved. It is therefore difficult to disentangle individual contributions to the various motions and their involvement in the membrane structure-dynamics correlation, especially in situ and under operando conditions.

Neutron scattering is ideal for this type of study because it allows a unique view of structures of soft condensed matter systems. The nature of neutron-matter interaction provides a non-destructive approach, making it a perfect tool to investigate structurally delicate membrane structure-dynamics properties as well as biological systems. Cold neutrons, with wavelengths of a few Å and energies from  $\mu\text{eV}$  to several meV, allow investigations and correlations of structure on the Å- to nano-scale combined with molecular motions on a nano- to pico-second time regimes. Furthermore, because of the difference in neutron scattering cross section between H and D, isotopic contrast experiments can be used to highlight different spatial/dynamic regions under varied chemical and physical conditions.

Here we present our journey using advanced neutron scattering techniques to shed light on the structure-dynamical interplay, while developing a new understanding by correlating energy, time and space to resolve structure to function interplay. We apply this approach not only to guide the design of new materials with improved performance characteristics but also to enhance our understanding and improve the recyclability of materials.

#### References

- [1] T.R. Willson et al., *J. Mater. Chem. A* **11**, 20724-20740 (2023).
- [2] K. Smith et al., *Adv. Funct. Mater.* **33**, 2304061(2023).
- [3] A. Gallastegui et al., *Polymer* **280**, 126064 (2023).
- [4] F. Foglia et al., *Nature Communications* **13**, 2809 (2022).
- [5] F. Foglia et al., *Nature Materials* **21** (5) 555 (2022).
- [6] F. Foglia et al., *Sci. Adv.* **6**, eabb6011 (2020).



## Neutroni & scienze della vita

### Cage dynamics revealed by EINS as a key quantities for pharmaceutical stability

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Simone Capaccioli<sup>1</sup>, Daniele Sonaglioni<sup>1</sup>, Alessandro Paciaroni<sup>2</sup>, Andrea Orecchini<sup>2</sup>  
Francesca Natali<sup>3</sup>

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<sup>2</sup> Department of Physics and Geology, University of Perugia, 06123 Perugia, Italy.

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Institut Laue Langevin, 38000 Grenoble, France.

Bioprotectant glassy matrices have been proven to induce a noticeable retardation and reduction of protein molecular movements, thus preventing thermal degradations. Recent studies [1] reported that the slow dynamic properties of levoglucosan (LG) greatly differ from those of glucose (G), a common bioprotectant. The more rigid structure of LG molecule has great impact on the molecular mobility:  $\alpha$ -relaxation becomes very sensitive to temperature and the secondary relaxation, responsible for the mobility in the glassy state, is suppressed. It is noteworthy that, despite its lower T<sub>g</sub>, LG preserves and stabilizes freeze-dried proteins better than usual excipients [2]. To investigate how this reflects in fast (ps) dynamics, we performed elastic and inelastic neutron scattering studies of Lysozyme in G and LG, in dry and hydrated conditions and in an extended T range. The overall scenario confirms recent findings that highlight the role of local dynamics in destabilization [3]: actually LG interaction strongly suppresses the local protein mobility.

Recently, we performed EINS experiments on co-amorphous mixtures of molecular pharmaceutical compounds, including eutectic concentration [4]. Mean square displacements showed a non-trivial trend vs the propensity of the coamorphous solution to recrystallize. Once again, the suppression of fast dynamics appears to control the stability to recrystallization from supercooled or glassy state.

#### References

- [1] K. Kaminski, et al. *J.Phys.Chem.B* **114**, 11272 (2010).
- [2] Y.H. Liao, et al. *Pharm. Res.* **19**, 1854 (2002).
- [3] M.T. Cicerone, C.L. Soles, *Biophys. J.* **86**, 3836 (2004).
- [4] K. Lobmann et al., *Mol. Pharmaceutics* **8**, 1919 (2011).

# **Abstract dei talk**

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## **Nanostructural characterisation of glycosylated protein biomarker interaction with lipid bilayer membranes: basis for biosensor development**

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Beatrice Barletti<sup>1,3</sup>, Nicolò Paracini<sup>1</sup>, Giovanna Fragneto<sup>2</sup>, Donald K. Martin<sup>3</sup>,  
Bruce Cornell<sup>4</sup>, Marco Maccarini<sup>3,5</sup>

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<sup>2</sup>*ESS, Partikelgatan 2, 224 84 Lund, Sweden.*

<sup>3</sup>*TIMC, Rdpt de la Croix de Vie, 38700 La Tronche, France.*

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In cancer's tests, the detection of protein biomarkers is still challenging due to their low abundance and glycosylated state which is believed to favor protein-lipid complexes. The study and understanding of protein-lipid interactions is of great importance, especially to optimise the sensitivity of biosensing techniques to identify protein biomarkers, in particular when present in their glycosylated forms. In the project we investigated at nanostructural level the interaction of glycosylated protein biomarkers with biologically relevant lipid bilayer membranes using neutron and x-ray reflectometry, particularly to identify how different lipids modulate this interaction to build a potential biosensor that is aimed for early detection of scarce biomarkers in blood samples. The glycosylated proteins of interest for the study are soluble vascular-endothelial cadherin (sVE) and alpha-fetoprotein, two clinical biomarkers found in the blood for the detection of vascular abnormalities and liver cancer respectively. Neutron and x-ray reflectometry results, together with QCM-D complementary data, showed significant changes in the lipid bilayer after the injection of glycosylated biomarkers, while smaller changes were reported in presence of non-glycosylated protein, BSA. Thanks to the study and glycosylation chemistry, it was possible to set the basis for the development of a lipid-based protein-biosensor in collaboration with the industrial partner of the project.

## **Determination of the fast and thermal neutron fields inside a shielding mock-up for fusion plants**

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A. Calamida<sup>1a</sup>, L. Russo<sup>2</sup>, M. A. Caballero Pacheco<sup>2</sup>, A. I. Castro Campoy<sup>2</sup>, R. Bedogni<sup>2</sup>,  
D. Flammini<sup>1</sup>, A. Colangeli<sup>1</sup>, G. Pagano<sup>1</sup>, S. Loreti<sup>1</sup> and A. Pietropaolo<sup>1,2</sup>.

<sup>1</sup>ENEA - Nuclear Department, Italy.

<sup>2</sup>Istituto Nazionale di Fisica Nucleare - Frascati National Laboratories, Italy.

A Neutronics benchmark experiment has been carried out at the Frascati Neutron Generator (FNG) in the framework of an EUROFUSION activity. The experiment aimed at assessing the thermal and fast components of the neutron field in selected positions inside an experimental shielding assembly by means of real time measurements. The measurements are very important for the assessment of the shielding effectiveness of the investigated material in a nuclear fusion plant environment. These were made using active detectors: the fast neutrons field was measured exploiting the inelastic  $^{12}\text{C}(n, \alpha) ^9\text{Be}$  ( $Q \cong -5.7$  MeV) and  $^{28}\text{Si}(n, \alpha) ^{25}\text{Mg}$  ( $Q \cong -2.66$  MeV) reactions occurring in a Silicon Carbide solid state detector. The thermal neutron field was measured using the thermal neutron radiative capture in  $^{113}\text{Cd}$  by means of a CZT (Cadmium Zinc Telluride) solid state detector. A comparison between experimental results and simulations is also shown.

## **SANS-driven insights into the self-assembly and optimization of metal-based superlattices**

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Alessandro Cangiano<sup>1,2</sup>, Noemi Gallucci<sup>1,2</sup>, Nathan S. Cowieson<sup>3</sup>, Apostolos Vagias<sup>4</sup>,  
Luigi Paduano<sup>1,2</sup>

<sup>1</sup>*Department of Chemical Sciences, University of Naples Federico II, 80126, Naples, Italy.*

<sup>2</sup>*CSGI, Center for Colloid and Surface Sciences, 50019, Sesto Fiorentino, Italy.*

<sup>3</sup>*Diamond Light Source, Didcot, Oxfordshire, England, United Kingdom.*

<sup>4</sup>*Institut Laue-Langevin, 71 avenue des Martyrs, CS 20156, 38042 Grenoble, France.*

Recently, metal-nanocrystals (M-NCs) attracted significant attention due to their unique optical, electronic, and catalytic properties, making them valuable in various fields and industries.

M-NCs Optimization has focused on manipulating NC shapes and dimensions to enhance surface energy, electronic structure, and environmental interactions.

A novel approach involves creating three-dimensional nanoscale-ordered assemblies, altering the plasmonic band by forming ordered structures like face-centered or hexagonal phases. We analyzed the effects of solvent choice and surface coverage on gold, silver, and platinum NCs' self-assembly, upon functionalization with oleic acid (OA) in water, and optical properties.

Solvent dielectric constants impact the  $R_h$  of nanocrystals, emphasizing the environment's role in aggregation. Optical property analyses showed that oleylamine-nanocrystals exhibit shifts in absorption maxima ( $\lambda_{max}$ ) due to solvent refractive indices, demonstrating the interplay between the environment and nanocrystal behavior. OA-coated NCs assembled into different superlattices depending on the starting solvent and the oleylamine degree of coverage. Moreover, different superlattices display variations in  $\lambda_{max}$  based on spatial organization, underscoring the influence of arrangement on optical properties. Through contrast-variation SANS experiments we investigated the interdigitation of oleylamine within the superlattice shedding light on the oleylamine role in the self-assembly process.

## **Preliminary results on an ongoing study of 28 fragments of equestrian gilded monumental-statuary complexes rediscovered near Parco dei Renai Signa, Firenze, Italy**

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F. Cantini<sup>1,2,3</sup>, F. Grazzi<sup>2,3</sup>, M. Galeotti<sup>4</sup>, S. Porcinai<sup>4</sup>, A. Scherillo<sup>5</sup>, A. Fedrigo<sup>5</sup>, A. Santagostino Barbone<sup>4</sup>, E. Tartaglia<sup>4</sup>, G. Rotondi<sup>4</sup>, A. Patera<sup>4</sup>

<sup>1</sup>*Università di Firenze, Dipartimento di Fisica e Astronomia, Sesto Fiorentino (FI), Italy.*

<sup>2</sup>*Consiglio Nazionale delle Ricerche - Istituto di Fisica Applicata Nello Carrara, Sesto Fiorentino (FI), Italy.*

<sup>3</sup>*Istituto Nazionale di Fisica Nucleare, sezione di Firenze, Italy.*

<sup>4</sup>*Ministero della Cultura, Opificio delle Pietre Dure, Firenze, Italy.*

<sup>5</sup>*UKRI- STFC Science and technology Facilities Council - ISIS Neutron and Muon Source.*

This work reports the results of the study of 28 fragments of bronze sculpture, some of which are gilded, made during the Roman Age. These fragments were found during the 1970s in a deposit near the Renai Park (Signa, Florence, IT). There is therefore no certainty regarding the geographical origin, the archaeological context, and the relative association of the various fragments. Thanks to the 2020 diagnostic and restoration campaign, at the Opificio delle Pietre Dure (OPD, Florence, IT), it was however possible to study these works of art with numerous techniques (ToF-ND, SEM-EDS, XRF, ICP-MS, etc.).

Here, we focus on ToF-ND performed on INES at ISIS Neutron and Muon Sources (Harwell, UK). In addition to preliminary characterizations of the materials, the main diagnostic questions we tried to answer during the work were mainly: 1) the possible relevance of the fragments to one or more groups of statues and 2) understanding the manufacturing process. One of the goals of the entire diagnostic campaign was indeed to understand any associations between the 28 pieces, making use of the autoptic and stylistic study, supported by the analysis on the metal alloy. This case study is an example of how metal alloy characterization and texture analysis in ToF-ND can provide a solid tool for the interpretation and reconstruction of an ancient technological process.

## Cage dynamics revealed by EINS as a key quantities for pharmaceutical stability

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Simone Capaccioli<sup>1</sup>, Daniele Sonaglioni<sup>1</sup>, Alessandro Paciaroni<sup>2</sup>, Andrea Orecchini<sup>2</sup>  
Francesca Natali<sup>3</sup>

<sup>1</sup> Physics Department, University of Pisa, 56127 Pisa, Italy.

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Bioprotectant glassy matrices have been proven to induce a noticeable retardation and reduction of protein molecular movements, thus preventing thermal degradations. Recent studies [1] reported that the slow dynamic properties of levoglucosan (LG) greatly differ from those of glucose (G), a common bioprotectant. The more rigid structure of LG molecule has great impact on the molecular mobility:  $\alpha$ -relaxation becomes very sensitive to temperature and the secondary relaxation, responsible for the mobility in the glassy state, is suppressed. It is noteworthy that, despite its lower T<sub>g</sub>, LG preserves and stabilizes freeze-dried proteins better than usual excipients [2]. To investigate how this reflects in fast (ps) dynamics, we performed elastic and inelastic neutron scattering studies of Lysozyme in G and LG, in dry and hydrated conditions and in an extended T range. The overall scenario confirms recent findings that highlight the role of local dynamics in destabilization [3]: actually LG interaction strongly suppresses the local protein mobility.

Recently, we performed EINS experiments on co-amorphous mixtures of molecular pharmaceutical compounds, including eutectic concentration [4]. Mean square displacements showed a non-trivial trend vs the propensity of the coamorphous solution to recrystallize. Once again, the suppression of fast dynamics appears to control the stability to recrystallization from supercooled or glassy state.

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- [4] K. Lobmann et al., *Mol. Pharmaceutics* **8**, 1919 (2011).

## **Design and physicochemical characterization of liposomes for enhanced intracellular delivery of therapeutics**

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Ilaria De Cristofaro<sup>1</sup>, Noemi Gallucci<sup>1,2</sup>, Alessandro Cangiano<sup>1,2</sup>, Nathan Cowieson<sup>3</sup>,  
Daniele D'Alonzo<sup>1</sup>, Marco Chino<sup>1</sup>, Pompea Giuseppina Grazia Del Vecchio<sup>1</sup>,  
and Luigi Paduano<sup>1,2</sup>

<sup>1</sup>*Department of Chemical Sciences, University Federico II, Naples, Italy.*

<sup>2</sup>*CSGI, Center for Colloid and Surface Science, Sesto Fiorentino, Italy.*

<sup>3</sup>*Diamond Light Source, Didcot, UK.*

With their ability to encapsulate therapeutics and release their content at the desired time, liposomes provide a valuable platform for the treatment of a variety of diseases, including cancer. In this regard, we developed liposomes using POPC, which is the main component of eukaryotic membranes, to improve the biocompatibility of the entire system.<sup>1,2</sup> Liposomes with different compositions have been designed to understand how each lipid (POPC, DOTAP, and cholesterol) affects the physicochemical properties of the system itself. This was done by combining several techniques, such as DSC,  $\zeta$ -potential, DLS, as well as SAS either with X-Rays or neutrons. The issue of specific targeting was also considered. In this regard, using scattering techniques, it was also studied the interaction between liposomes and T7 peptide. This is a targeting peptide, having a high affinity towards the human transferrin receptor, overexpressed on glioblastoma cells.<sup>3</sup>

The results obtained revealed that the composition does not affect liposomes size. On the contrary, it affects the charge, as well as the lipid transition temperature. Moreover, SAS analysis suggests that the interaction between liposomes and T7 peptide takes place, and it is probably driven by a charge redistribution on liposomes surface.

### **References**

- [1] R. Tenchov et al., ACS Nano **15**, 16982 (2021).
- [2] Y. Wu et al., Mol Ther Nucleic Acids **27**, 956 (2022).
- [3] L. Tanget al., Acta Biomaterialia, **155**, 521 (2023).



## Neutrons: powering the future of green energy

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Fabrizia Foglia

*Department of Chemistry, University College London,  
Christopher Ingold Building, 20 Gordon Street, London, WC1H 0AJ, UK*

Despite the widespread use (e.g. in healthcare, energy and water treatment applications) and the continued development of new materials and solutions for their implementation in advanced devices, improving membrane performance and durability remains a non-trivial problem. In large part this is due to the lack of a detailed understanding of the dynamics of the permeant confined within the membrane structures, that are typically multi-scale in terms of correlation lengths and relaxation timescales for the different processes involved. It is therefore difficult to disentangle individual contributions to the various motions and their involvement in the membrane structure-dynamics correlation, especially in situ and under operando conditions.

Neutron scattering is ideal for this type of study because it allows a unique view of structures of soft condensed matter systems. The nature of neutron-matter interaction provides a non-destructive approach, making it a perfect tool to investigate structurally delicate membrane structure-dynamics properties as well as biological systems. Cold neutrons, with wavelengths of a few Å and energies from  $\mu\text{eV}$  to several meV, allow investigations and correlations of structure on the Å- to nano-scale combined with molecular motions on a nano- to pico-second time regimes. Furthermore, because of the difference in neutron scattering cross section between H and D, isotopic contrast experiments can be used to highlight different spatial/dynamic regions under varied chemical and physical conditions.

Here we present our journey using advanced neutron scattering techniques to shed light on the structure-dynamical interplay, while developing a new understanding by correlating energy, time and space to resolve structure to function interplay. We apply this approach not only to guide the design of new materials with improved performance characteristics but also to enhance our understanding and improve the recyclability of materials.

### References

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- [3] A. Gallastegui et al., *Polymer* **280**, 126064 (2023).
- [4] F. Foglia et al., *Nature Communications* **13**, 2809 (2022).
- [5] F. Foglia et al., *Nature Materials* **21** (5) 555 (2022).
- [6] F. Foglia et al., *Sci. Adv.* **6**, eabb6011 (2020).

## **CeO<sub>2</sub> nanoparticles coated with a dopamine-derivatized molecule: the role of surface functionalization on the structural organization**

Noemi Gallucci<sup>1,2</sup>, Alessandro Cangiano<sup>1,2</sup>, Massimo Melchiorre<sup>1</sup>, Francesco Ruffo<sup>1</sup>,  
Giuseppe Vitiello<sup>2,3</sup>, Luigi Paduano<sup>1,2</sup>

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Production Engineering, Naples, Italy.

Cerium oxide nanoparticles (CeO<sub>2</sub> NPs) are widely used for many technological applications.<sup>1,2</sup> Recently, they have attracted great interest in the biomedical field, as anti-cancer, antioxidant, and antibacterial agent, due to their red-ox properties, which can be opportunely modulated to inhibit (antioxidant) or promote (pro-oxidant) oxidation processes. To exploit the anti- or pro-oxidant properties of CeO<sub>2</sub> NPs it is crucial to obtain single functionalized NPs stable in water. To obtain them, it is necessary to modulate the ratio of CeO<sub>2</sub> NPs coated with the first organic layer, used during the synthesis, with the functionalized molecule.

Based on these, we have prepared very small CeO<sub>2</sub> NPs (core radius ~2.5 nm), with a high colloidal stability, and antioxidant properties.<sup>3,4</sup> These NPs have been functionalized by exchanging ligands, replacing the organic layer used in the synthesis phase (oleylamine) with a synthetic bifunctional molecule (derivatized-dopamine). The chemical structure of this molecule is characterized by a double functional group, one able to interact with the surface of NPs and replace oleylamine, the other able to disperse them in water and at the same time being suitable for further functionalization. For example, functionalizing with a fluorophore the CeO<sub>2</sub> NPs coated with the derivatized-dopamine can obtain a multi-functional system, in which the fluorophore allows us to localize the NPs and the CeO<sub>2</sub> acts as an anti-tumor agent. However, optimizing the coverage of NPs with functionalizing molecules is essential. SANS measurements were conducted to determine the optimal CeO<sub>2</sub> to derivatized-dopamine ratio for biomedical applications. Using the contrast-match technique, we evaluated the organic coating and the relative ratio between oleylamine and the derivatized-dopamine.

### **References**

- [1] T. Montini et al., Chem Rev. **116**, 5987-6041 (2016).
- [2] N. Gallucci et al., J. Environ. Chem. Eng. **10**, 107866 (2022).
- [3] N. Gallucci et al., Nanomaterials **11**, 542 (2021).
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## **Non-invasive characterization of ancient bronzes and of their manufacturing techniques through neutron advanced techniques: an overview and a peculiar case studio from ancient Japan**

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The technology of solid bronze casting is one of the most ancient systems in history for the creation of specifically shaped metal artefacts, which can be used to produce specific tools or wonderful piece of art. Discriminating which casting method was used can be critical for understanding the technological process and reconstructing its historical context.

Those artefacts often are heavily corroded or artificially patinated and direct investigation of sound metal is difficult unless severe sampling is applied. Neutron techniques offer the possibility to characterize the metal applying a non-invasive approach, allowing to obtain morphological, microstructural, and compositional details by exploiting a combination of neutron diffraction and imaging methods.

An overview of the neutron methods and their application to bronze artefacts will be presented.

I will also present the preliminary results of the neutron analysis performed on a large set of bronze arrowheads from archeological burial mounds of Okayama prefecture in Japan (Kofun and Yayoi periods), in the frame of a collaboration project between CNR, INFN, Università di Torino and Okayama University.

All results aim to identify the particular casting methods and distinguish the possible evolution of technology through time, revealing new details about bronze casting during the period of state formation in Japan.

## Link between permanent shear-banding and local concentration fluctuations in suspensions of compressible microgels

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We uncover the occurrence of shear banding in dense suspensions of compressible microgels by combining velocimetry, rheology and small angle neutron scattering under shear [1,2]. Velocimetry measurements evidence the presence of permanent but unsteady shear-banding for sufficiently small Peclet numbers, with the formation of a plug-like flow in the central region of the gap of the concentric cylinder geometry. Small-angle neutron scattering experiments under shear link the observed banding phenomenon to structural variations along the velocity gradient, providing a connection between the formation of the arrested band and the increase of structural correlations, determined through the integral of excess scattering under shear. The structural variations can be directly associated to changes in the local packing fraction through transmission measurements. These results provide unique evidence of a shear-concentration coupling mechanism in jammed systems of compressible particles. Additionally, our study opens the route to investigate the effects of particle compressibility on shear-concentration coupling in a variety of dispersions of soft colloids, with important consequences in applications related to the flow and processing of dense suspensions.

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## Small Angle Neutron Scattering investigation of ageing in CuCrZr alloy for fusion reactor technology

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In the framework of the EUROfusion Programme, small-scale W/CuCrZr monoblocks are being investigated through different experimental techniques as prototypes of the *divertor*, the large plasma-facing component designed to contain plasma instabilities and disruptions [1]. Their reliability in service under cyclic and intense thermal loads, can be efficiently assessed through experimental microstructural characterization. Understanding the influence of microstructures or precipitates on the material elastic properties is of great interest for the application of metallic materials in many industrial fields. Providing new insights into microstructural changes produced in the CuCrZr alloy by thermal treatments is therefore imperative to assess the resistance of such cooling pipes [3].

Information on the microstructural changes and precipitate formation in similar alloys can be obtained through Small-angle Neutron Scattering (SANS), thus providing useful tools for investigating metallurgical problems of interest for nuclear applications [4]. SANS technique has been recently exploited to investigate the occurrence of Cr-rich precipitates in CuCrZr alloy samples submitted to thermal treatments. In particular, precipitate formation was observed after ageing at 580°C, where the SANS cross-section suggests the occurrence of a new population of small precipitates. This demonstrated the potential of efficiently using SANS to resolve the state of CuCrZr precipitates in fusion reactor divertor components.

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## **A multipurpose compact neutron generator for applications in nuclear medicine and nuclear forensics**

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Compact neutron generators can provide a high flux of neutrons with energies ranging from thermal (0,025 eV) to 14 MeV. The application of the D-D, D-<sup>10</sup>B, and D-<sup>7</sup>Li nuclear reactions and new advancements in high-flux neutron generator technology along with the commercial availability of high-voltage direct current power supplies enables the production of high-flux 2,45 MeV, 6 MeV, 10 MeV, and 13 MeV neutrons. The high-energy neutrons or the moderated epithermal neutrons from the new compact neutron generator can greatly advance cancer therapy, radioisotope production, neutron yield measurement, special nuclear materials detection, and neutron transmutation doping of silicon. This work is focused on application for cancer therapy and special nuclear materials detection. The first two prototype of a longitudinal compact neutron generators, designed for neutron intraoperative radiotherapy (nIORT) are going to be installed at ENEA Research Centre in Brasimone, in the frame of the LINC-ER project.

## **Update on the SORGENTINA Project**

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Antonino Pietropaolo

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The SORGENTINA project aims at developing a 250 kW power 14 MeV neutron source. The main focus is the production of medical radioisotopes, especially  $^{99}\text{Mo}$  as precursor of  $^{99\text{m}}\text{Tc}$ , a radiotracer widely used in Single Photon Emission Computed Tomography.

The neutrons made available at the plant can also be used for different applications, ranging from irradiation of materials and electronics as well as for investigations on materials thanks to the presence of a moderated neutron field.

The project entered in its final year. This contribution aims at presenting the status of the implementation of the two main components of the facility:

- 1 the rotating target;
- 2 the ion accelerator.

The experimental campaign on the rotating target is close to be approached and, possibly, preliminary experimental results might be presented.

The ion source is going to be tested at 50 kW before full test commissioning within the end of the year. The results of the test will be presented.

## **Structural and dynamical properties of PS-PNIPAM block copolymer micelles in concentrated samples**

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Concentrated solutions and gels of block copolymer micelles demonstrate both the cohesive strength of solids and the diffusive transport characteristics of liquids, and are subject of theoretical and technological interest. Special attention is devoted to polymers containing a stimuli-responsive "switching" block that imparts the system the ability to undergo reversible changes in response to variation of external control parameters. Among them, poly-N-isopropyl acrylamide (PNIPAM) is attractive due to thermoresponsive behaviour, with a lower critical solution temperature (LCST) in water close to physiological range (LCST  $\approx$  32°C). Current applications of PNIPAM-based block copolymer micelles include targeted drug carriers, engineered tissues, and "switching" membranes. We recently synthesised block copolymers containing thermoresponsive PNIPAM and hydrophobic polystyrene (PS) blocks. In diluted aqueous solution, PS-PNIPAM diblock and PS-PNIPAM-PS triblocks form respectively starlike and flower-like micelles. In the latter case, both the PS end blocks are sticking in the same micellar core as the PNIPAM block folds in a loop. However, such a configuration is entropically unfavourable and one of the two PS blocks might stick out of the original core, eventually forming a network of interconnected micelles at high concentration. The existence of bridges is thought responsible for the formation of physical gels in concentrated PS-PNIPAM-PS samples, although the relative contribution of loops and bridges is debated, as well as the influence of structural parameters such as block length and composition. Moreover, there are surprisingly few studies on the dynamical properties on such microscopic scales. Connecting mechanical stability to local mobility is important e.g. to quantify transport properties within the gel. Here we use rheology to investigate the mechanical properties of concentrated PS-PNIPAM diblock and PS-PNIPAM-PS triblock copolymers in water, and we connect them to structural and dynamical information on the microscopic level, obtained by combining small-angle neutron scattering with neutron spin echo and neutron backscattering spectroscopy.



## **Application of neutron science in the study of ancient Iranian weaponry**

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Neutron techniques such as neutron diffraction and neutron tomography allow for non-invasive analysis of complex metal artefacts, providing information about their internal structure, conservation status and, via Neutron Resonance Capture Analysis, elemental composition. In this talk we discuss the application of neutron science at ISIS Neutron and Muon Source to the study of Iranian swords from the Iron Age (1250-550 BC). The objects were recovered by the Border Force after being seized on entry to the UK and will be repatriated to Iran, providing an opportunity to investigate both ancient manufacture and modern modifications. Neutron tomography allowed us to discover remnants of iron tangs preserved inside bronze hilts, while neutron diffraction provided information on the crystalline phases present in these metals without sampling. Similarly, iron swords were analysed with neutron diffraction to examine the crystalline phases of iron and estimate carbon content. The non-invasive nature of this technique allows for analysis of many spots throughout the object, which would not be possible if sampling was required. The results provide information about Iron Age metallurgy in northwestern Iran and together form a comprehensive picture of both assembly methods and phase/elemental composition, allowing us to understand better the technological choices of ancient metalworkers.

## **Study of the effects of chronic neutron exposure on plants for agrospace-related activities**

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The exposure of biological organisms to cosmic rays during future space missions to the Moon and Mars is a well-known problem. Primary cosmic radiation produces, in the presence of targets of different types, swarms of secondary radiation including neutrons. The presence of plants on future space missions will have a dual purpose, the production of fresh food (through microgreen growth) for the astronauts and the production of oxygen.

At the ENEA-NUC-INMRI neutron laboratory at Cr-Casaccia contains a room in which several shielded neutron sources are stored, some of which have energy spectra partly similar to those of cosmic neutrons, it is possible to irradiate samples under neutron flow for long periods (from a few weeks to several months). Irradiations were carried out on plant samples with neutron fluxes that reproduce similar environmental equivalent dose rates that should be found in space travel and on the surfaces of the Moon and Mars.

After exposure of the plant samples to neutrons, the effects on germination and seedling growth were evaluated by morphological, flow cytometric and metabolomic analyses. Some results will be presented.

## The ENEA TRIGA RC-1 neutron source: from activation analyses to radioisotopes production

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The TRIGA RC-1 research reactor is 1 MW thermal power neutron source located at the ENEA Casaccia Research Centre (RM). Pool-type design, its core is at the bottom of a cylindrical tank filled with 7 meters of water [1].

The reactor embraces those areas of applied research where an intense thermal neutrons source is required. Several irradiation channels are installed in the pool (Central Thimble, Rotary Rack and Rabbit system) with higher neutron fluxes but limited volumes; some other (horizontal extraction lines) are targeted for out-of-core experiences with larger spaces for experimental devices but less intense neutron fluxes. Spectral characterization of neutron fluxes is performed by different methods according to the required target objectives.

One of the main applications of TRIGA RC-1 is the Neutron Activation Analysis: a non-radioactive material is exposed to neutrons to generate radioactive nuclei. Such radionuclides are characterized to study the irradiated sample, e.g. analytical determination of elemental traces concentration [2].

With the same concept, it is possible to produce radioactive sources for nuclear medicine or industry also. With this focus in mind the TRIGA RC-1 team joined the EU funded SECURE Project. The ENEA investigation focused on the possibility to produce  $^{161}\text{Tb}$  by neutron activation of gadolinium target (highly enriched in  $^{160}\text{Gd}$ ) [3,4]. After appropriate chemical processes,  $^{161}\text{Tb}$  (precursor of the radiopharmaceuticals for cancer therapy) and  $^{160}\text{Gd}$  oxide (to start new cycles) are extracted. As to study the production capabilities of the TRIGA RC-1, simulations are performed by MCNP and FISPACT-II codes, along with irradiation experiments for validation.

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## **Neutrons for painting conservation: addressing varnish blanching through scattering techniques and optical methods**

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Varnish blanching poses a significant challenge in paintings conservation, altering their appearance over time. It occurs when paintings are kept in high-humidity environments or exposed to water. The moisture penetrates and modifies the structure of pre-existing nanoscopic pores in the polymeric varnish. Thus, the pores grow to a size that scatters visible light, causing the varnish to opacify. This study aims to deepen the knowledge of this degradation process by relating the alterations in the polymer structure with the optical changes.

Our approach combines small-angle neutron scattering (SANS) and optical coherence tomography (OCT) to get complementary information of the structure and optical properties of the varnish. In this preliminary study, mastic varnish mock-ups are applied directly onto silicon wafers. The progress of the degradation is monitored through dynamic measurements using SANS and OCT on samples immersed in D<sub>2</sub>O and H<sub>2</sub>O, respectively.

One finding is the observation of two distinct processes occurring on two different time scales: a visible but reversible process happens within the first 30 hours after immersion, while irreversible blanching is noticed after 3 days of soaking. The methods also allow us to monitor the size changes of the nanoscopic pores, and the swelling of the varnish layer on the two timescales. This research aims to provide valuable knowledge of the blanching process to develop conservation strategies for protecting our cultural heritage.

# **Abstract dei poster**

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## **SANS characterization of nanocomposites based on polymer containing Inorganic nanoparticles**

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The nanocomposites based on polymer containing inorganic nanoparticles are a kind of composite materials comprising of nanometer-sized inorganic nanoparticles (1-100 nm), which are uniformly dispersed in fixed polymer matrix. The incorporation of structured nanomaterials with specific physical properties in the gel matrix allows this type of material to have multifunctionality. Our work focused on two systems based on: Hydroxypropylcellulose (HPC) with zinc oxide NPs, and Chitosan (Ch) with silver NPs. Firstly, composite based on HPC/ZnO, HPC is water-soluble cellulose derivative forming hydrogel that shows excellent biocompatibility and biodegradability. It has been chemically cross-linked with sodium triphosphate (STP) as cross linker and obtained microgel of  $R_h 560 \pm 20 \text{ nm}$  while it does not show any optical properties. The ZnO NPs having good optical properties, have been introduced with varying w/w ratios to the gel matrix. Through dynamic light scattering (DLS), the 0.025% weight ratio of nanoparticles was found the best (stable for long time) and it has  $R_h 410 \pm 40 \text{ nm}$  lower than microgel due possible contraction of HPC free chains when ZnO NPs surrounds them and/or somehow electrostatic/van der Waals interaction between -OR (R=CH<sub>2</sub>CH(OH)CH<sub>3</sub>) group of HPC and ZnO NPs. In the absorption spectra we see a clear peak at 350nm indicates the presence of ZnO NPs in the gel matrix. Then Fluorescence over the range of 20-60°C was performed to check their temperature behavior and decrease in intensity was observed due to nanoparticles motion and gel cluster formation. Secondly composite based on Ch/Ag NPs, chitosan is a promising material for wound healing and silver nanoparticles (AgNPs), having attractive biological activities (anti-bacterial, antioxidant etc.) synthesized together by reduction of silver nitrate (AgNO<sub>3</sub>). Through Dynamic Light Scattering (DLS), we observed formation of a formation monodisperse system having  $R_h 1100 \pm 120 \text{ nm}$  and UV spectra show a sharp peak at 427nm confirm the presence of Ag nanoparticles inside microgel. SANS measurements were carried out to get more details information about the structure of system. The preliminary results suggest the interaction of nanoparticles with the polymer chains, this plays a crucial effect in ruling the structural organization of nanocomposites.

## ***Determination of the multiple scattering contribution in inelastic neutron scattering: the case of disordered materials***

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Thermal neutron scattering is a powerful technique for investigating the atomic structure and dynamics of matter. In particular, inelastic scattering experiments provide valuable insights into atomic dynamics by probing the system space- and time-dependent density correlations. Background subtraction and data reduction are crucial points for extracting meaningful information from experimental measurements. Here, multiple scattering draws up the most challenging correction, yet is dominant, especially in disordered systems where the aim is to map the entire scattering function. This poster presents the theoretical framework, as well as the practical implementation, for applying Monte Carlo methods to quantify the contributions of multiple versus single scattering, using the case of scattering from a d-Benzene cylinder as an example.

The simulation involves modelling the incident beam as a spatially homogeneous set of  $N$  neutrons, each travelling perpendicularly to the sample until they reach a random scattering position. The relevant probability density function for this process is governed by the Lambert-Beer law. Single scattering intensity is determined by calculating the probability of detecting a scattering event at a given angle and energy shift, that is the double differential cross-section, which is related to the system's dynamic structure factor  $S(Q,E)$ . Differently, to model a double scattering event we extract an initial scattering direction and energy shift from the  $S(Q,E)$  probability density function. A second scattering position within the sample is then randomly selected, and the final double scattering intensity is calculated as in the single scattering scenario.

We implement the simulation in Python. It needs few computational resources and exhibits running times of about a few seconds per point in the  $Q$ - $E$  space.

## **Thermal Neutron Energy Determination with Multilayer Detection**

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Thermal neutrons are detected by nuclear interactions, in which their energy information is lost. This project, following on from a proof of concept and a statistical investigation of using the cross section variation of the interaction with energy to extract the neutron energy, will use this in conjunction with AI/machine learning to produce a workable algorithm to determine the neutron energy and the limitations of the technique with multilayer detectors. This builds on a proof of concept and statistical investigation of using the cross-section variation of the interaction with energy to extract the neutron energy. A unique chance to take use of this option is provided by the innovative multi-layer <sup>10</sup>B thin film detector technology, which uses the different neutron penetration depths to retrieve energy information. Additionally, the experimental implementation and verification of this will be examined. The result is an algorithm to calculate the energy of thermal neutrons in a realisable detector. The goal is to create a machine learning model to validate and optimize the results of a basic model for neutron absorption derived from simulations using Geant4 and Ncrystal toolkit. The input parameters – that is, the inelastic neutron scattering cross section – will be the crucial choice for the model. The purpose of this work (just starting) is to apply the conceptually proven results to the real-world applications and useful algorithms as a possible supplementary tool for neutron scattering beyond time-of-flight measurements.



## **Neutron imaging investigation of stainless steel scaffolds for biomedical applications**

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The use of neutron tomographic imaging is emerging as a promise method to study bone - metal implant interface at medium-high resolution, in terms of material density and distribution. In this experimental work, neutron tomography was extended to the investigation of cellularized scaffolds for bone tissue engineering. 316L stainless steel scaffolds were produced with a graded lattice geometry by Laser Power Bed Fusion (L-PBF) designed by reducing of approximately 50% in size a previously validated dense-out (DO) geometry. Reduced scaffold with DO geometry (rDO) were analyzed after immersion in two different cell culture media, such as Dulbecco's Modified Eagle Medium (DMEM) and DMEM + b-glycerophosphate + ascorbic acid, for 7 days. Scaffolds in both the culture soils were also charged with human MG-63 human osteosarcoma cells, in order to evaluate the development of extracellular matrix after 7 days of culture. The aim of the study is to design a LPBF bone scaffold with enhanced graded lattice geometry, crucial for optimizing tissue regeneration strategies. Additionally, the study aims to characterize the in vitro performances of rDO scaffolds, to evaluate the development of ECM produced by MG-63 cells after 7 days of culture. Neutron tomography analysis allows identifying rDO scaffold in DMEM with MG-63 cells as the environment with the highest amount of organic compound.

## **Mimicking the interface between mammalian plasma membrane and extracellular matrix: chondroitin sulfate-decorated supported lipid bilayers**

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Many vital processes, such as the interaction with pathogens or drugs, take place at the interface between the plasma membrane (PM) and the extracellular-matrix (ECM). The zwitterionic phosphatidylcholine (PC) and the negatively charged phosphatidylserine (PS) are among the most abundant lipids in the PM. The ECM is made of flexible carbohydrates and proteins and is responsible for the cell organisation within tissues. Chondroitin sulphates (CSs) are present in the ECM of animal cells and are composed of a disaccharide unit (i.e. glucuronic acid and galactosamine), which can be sulfonated at different positions. Mono-sulfonation at position 4 or 6 is the most common, resulting in CS-A and CS-C species, respectively. Typically, CS-A is the most abundant form in human cells, however CS-C is overexpressed in cancer cells. There is few information on the structural arrangement of CS molecules onto the PM surface and how this is affected by the status of the cell, e.g. healthy cells vs cancer cells vs inflammation response. This project is aimed at developing supported lipid bilayers (SLB) functionalised with CS molecules to investigate the impact of the bilayer lipid composition on the structural arrangement of CS. To produce said bilayers, we optimised a recently reported protocol, which consists in adding a modified phospholipid that bears an ammino group exposed to the bulk solvent (18:1 Dodecanylamine PE, DOPE-NH<sub>2</sub>) to the SLB to form an amide bond with CS-C. We investigated the CS-SLBs interaction for SLBs composed of either pure PC lipids or a mixture of PC and the negatively charged PS. These systems let us investigate the response of the CS layer structure to the exposure of PS lipids on the PM surface, which occurs in case of inflammation. The produced samples were characterized with quartz crystal microbalance with dissipation monitoring (QCM-D) and neutron reflectometry (NR).

## **Integrating Plasma-Based Techniques in the Production of PEM Electrocatalysts**

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Hydrogen, produced by electrolysis, is considered a clean fuel alternative, essential for achieving decarbonisation targets in various sectors. Among the different types of electrolyzers, Proton Exchange Membrane (PEM) electrolyzers stand out for their efficiency, solidity, higher purity hydrogen production and better integration with variable renewable energy sources. In this regard, plasma-based physical (PVD) and chemical vapor deposition techniques (such as plasma enhanced chemical vapor deposition and atomic layer deposition techniques, PE-CVD and PE-ALD, respectively), can serve as suitable tools for the development of innovative, functional and nanostructured electro-catalyst materials. In particular, these techniques allow precise control of the synthetic parameters and exclude the use of solvents or other harmful chemical reagents, making them green and industrially scalable processes. The core of a PEM electrolyzer is the membrane electrode assembly (MEA), that houses the electrode materials. One of the advantages of PVD and CVD techniques is the suitability in manufacturing the MEA by directly depositing (or decorating) the catalyst material on the solid polymeric electrolyte, as well as over powdered substrate, suitable for the production of catalytic ink. Our work shows the implementation of plasma-based techniques in the development process of MEA (consisting of the synthesis and the characterization of electrode materials), for oxygen and hydrogen evolution reactions through PEM electrolyzer technique.

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