XXXII Congresso Annuale
SISN
7-8 Ottobre 2021

Programma definitivo

Giovedì 7 Ottobre 2021

14:30 - *Apertura della sessione Zoom: https://us02web.zoom.us/j/84127131569?pwd=aTJPU2FkQVN1Y2x0SlNueEtUejh1UT09*

14:35 - *Benvenuto e Saluti*

14:40 - 15:00 ***Leonardo Del Rosso*** (*invited*)
"The phase 2 of the VESPA project: design and construction challenges"

15:00 - 15:20 ***Andrea Orecchini*** (*invited*)
"An update on the T-REX project for ESS"

15:30 - *Assemblea dei soci SISN*

18:00 - *Conclusione dei lavori della giornata*

Venerdì 8 Ottobre 2021

14:00 - *Apertura della sessione Zoom: https://us02web.zoom.us/j/85847360452?pwd=Z0pIR3FxRWJQSGxpTmhIcU9PV2JLdz09*

14:10 - *Sessione scientifica "Patrick Zaki" - PhD students*

14:10-14:20 ***Francesco Cantini,* Università degli Studi di Firenze**
"Alloys characterization and technological interpretation of the manufacturing process of the Vittoria Alata di Brescia by means of neutron techniques".

14:20-14:30 ***Domenico Cavasso,* Università degli Studi di Napoli Federico II**
"Effect of mixed solvent and temperature on the phase behavior of hydroxypropyl cellulose in the presence of SDS".

14:30-14:40 ***Arianna D'Angelo,* Laboratoire de Physique des Solides di Orsay**
"Order-disorder transition in geo-inspired nanotubes".

14:40-14:50 ***Noemi Gallucci,* Università degli Studi di Napoli Federico II**
"Hierarchical structuring of cerium oxide nanoparticles driven by amphiphilic coating".

14:50-15:00 ***Pallavi Kumari,* Università degli Studi Roma Tre**
"Stiffening effect of an ionic liquid on the bending modulus of a model lipid nanoparticle".

15:00-15:10 ***Valeria Libera,* Università degli Studi di Perugia**
"Porphyrin binding and irradiation promote G-quadruplex DNA dimeric structure".

15:10-15:20 ***Valentina Lorusso,* Università degli Studi di Parma**
"A Neutron Reflection study of nanoparticle-surfactants layers".

15:20-15:30 ***Giulia Marcucci,* Università degli Studi di Milano Bicocca**
"Implementation of a neutron imaging technique for elemental characterization of inhomogeneous samples".
15:30-15:40 ***Oriol Sans Planell,* Università degli Studi di Torino**
"Design and test of a novel compact thermal neutron collimator".
15:40-15:50 ***AndreasSantamaria,* Institut Laue-Langevin (ILL) di Grenoble**
"Structure and function investigation on membrane-binding proteins: a Neutron Reflectometry study".

15:50-16:20 *Coffee break*

16:30 - *Sessione scientifica – Post Doc*

16:30-16:40 ***Alessandro Calamida,* Istituto di Fisica Nucleare - Laboratori Nazionali di Frascati**
"Moderation of neutrons using monochromatic neutron sources: a comparison using fusion and spallation neutrons".
16:40-16:50 ***Michael Di Gioacchino,* Università degli Studi Roma Tre**
"Two is better than one".
16:50-17:00 ***Umbertoluca Ranieri,* Università di Roma La Sapienza**
"Self-dynamics of supercritical methane at high pressure".
17:00-17:10 ***Benedetta Petra Rosi,* Università degli Studi di Perugia**
"Cosolvent-induced effects on the protein-like dynamical transition of PNIPAM: a neutron scattering study".
17:10-17:20 ***Eleonora Vottero,* Università degli Studi di Torino**
"H_2 induced reconstruction phenomena in a Pt/Al_2O_3 catalyst: an INS spectroscopy and DFT study".
17:30-17:20 ***Dario Moricciani,*** *I*stituto N**azionale di Fisica Nucleare - LNF di Frascati** (*invited*)
"Progress towards a Bell-type polarization experiment with thermal neutrons".

18:00 - *Conclusione del XXXII Congresso della Società Italiana di Spettroscopia Neutronica*
Si procederà con l'assegnazione dei riconoscimenti alle due migliori presentazioni scientifiche:

- **Premio "Elisa Barzagli"** per la migliore comunicazione categoria *PhD student*
- **Premio "Marco Zoppi"** per la migliore comunicazione categoria *Post Doc*

Ciascuna presentazione dovrà prevedere una **durata massima di 10 minuti** (8' + 2' per domande).

Le ***slides*** dovranno essere preferibilmente in **lingua inglese**, mentre la **presentazione** potrà essere proposta in lingua **italiana** o, eventualmente, in lingua **inglese**.

The phase 2 of the VESPA project: design and construction challenges

Leonardo del Rosso[1], Daniele Colognesi[1]

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Among the 16 neutron beam instruments making up the starting suite of the new European Spallation Source (ESS), VESPA is the only instrument fully dedicated to neutron vibrational spectroscopy (NVS). VESPA will efficiently exploit the long pulse produced by the ESS source by means of the wavelength frame multiplication principle, measuring in one single ESS pulse the full spectrum in a broad energy-transfer band (0-500 meV) and with a relative energy resolution up to 1% in the energy range of the so-called “fingerprint region” (i.e., 60÷220 meV). Here we show an update concerning the status of the project, that is currently in the Phase 2 (i.e., detailed design). We present the progress to date of the design work and the construction strategy for some of the sub-systems of the VESPA beamline, that is expected to produce the first scientific results at the beginning of the 2026.

An update on the T-REX project for ESS

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T-REX is a bi-spectral direct-geometry time-of-flight spectrometer for the European Spallation Source.

Thanks to the long ESS pulse and the use of both cold and thermal moderators, the instrument will explore a wide dynamic range, extending from 0.020 to 140 meV in exchanged energy and from 0.01 to 17 ≈-1 in wavevector transfer. By tuning the choppers frequencies, the elastic energy resolution (FWHM) can be freely adjusted from 1% to 3% at 3meV incident energy, and from 4% to 6% at 100meV incident energy. Simulation benchmarks against existing state-of-the-art neutron ToF spectrometers predict gain factors between one and two orders of magnitude for T-REX.

T-REX will implement polarization analysis as a standard tool, which will enable the separation of magnetic and nuclear scattering, the analysis of polarization and eigenvectors of magnetic excitations, and the separation of coherent and spin-incoherent scattering in organic and biological samples.

T-REX has recently entered the ESS Phase 2, that consists in the development of the detailed engineering design and in the actual production of the corresponding components.

Alloys Characterization and Technological Interpretation of the Manufacturing Process of the Vittoria Alata di Brescia by means of Neutron Techniques

F. Cantini[1,2,3,4] *, F. Grazzi[2,3], A. Scherillo[5], A. Fedrigo[5], A. Brini[4], M. Galeotti[4]

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The "Vittoria Alata" (Winged Victory) of Brescia, dated around the 1st Century AD, is one of the most important Roman bronzes rediscovered in Italy, and has recently undergone a restoration coordinated by the Opificio delle Pietre Dure di Firenze (OPD) [1]. This major restoration campaign offered a unique opportunity for a thorough study of the statue. In this work, results of the study of the metal alloy are shown, obtained by both neutron techniques and SEM-EDS analysis. ToF-Neutron Diffraction and Neutron Imaging measurements are performed at the ISIS neutron spallation source (Didcot, UK) [2]; SEM-EDS analysis were carried out at the OPD Scientific Laboratory (Florence, IT). Given the neutrons deep penetrability into the matter and their high sensitivity with respect to the elements, they are eligible as a promising probe to investigate metal artefacts in the field of cultural heritage, allowing to analyse even geometrically complex artwork, in a totally non-invasive way. Time of Flight Neutron Diffraction allows to measure selected areas of the samples - ranging in size from a few mm to a few cm - and to quantitatively determine the concentration of the crystalline phases in the investigated volume regardless the sample corrosion. Furthermore, by studying the shape and relative intensity of the diffraction peaks in the metal phases, it is possible to obtain indirectly information on the grain size, on the presence and density of flaw and internal stress and on the cold working methods or on the direction of solidification [3]. Alongside the investigations carried out by ToF-ND, the Neutron Resonance Capture Analysis (NRCA) - also available on ISIS facility - was performed, providing a semi-quantitative analysis of the elements present in the volume of the samples investigated [4].

A detached feather of the right wing of the statue was also investigated through neutron radiography allowing to highlight some morphological characteristics and to map the conservation state of the artefact. The mineralized phases are characterized by light elements often associated with the presence of hydrogen which, due to its strong interaction with neutrons, appears dark or black in the neutron radiography, strongly highlighted in comparison with the lighter tones of the metallic phase [5]. Although limited to the analysis of a single stratigraphic plane of the sample, the SEM-EDS analysis can provide valuable information about the morphology and microstructure of the metal alloy, and also allowed to clearly understand the stratigraphy of mineralization patinas. An elemental quantitative analysis can also be carried out even if intergranular corrosion and decuprification phenomena can affect the reliability of the result [6].

This study, performed both on small samples taken from the various parts of the statue, and on macro-fragments already detached from the artefact, allowed to characterize the composition of the alloy and also provided relevant clues relating to the manufacturing methods. Moreover, thanks to the comparison of these complementary techniques it was possible to highlight the strengths of the employed methods in the analysis of a work of art as complex as an archaeological bronze.

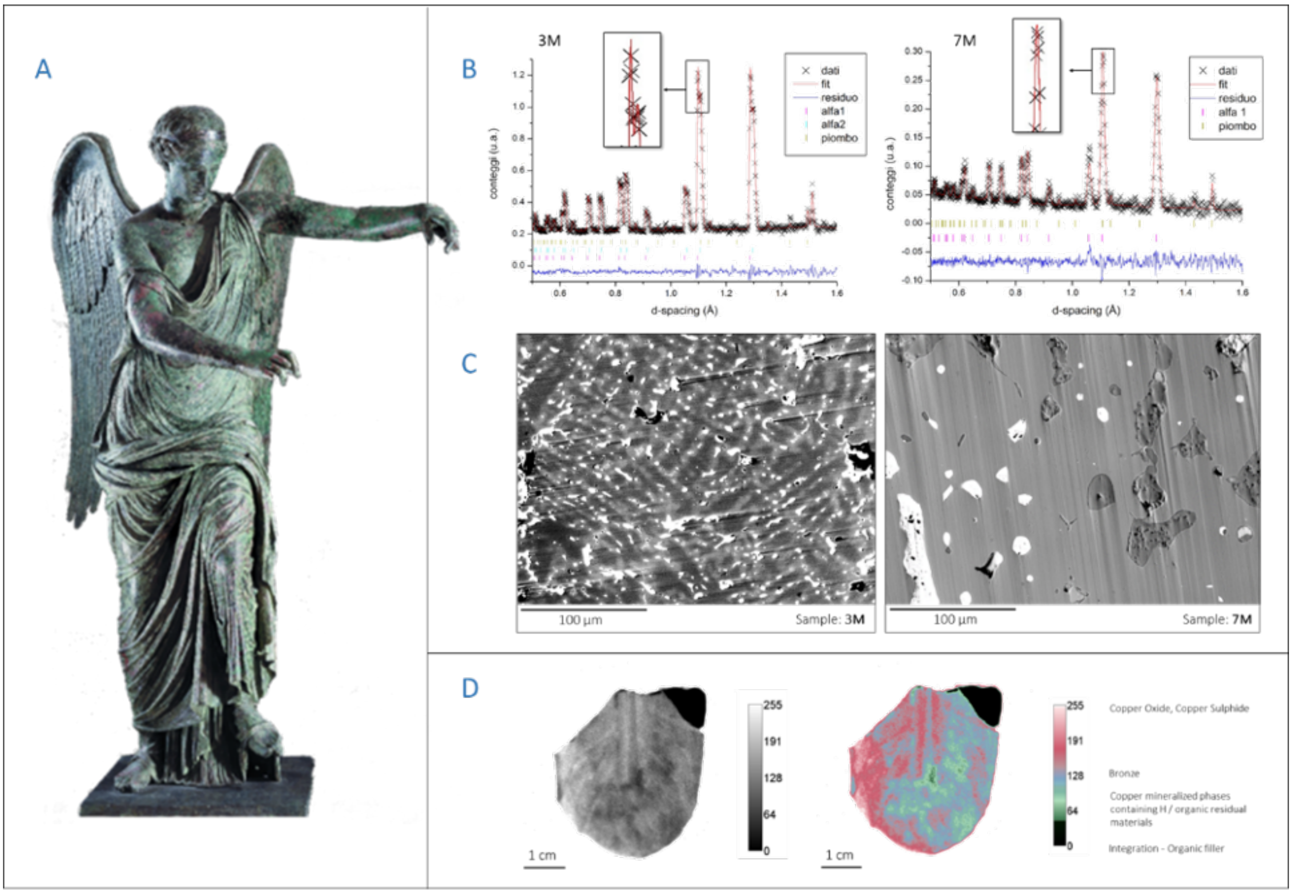

Figure 1 **A)** The “Vittoria Alata di Brescia” before the last restoration. **B)** and **C)** shows the study of dendritic microstructures in samples 3M and 7M using both ToF-ND and SEM-EDS Analysis; **B)** Neutron Diffraction Spectra of samples. The presence of dendritic structure is highlighted by the diffraction peaks of the alpha phase that appear double, indicating the presence of two bronze phases: alpha 1 and alpha 2 (sample 3M). As highlighted by the close-up details, this is not observable in the peaks of the 7M sample. **C)** The figure shows Electron Scan Microscopy BSE images of the sample 3M - which has a dendritic structure - and of sample 7M - in which it is absent. **D)** The neutron radiograph of the feather fragment, and the false color mapping of its state of conservation are shown.

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Effect of mixed solvent and temperature on the phase behavior of hydroxypropyl cellulose in the presence of SDS

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Hydroxypropylcellulose (HPC), one of the most well-known cellulose derivatives, is a surface-active non-ionic polymer. Nowadays HPC is used as emulsifier, stabilizer, thickener and film former in foods, cosmetics and paints. Because of this it is relevant its behaviour in commonly used co-solvent such as glycerol. Indeed one of the most interesting property of this polymer is its thermo-responsivity, HPC can change its solubility as a function of temperature. This feature allows the HPC to be considered for stimuli responsive foams, where macroscopic properties need to be reversibly changed on demand. Thermo-responsivity from HPC is substantially associated to the lower critical solution temperature (LCST) of the polymer in aqueous solutions. The presence of cosolvent can drastically modify this temperature and the size and morphology of the aggregate above the LCST. Furthermore, this kind of polymers typically form complexes with anionic surfactants~~.~~ Here we have investigated the complexation process between HPC and SDS at different temperature and surfactant concentration in the mixed water/glycerol solvent. The collected experimental data show that the presence of glycerol drastically chances the aggregation process, ruling the morphology and the size of the aggregates and the value of the LCST with respect to that observed in pure water. We investigated the effect of sodium dodecyl sulfate (SDS), a widely used surfactant, on the transition temperature (LCST) of the hydroxypropyl cellulose (HPC) in aqueous solution and in mixed solvent water/glycerol 7/3 w/w by Fluorescence Spectroscopy, Dynamic Light Scattering and Small Angle Neutron Scattering using a temperature gradient. The fluorescence spectroscopy has been conducted using the ANS (8-Anilinonaphthalene-1-sulfonic acid) as a probe. The analysis of the spectra shows a blue signal shift upon formation of polymer-surfactant aggregates and reveals an opposing effect between increasing the SDS concentration and adding glycerol. In particular SDS causes an increase in the LCST value while the presence of

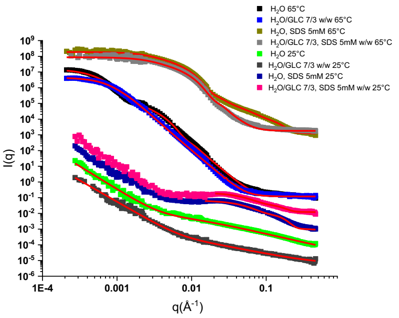

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Figure1. SANS scattering profiles at 25 and 65°C.

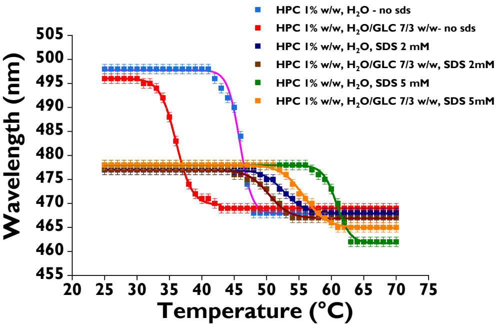

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Figure 2. *The values of the wavelength corresponding to the maximum emission peak reported as a function of temperature*

glycerol causes a reduction in LCST. This suggests a significant role of glycerol, a nonaqueous hydrogen-bonding solvent, in determining the properties of the system. Furthermore with the Dynamic Light Scattering and SANS experiments, we have studied the change, in morphology and dimension, of the aggregates in solution in the presence of the glycerol and SDS before and after the transition temperature.

Order-disorder transition in geo-inspired nanotubes

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Imogolite is a nanotubular clay material, with stoichiometry $(OH)_3Al_2O_3Si(OH)$. Thanks to its small inner diameter (~1.5 nm), it is a model system for studying the dynamics of nanoconfined water, which can exhibit radically different properties in comparison to those of bulk water. An imogolite nanotube is hydrophilic because its inner wall is covered with hydroxyl groups.

Recent investigations on an imogolite-like nanotube with inner diameter ~2.8nm, where silicon was replaced by germanium, showed that H_2O molecules in contact with the surface are stabilized by the formation of three H-bonds with the nanotube wall, resulting in a single water wetting-layer strongly bound and solid-like up to 300K [1].

As it seems that the flexibility and mobility of the inner hydroxyls are the main responsible for water structuring, our study focuses on the study of a tube in dry conditions. The results presented here were obtained by Elastic, Inelastic and Spin-Echo Neutron Scattering Experiments, combined with Molecular Dynamics (MD) simulations using a pre-existent parametrization for the interaction potential of the imogolite [2].

A transition from a state where inner OH bonds have the same orientation (as shown in Fig. 1) to a disordered state is evidenced as a function of temperature.

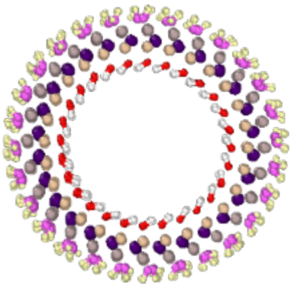

Figure 1 Top view of an imogolite nanotube in its low temperature state, having the inner hydroxyls (inner oxygen in red; inner hydrogen in white) aligned in the same direction.

References
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Hierarchical structuring of cerium oxide nanoparticles driven by amphiphilic coating

Noemi Gallucci,[1,2,*] Giuseppe Vitiello,[2,3] Rocco Di Girolamo,[1] Filomena Sica,[1] Marie-Sousai Appavou,[4] Nathan Cowieson,[5] Artem Feoktystov,[4] Luigi Paduano,[1,2]

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In recent years, the controlled clustering of nanoparticles (NPs) building blocks into defined geometric arrangements opens a new research area in soft-materials with original physico-chemical properties. NP clusters not only allow the combination of properties of individual NPs but also takes advantage of the interactions between neighboring NPs which can result in new properties (optical, magnetic, catalytic) not present in the original constituents [1]. Here, a button-up approach led to clusters of coated cerium oxide nanoparticles (CeO_2-NPs) dispersed in water [2]. Through hydrophobic interactions between the alkyl chains of organic coating, aggregates can be obtained with a more or less complex order, passing from faces cubic structures or body-centered cubic structures to Frank-Kasper phases [3]. In this study, the analysis of SANS, SAXS, and Cryo-TEM data is of crucial importance to determine the structure obtained. These structures are discussed in terms of geometrical parameters including NPs diameter, distance between neighboring NPs, and ligand length. In particular, the length of the amphiphilic molecules in the coating layer of the NPs have a crucial effect in ruling the ordering phases, and so the final physico-chemical properties of clusters of nanoparticles.

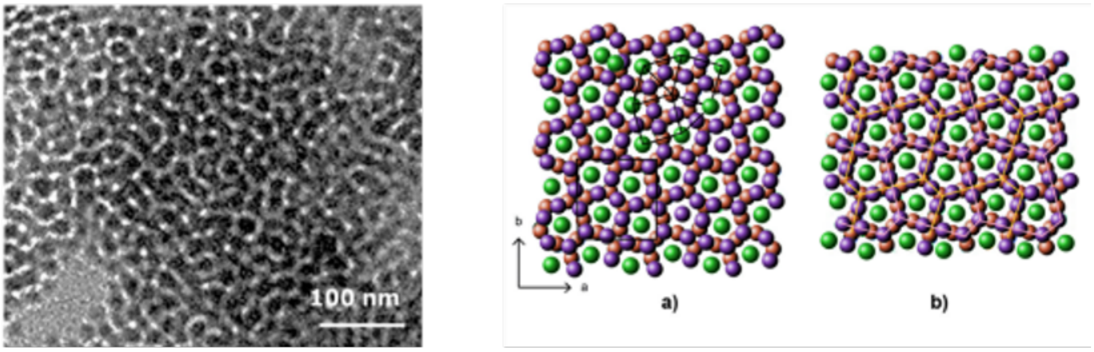

Figure 1. CryoTEM image of an ordered cluster of coated CeO_2-NPs and its schematic representation.

References

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Stiffening Effect of an Ionic Liquid on the Bending Modulus of a Model Lipid Nanoparticle

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The viscoelasticity of cell membrane plays a crucial role in life. Its alteration has been observed in several diseases and being able to control it has been suggested as a route for new therapeutic and diagnostic approaches. The new vast class of complex organic electrolytes known as ionic liquids (ILs) may play an important role in this context.[1] In this talk, I will present the results of a recent neutron scattering study performed on DMPC lipid nanoparticles doped with the model IL [bmim][Cl].[2] In this study, small-angle neutron scattering (SANS) has been used first to determine the partitioning of the IL between lipid and aqueous phases. We have found that the IL, dispersed at low concentrations at the lipid nanoparticle-aqueous interface, diffuses into the lipid region, accounting for five IL-cations for every eleven lipids (Figure 1). Then we recover to neutron spin-echo (NSE) spectroscopy to assess the effect of the IL on the bending modulus of the lipid nanoparticle. It turned out that the presence of IL-cations in the lipid phase causes an increase of the lipid nanoparticle bending modulus up to 60% compared to the neat nanoparticle (Figure 1).

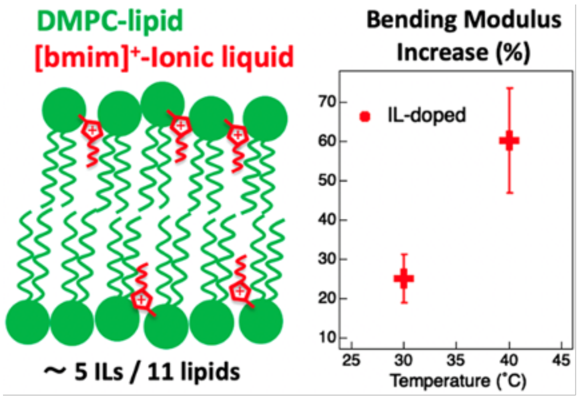

Figure 1. On the left, a cartoon summarizing the main SANS result: about 5 IL-cations per 11 lipids diffuse into the lipid region. On the right, the bending modulus percentage deviation of IL-doped lipid nanoparticles with respect to the neat, 100($\varkappa_{IL} - \varkappa_{neat}$)/ $\varkappa_{neat}$, at 30 and 40 °C, showing the IL-induced increase in bilayer bending modulus.

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Porphyrin Binding and Irradiation Promote G-quadruplex DNA Dimeric Structure

Valeria Libera,[1,2,3,*] Elena A. Andreeva,[4] Anne Martel,[5] Aurelien Thureau,[6] Marialucia Longo,[7] Caterina Petrillo,[1] Alessandro Paciaroni,[1] Giorgio Schirò,[4] Lucia Comez[3]

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The human telomeric guanine-rich sequences, known as G-quadruplex (G4), can be considered a new and promising target for anticancer therapeutics. It was increasingly recognized, indeed, that the presence of G4 structures can inhibit the telomerase action. As telomerase is an enzyme able to overcome telomere-dependent cell death, which is present in 85% of the cancer cells making them immortal [1], interfering with its activity is vital in molecular biology and biomedicine. This discovery has lighted up the interest in testing and designing small molecules with high affinity to G4, able to stabilize their structure for therapeutic purposes [2].

The interaction of G4 with binders is really challenging because their folded topology, i.e. the geometry of the loops connecting the guanine segments [2][3], is greatly affected by many environmental factors, such as temperature, ionic strength and DNA/ligand concentration.

Among various ligands, porphyrins are very attractive due to their light activation that can make them valuable G4s *conformational regulators*. Here, a structure-based strategy [4], integrating complementary probes, SANS,SAXS and circular dichroism, is employed to study the interaction between TMPyP4 porphyrin and a human telomeric sequence (Tel22) before and after irradiation with blue light [5]. Porphyrin binding is discovered to promote Tel22 dimerization, while light irradiation of the Tel22-TMPyP4 complex controls the dimer fraction (Figure 1).

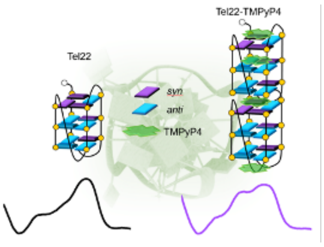

Figure 1. Schematic view of Tel22 beafore and after binding with TMPyP4.

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A Neutron Reflection study of nanoparticle-surfactants layers at the liquid-liquid interface

Valentina Lorusso [1], Davide Orsi [1], Andrea Tummino [2], Philipp Gutfreund [2] , Armando Maestro[2], Libero Liggieri [3] , Francesca Ravera [3], Eva Santini [3], Katarzyna Dziza[3] and Luigi Cristofolini [1,3]

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Hydrophilic silica nanoparticles (SiNP) are commonly used nanomaterials. The adsorption of extremely low amounts of proper surfactants on these particles can result in the formation of amphiphilic complexes, able to segregate at liquid interfaces.

The features of these layers, such as their capability to stabilize emulsions and foams, primarily depends on their structure on the nanometric scale, which is still poorly understood. In order to investigate the interfacial properties, we have performed a Neutron Reflectivity (NR) measurements on liquid-liquid interfacial layers between dispersions of SiNP in water, CTAB and dodecane. SiNP and surfactants interact and form complexes directly at liquid-liquid interface.

Thus the studies are mostly aimed at understanding the difference in the rearrangement of the surfactant within the interfacial layer and its distribution between the water-oil, particle-water and particle-oil interfaces.

Preliminary characterizations have been performed by DLS and by Small Angle Neutron Scattering (SANS) to determine the size and scattering of the SiNP alone and when forming complexes with CTAB. The NR studies are performed with the FIGARO instrument at ILL-Grenoble, by using a cell for the investigation of interfacial layers at liquid-liquid.

To disentangle the complex interfacial structures, we employed four different isotopic contrasts, all with D_2O as the aqueous phase:

1) hydrogenous oil and hydrogenous surfactant
2) hydrogenous oil and deuterated surfactant
3) Silicon matched oil and H-surfactant
4) Silicon matched oil and D-surfactant

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Implementation of a neutron imaging technique for elemental characterization of inhomogeneous samples

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Neutron Resonance Transmission Imaging (NRTI) is an innovative non-destructive radiographic technique based on the presence of resonance structures in the neutron-induced reaction cross-sections[1], which allows for 2D (and potentially 3D) mapping of isotopes and elements within the bulk of the analysed sample. NRTI has been performed at the INES (Italian Neutron Experimental Station)[2] beamline of the ISIS spallation neutron source, where a time and spatial-resolved detector is employed for Time-of-Flight (ToF) measurements of the neutron beam transmitted through the object).

ISIS is a large-scale facility consisting of a 50Hz source producing 50 sharp neutron pulses every second by a spallation process[3]. The neutron beam at the INES beamline is moderated at thermal-epithermal energies by a 295 K water moderator.

The detector is based on the neutron Gas Electron Multiplier technology (nGEM)[4], originally developed at CERN[5] to achieve high rate, high accuracy detection and localization of fast charged particles in High Energy Physics. However, due to their versatility, they can be properly adapted as neutral particles detectors. The advantage of this technology is the good space resolution combined with a large active area (10 x 10 cm^2 for the nGEM detector used at INES).

The observed quantity in NRTI measurements is the fraction of the neutron beam that traverses the sample without any interaction.

The peculiarities of NRTI make this technique suitable for the characterization of inhomogeneous samples[6,7]. In order to deepen the feasibility of NRTI in the field of Cultural Heritage, a set of crucible fragments, connected to bronze and brass production and dated back between the end of I and the beginning of II century AD[8], has been investigated through Neutron Resonance Transmission Imaging. Crucibles consisted of mass-produced terracotta pots, coated with a thick layer of refractory clay. Inside, the copper and zinc alloy were usually heated up to high temperature, liquefied and then thrown into molds to make appliques for furniture and ornamental objects. Moreover, the presence of impurities such as tin and iron are connected to the use of scrap materials while lead indicates that the alloy produced was a leaded brass and/or leaded bronze.

NRTI analysis returned the elemental composition of the fragments, disclosing the presence of brass and bronze. In addition, also silver was detected in the bulk of the crucible's fragments. NRTI can provide bidimensional maps of the elemental distribution inside the bulk, which will be useful to reveal the spatial position and the size of the brass inclusion within the crucible fragments. In fact, not all the fragments show metallic depositions on their surface.

The NRTI measurements have been compared with Neutron Resonance Capture Analysis (NRCA), performed at the INES beamline. NRCA results are helpful in the data analysis of NRTI maps, in order to focus the attention in the data treatment on selected elements.

NRCA exploits the prompt-gamma emission that can follow the resonant capture of neutrons and provides qualitative elemental composition of the samples. The energy of the resonance is characteristic of the element and isotope producing the gamma rays, and can be used to identify the chemical composition of the investigated sample by the comparison with (n,γ) cross section libraries[1] in a non-destructive manner.

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Design and test of a novel compact thermal neutron collimator

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In this work a novel design for a thermal neutron collimator and the the first experimental results are presented. The concept is based on the decoupling of the device's field-of-view from its collimation power. A multi-channel geometry is proposed consisting of a chess-board structure where highly neutron-absorbing channels are alternated with air channels. A borated polymer was purposely developed to produce the attenuating components in the form of square-sectioned long rods. A scalable structure consisting of multiple collimation sectors can be arranged. The geometrical parameter L/D, corresponding to the ratio between the length of a channel and its width, defines the collimation power. Several sectors can be arranged one after the other to reach relevant collimation powers. Each sector, 100 mm long, is composed by several channels with D = 2.5 mm corresponding to an L/D coefficient of 40. The target field of view is 50x50 mm^2. The prototype presented consists of 4 stages, comprising a total L/D of 160. This novel collimator, developed inside the INFN-ANET collaboration, due to its intrinsic compactness, will be of great importance to enhance the neutron imaging capability of small to medium-size neutron sources.

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Structure and Function Investigation on Membrane-Binding Proteins: a Neutron Reflectometry Study

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This PhD project is focused on investigating the interaction of model membranes with proteins from two different sets: (*i*) proteins from **Clathrin-mediated endocytosis** (**CME**) and (*ii*) peptides from **SARS-CoV-2 Spike protein**. (*i*) **CME** is the main mechanism by which eukaryotic cells internalize membrane proteins and is driven by different proteins that interact with the inner leaflet of the cell membrane. The aim of this work has been to investigate the structures formed by the proteins **CALM** and **FCHo2** on association with lipid monolayers. Neutron Reflectometry (NR) allowed us to determine the orientation of both CALM (**Figure 1(*i*)**) and FCHo2 with respect to the membrane. (*ii*) The **SARS-CoV-2** is an encapsulated virus, indeed it has a lipid envelope with membrane proteins such as the **Spike protein**, which is responsible for receptor recognition. Besides, the **fusion domain of the Spike**, which can be divided in four **Fusion Peptides** (**FP**), is responsible for triggering the fusion between viral and host membranes, a critical stage of the infection. The aim of this work has been to investigate the role of the different FP in the fusion process, also exploring the influence of calcium. Neutron Reflectometry, using model membranes composed of natural lipids, shed light on the critical role of **FP1** (i.e. the N-terminal of the Spike fusion domain), which is able to cross membranes in a calcium dependent manner[1] (**Figure 1(*ii*)**).

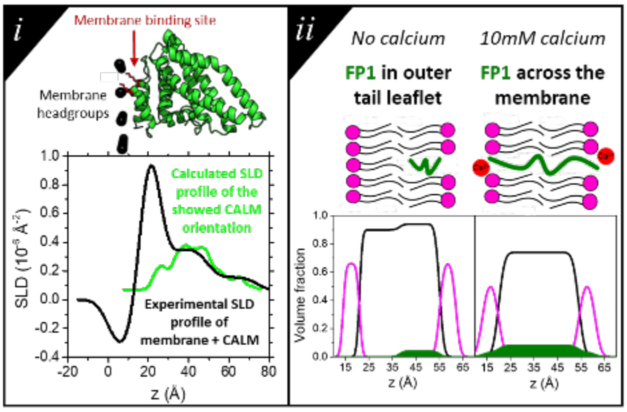

Figure 1. (***i***) SLD profiles showing the best orientation of CALM obtained from Neutron Reflectometry. (***ii***) volume fraction profiles obtained from Neutron Reflectometry, showing the insertion of FP1 in the mebrane.

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Moderation of neutrons using monochromatic neutron sources: a comparison using fusion and spallation neutrons

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Starting from two different neutron production reactions, namely the deuterium-tritium (DT) fusion and the proton induced spallation on a tungsten target, a neutronic analysis is carried out considering the same reflector-thermal moderator assembly. The rationale subtending this investigation is to evaluate and compare the slowing down effect of a typical moderator assembly used at a spallation neutron source on the almost monochromatic spectrum of a DT reaction. The results are eventually compared in terms of moderator brilliance. As far as the neutron spectral analysis is concerned, it is shown that, for the same setup, the slowed down spectra resulting from 14 MeV neutrons have similar features as compared to that obtained from spallation: a Maxwellian peak and an epithermal neutron tail featuring a comparable slope. The spectral intensity deserves further discussion on engineering bases. Although neutrons spallation sources are largely used for the production of beams for neutron scattering purposes, nevertheless, the results obtained in this study highlight that is in principle feasible the thermalization of monochromatic

Two is better than one

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The tripeptide Glycyl-L-prolyl-glycinamide HCl (GPG-NH2) is considered the simplest model system to investigate β-turns formation in aqueous solutions[1]. Here we investigate, by neutron diffraction augmented by Monte Carlo simulations, the interaction of water, trehalose and glucose with GPG-NH2 in two ternary (water, carbohydrate, peptide) solutions. The rationale behind the choice of trehalose and glucose is that the first is known as the most effective carbohydrate in preserving the native structure and functionality of biomolecules, and thus of β-turns, in drought

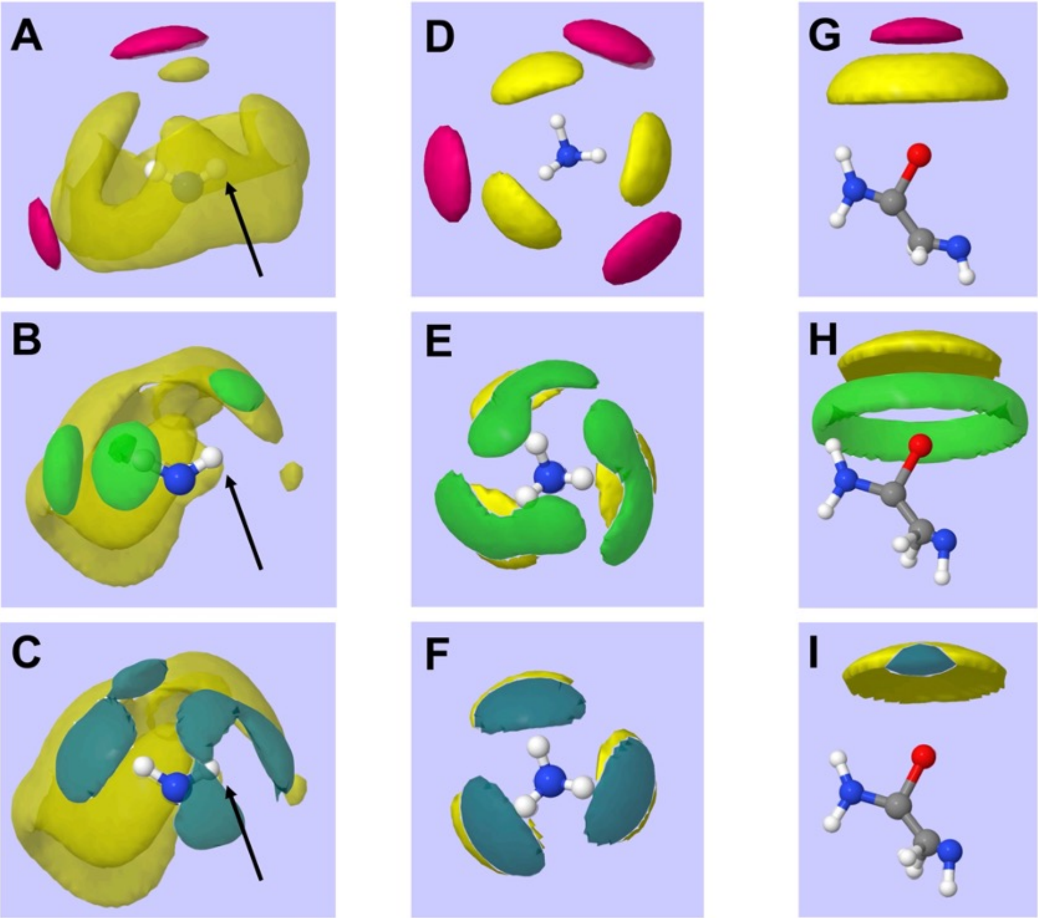

Figure 1. Spatial density functions, showing in 3D the interaction of the GPG-NH2 groups with the water (yellow clouds) and trehalose, α- and β- glucose (magenta, light and dark green clouds) in the ternary solution. Panel A, B and C show the interaction of the NH_2 group with water and trehalose, α-glucose and β- glucose, respectively. The black arrow indicates the Hn2 site, that is involved in the β-turn and is the less hydrated. Panel D, E and F show the

interaction of the NH_3 group with water and trehalose, α-glucose and β- glucose, respectively. Panel G, H and I show the interaction of the CO group with water and trehalose, α-glucose and β-glucose, respectively.

conditions[2], while glucose does not, although being the building block of trehalose[3,4].
These experiments show that glucose occupies the first neighbours shell of GPG-NH2 in competition with water, while trehalose entraps a layer of water molecules in the first neighbours shell of GPG-NH2, without direct bonding with it (Figure1).[5,6] Furthermore, we observe that the presence of trehalose stabilizes the β-turns formation with respect to the GPG-NH2-water binary mixture (Figure2), contrarily to glucose.[5,6]
Our findings suggest that, when two glucose rings bind in a 1α -1'α the rearrangement of the electronic clouds determine a reduction of the ability of forming H-bonds with both water and biomolecules. This determines also the strongly different taste of trehalose compared to glucose[4].
Finally, these results suggest that the preferred bioprotection mechanism, adopted by trehalose is the containment one.[5]

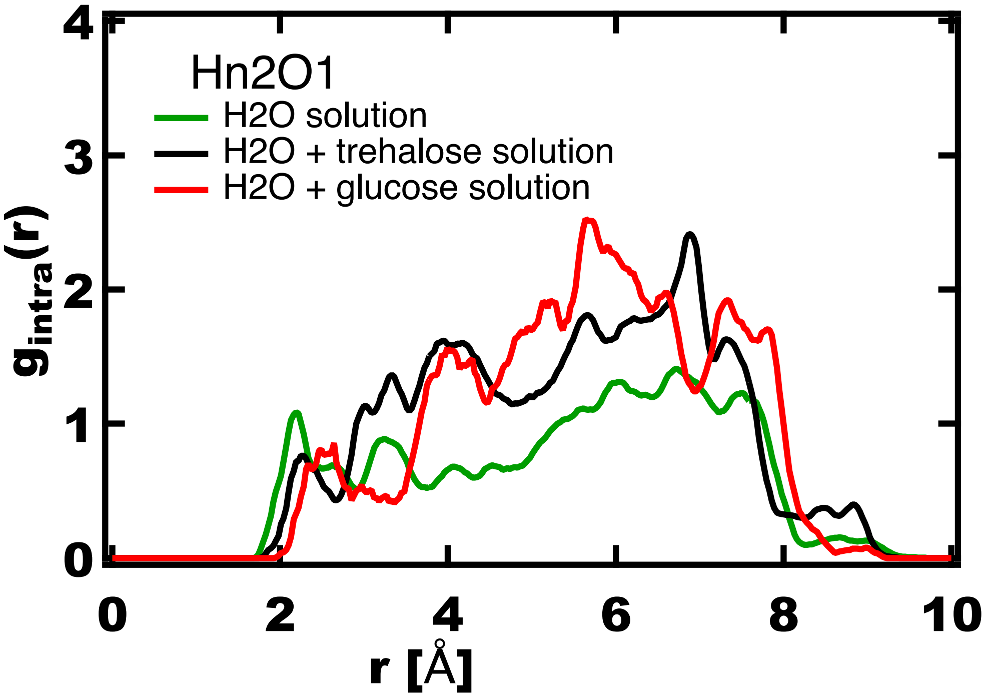

Figure 2. Comparison of the intra-molecular g_{Hn2O1}, sites involved in the β-turn formation, in the three GPG-NH2 solutions, namely in pure water (green line)[5], in a water-trehalose solution (black line)[5] and in the water-glucose solution investigated here (red line)[6].

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Self-dynamics of supercritical methane at high pressure

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Methane is one of the most important molecules for human life and technology. It is the chemical we use to heat up our houses, drive some of our vehicles, and even fuel rockets to space. Outside Earth, the chemical-physical properties of methane also have critical planetary consequences. Due to its quasi-sphericity and to the lack of hydrogen bonds, experimental findings for methane can be easily compared to computationally derived values and simple models such as the hard-sphere model or the Lennard–Jones model often apply.

We recently measured the single-particle diffusion coefficient of supercritical CH_4 at the constant temperature of 300 K and pressures between 0.1 and 1.4 GPa, i.e. up to the freezing pressure.[1] The self-diffusion coefficient is among the main transport properties of a fluid but there are generally fewer high-pressure data available in the literature for the diffusion coefficient than, say for viscosity. The experiments were performed by quasi-elastic neutron scattering at the IN6-SHARP spectrometer installed at the Institut Laue-Langevin in Grenoble, France.

The self-diffusion coefficient of methane at 300 K and 1.4 GPa turned out to be comparable to that of liquid methane at ambient pressure and 100 K. Breakdown of the Stokes–Einstein–Sutherland relation was observed. A fractional Stokes–Einstein–Sutherland relation correctly represents our data over the entire pressure range with a power-law exponent of 0.73±0.02, namely a value much lower than that of the Lennard–Jones fluid (0.92). We also found that the pressure dependence of the diffusion coefficient departs from that expected for a dense fluid of hard spheres for any constant sphere diameter. These findings underpin the lack of a simple model for predicting the pressure dependence of the self-diffusion coefficient of dense fluid methane [1].

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Cosolvent-induced effects on the protein-like dynamical transition of PNIPAM: a neutron scattering study

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The dynamical transition[1] (DT) is a ubiquitous phenomenon observed in several proteins and other biomacromolecules that consists in the activation at $T_d \approx 220$ K of anharmonic fluctuations occurring on the ps – ns time scale. Such a fast dynamics is made accessible by neutron scattering techniques, including Elastic Incoherent Neutron Scattering (EINS). The extra mobility above T_d is reflected in a sudden change in the temperature dependence of the macromolecular mean square displacements (MSD). It is believed that, in order to gain the necessary flexibility to undergo the transition, a prominent role is played by the *plasticizing* effect exerted by the protein hydration water. On the one hand, in fact, the transition is not observed in completely dry proteins, on the other hand, the protein hydration water itself is found to undergo a DT. The connection between protein and solvent dynamics is also manifested in a strong sensitivity of the DT to the solvent composition, in particular, the presence of *stabilizing* compounds (sugars, polyols) causes a sensible reduction of the macromolecular flexibility that is reflected in a shift of T_d toward higher values with respect to pure water. Sugars and polyols are also known for their ability to preserve proteins against unfolding and degradation, and a relationship has been speculated between inhibition of protein dynamics on fast time scales and preservative action on longer time scales, although the details of such a connection have not been fully clarified[2]. A "protein-like" DT has also been recently observed[3] in poly(N-isopropylacrylamide) (PNIPAM), i.e. a thermoresponsive polymer that undergoes a coil-to-globule transition around 305 K in water, reminiscent of the protein cold denaturation. The similarities between protein and PNIPAM behavior in the aqueous media make PNIPAM an excellent model system to identify general mechanisms at the basis of the DT and to help at elucidating the relation between solvent characteristics, macromolecular flexibility and conformational stability. By means of EINS techniques we studied how aqueous mixtures of stabilizing compounds (glycerol, glucose) impact on the dynamics of PNIPAM over fast time scales (Figure 1). The analysis of the MSD marks the existence of a tight coupling between the dynamics of PNIPAM and that of the solvent, revealing strong analogies with the protein behavior

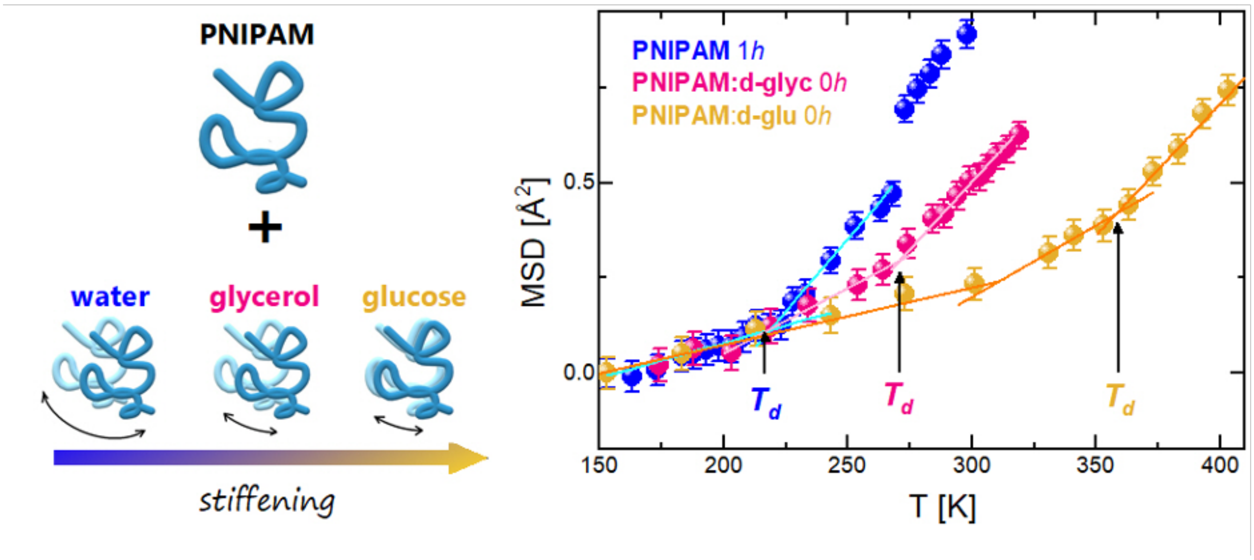

Figure 1. Mean square displacements (MSD) of PNIPAM in pure water (PNIPAM *1h*), pure glycerol (PNIPAM:d-glyc *0h*) and pure glucose (PNIPAM:d-glu *0h*). According to the characteristics of the employed spectrometer (IN13), the reported MSD are associated with motions faster than τ_R=150 ps. For each sample, the activation of the DT at the corresponding value of T_d is indicated with an arrow.

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H_2 induced reconstruction phenomena in a Pt/Al_2O_3 catalyst: an INS spectroscopy and DFT study

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The catalytic activity of supported platinum nanoparticles has been well known for a long time, but a complete understanding of the related phenomena at an atomic scale is still missing. In this work, we highlight the dynamics of the hydrogenated nanoparticles on a Pt/Al_2O_3 catalyst under different H_2 partial pressures, obtained by Inelastic Neutron Scattering (INS) spectroscopy and Density Functional Theory (DFT) simulations. This work is part of a collaboration with the industrial partner Chimet S.p.A. (Arezzo, Italy).

INS spectra of Pt/Al_2O_3 in H_2 provide important information about the Pt-H species formed. We measured the INS spectra under two different H_2 partial pressures and temperatures, corresponding to a high and low H-coverage of the Pt nanoparticles (Figure 1 A and B). The differences between the two spectra were interpreted on the basis of complementary DFT simulations. As calculated in ref[1], Pt nanoparticles supported on γ-Al_2O_3 are expected to undergo a significant morphological reconstruction when changing the hydrogenation conditions, passing from biplanar structures in strong interaction with the support at low H-coverage to cuboctahedral geometries completely solvated by H atoms at high H-coverage. The INS spectra of these models were simulated and compared with the experimental ones, showing a good matching between the completely solvated models and the high H-coverage experimental spectrum (Figure 1A) and between the 450 cm^{-1} band of the low H-coverage experimental spectrum and low H-coverage models (Figure 1B). This second

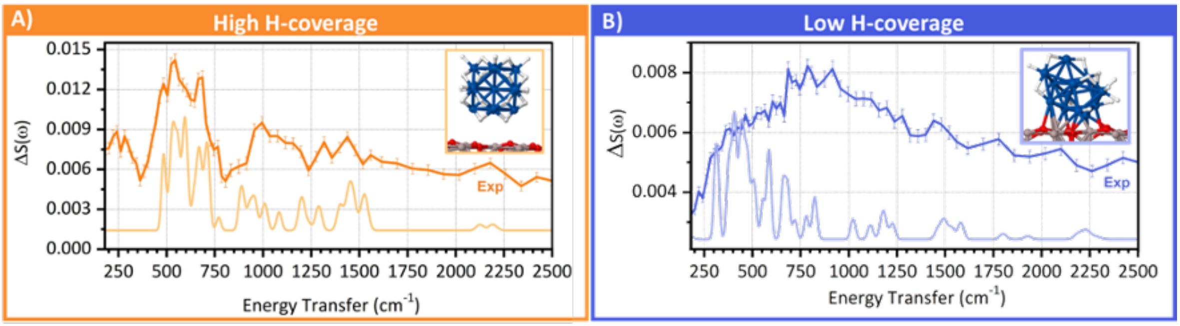

Figure 1. A) INS fingerprint of Pt-H species collected under a high H_2 pressure, compared with the theoretical spectrum of the cuboctahedric $Pt_{13}H_{32}$ cluster. B) INS spectrum collected at very low H_2 pressure compared with the simulated spectrum of the biplanar $Pt_{13}H_{16}$ model.

INS spectrum also shows the formation of a signal at 800 cm^{-1} compatible with -OH groups generated by H-spillover (not shown) onto the Al_2O_3 support. This comparison supports the reconstruction of Pt nanoparticles in the presence of H_2 predicted in ref[1] and complements the previous experimental evidences collected by means of FT-IR and XAS spectroscopies[2].

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Progress towards a Bell-type polarization experiment with thermal neutrons

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Experimental tests of Bell-type inequalities distinguishing between quantum mechanics and local realistic theories remain of considerable interest if performed on massive particles, for which no conclusive result has yet been obtained. Only two-particle experiments may specifically test the concept of spatial nonlocality in quantum theory, whereas single-particle experiments may generally test the concept of quantum noncontextuality.

Here, we have performed the first Bell-type experiment with a beam of thermal-neutron pairs in the singlet state of spin, as originally suggested by J.S. Bell. These measurements confirm the quantum-theoretical predictions, in agreement with the results of the well-known polarization experiments carried out on optical photons years ago.