Società Italiana di Scienze Neutroniche
Associazione di Promozione Sociale

XXXIV Congresso Annuale SISN
I neutroni e le sfide globali: clima, salute e nuove tecnologie

13 - 15 settembre 2023
Sala Olimpica – Teatro Vittoria
Bosco Chiesanuova (VR)

Il Congresso Annuale SISN è un momento d'incontro e confronto per i ricercatori attivi nella neutronica, sia dal punto di vista fondamentale che tecnologico.
Le sessioni scientifiche, come sempre interdisciplinari, saranno intervallate da spazi di discussione che possano favorire la nascita di nuove idee, progetti e collaborazioni.
Inoltre, in questa edizione sarà celebrato il trentennale della costituzione della Società con una sessione speciale che mostri il contributo che i neutroni possono dare nell'affrontare le sfide globali.

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Mercoledì 13 settembre 2023

Sala Olimpica, Teatro Vittoria
Bosco Chiesanuova (VR)

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Barbara Asinari, Consigliere Comunale con delega al Turismo e Commercio
Carmelo Melotti, Vicepresidente della Cassa Rurale Vallagarina

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16.10
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Hotel Lessinia
Piazza degli Alpini 3, Bosco Chiesanuova

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Sala Olimpica, Teatro Vittoria
Bosco Chiesanuova (VR)

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9.30
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9.50
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10.10
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10.30 **Coffee Break**

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Luca Bertini

11.20
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11.40
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Francesco Spinozzi

12.00
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Giulia Marcucci

12.20
Tecniche di Luce di Sincrotrone per la Scienza dei Beni Archeologici
Franco Zanini

13.00 **Pranzo**

Hotel Frizzolan
Piazza Borgo 5, Bosco Chiesanuova

Trent'anni di SISN

Chair: Marco Zanatta

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15.00
Ancient Egypt bronze coffins investigation by Neutron Imaging
Francesco Cantini

15.30
Dynamic personality of proteins and effect of the molecular environment
Valeria Libera

16.00
A spectrometric transfer instrument for neutron metrology
Alessandro Lega

16.30
IN13+: more flux, more science
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17.00

Poster session

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  Erica Alfinelli

- *SAXS characterization of gel nanocomposite containing fluorine doped zinc oxide nanoparticles*
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- *Purification and SAXS analysis of the Nucleocapsid Protein of the SARS-CoV 2 virus*
  Yessica Roque Diaz
- *GO/silica nanocomposites for white light sources*
  Chiara Giustini
- *Sonobioreactor: a novel platform to study ultrasounds-induced bioeffects*
  Tommaso Mancini
- *Innovative neutron guide replacement at the ILL*
  Giuliana Manzin
- *Development of drug delivery systems for hydrophobic metastatic melanoma inhibitors*
  Pietro Milesi
- *Purification and characterization of iron oxide nanoparticles (IONs) and their potential use as drug delivery vectors*
  Paolo Moretti
- *Development of topoelectric circuits via transmission lines*
  Denis Nabari
- *Characterization of 3D micro-structured TIMEPIX detectors for neutron imaging*
  Matteo Polo
- *Laboratorio di Metrologia dei neutroni dell'INMRI-ENEA: Simulazioni a supporto delle attività sperimentali*
  Lucrezia Spagnuolo
- *Scientific analysis of a Classic Maya ceramic vessel: insights into composition and pottery technique*
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18.00 **Chiusura dei lavori**

20.00 **Cena sociale**

Agriturismo la Marmacola
Contrada S. Margherita, Bosco Chiesanuova

Venerdì 15 settembre 2023

Sala Olimpica, Teatro Vittoria
Bosco Chiesanuova (VR)

9.00

Assemblea dei soci SISN

11.00 **Coffee Break**

11.30 **Tavola rotonda**

Società Italiana di Scienze Neutroniche:
quali sfide per i prossimi anni

12.30 **Conclusioni e saluti**

Abstract dei contributi orali

Effect of Polymorphism and Ligand Binding on G-quadruplex Fast Dynamics probed by Elastic Incoherent Neutron Scattering

Luca Bertini[1], Valeria Libera[1], Francesca Ripanti[1], Francesca Natali[2], Marco Paolantoni[3], Andrea Orecchini[1], Alessandro Nucara[4], Caterina Petrillo[1], Lucia Comez[5], Alessandro Paciaroni[1]

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G-quadruplexes (G4s) formed by the human telomeric sequence $AG_3(TTAG_3)_3$ (Tel22) play a key role in cancer and ageing. G4 structures are known to display a variety of topologies, which are determined by several factors, resulting in structural polymorphism. Neutron Scattering techniques are a valuable tool to investigate how G4 structural polymorphism and ligand binding affect their sub-nanosecond dynamics. Within this context, we combined FTIR spectroscopy to monitor the Tel22 conformation and EINS to assess the corresponding dynamical properties. K+ and Na+ stabilized G4s were found to be in the parallel and mixed parallel-antiparallel topologies, respectively, with the latter resulting to be dynamically more stable. This result is compatible with the presence of ordered hydration-water structures in the antiparallel conformation. Complexation with the model ligand BRACO19 (BR19) resulted in an overall increase of Tel22 mobility. Such a dynamical enhancement, which is uncorrelated to the G4 topology, can be ascribed to a preferential binding of water molecules to Tel22 rather than to BR19.

Single photon emitters:
GaAsN:H quantum dots and color centers in silicon

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Quantum-light emitters are a fundamental building block for the large-scale implementation of photon-based quantum information technologies. After a brief review of the current state of the art, I will present two types of these emitters recently studied in our laboratories: GaAsN quantum dots (QDs) and color centers in Silicon.
A novel and versatile approach for the fabrication of site-controlled QDs is presented [1,2]. Hydrogen incorporation in GaAsN results in the formation of N-H complexes, which neutralize all the effects of N on GaAs, including the N-induced large reduction of the bandgap energy. The N-H bonds located within an intense light spot (generated by a scanning near-field optical microscope tip or a photonic jet) are broken, thus obtaining a selective removal of hydrogen and the creation of site-controlled GaAsN QDs with tunable emission wavelength.
Luminescent point-defects in semiconductors are another type of quantum-light emitters. In particular, silicon platform is very attractive because of its widespread adoption and advanced technologies for microelectronics and photonics. The control of the electronic states of carbon-related defects (G-centers) in silicon via strain engineering will be presented [3]. By embedding these defects within patches of silicon on insulator and topping them with SiN_x, symmetry breaking is demonstrated, resulting in a controlled splitting of the zero phonon line (ZPL) and in the full polarization of its emission.

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Advanced Quantum Technologies, 4 (2021), 2100045.
[2] F. Biccari, *et al.* "Site-controlled single-photon emitters fabricated by near field illumination".
Advanced Materials, 30 (2018), 1705450.
[3] A. Ristori, *et al.* "Strain engineering of the electronic states of silicon-based quantum emitters".
Advanced Optical Materials. *Accepted for publication* (2023).

Science in a Cup of Coffee: A Structural Study of a Trigonelline Aqueous Solution

Fabio Bruni[1], Michael Di Gioacchino[1], Maria Antonietta Ricci[1]

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For sheer sensory enjoyment, few everyday experiences can compete with a good cup of coffee. The alluring aroma of steaming hot coffee just brewed from freshly roasted beans can drag sleepers from bed and pedestrians into cafés. But underlying this seemingly commonplace beverage is a profound chemical complexity that demands detailed knowledge of its composition [1]. Caffeine, trigonelline and nicotinic acid are three important bioactive components of coffee [2-4]. In particular, trigonelline belongs to major components of coffee, where it is present in amounts similar to those of caffeine [5-7]. In the present report, we have looked at the atomic structure of an aqueous solution of trigonelline exploiting Neutron Diffraction with Isotopic Substitution (NDIS) augmented with computer simulations. Regarding the coffee making process, the outcome of the present study could provide a basic framework essential to carry on future studies on the extraction efficiency of trigonelline from ground coffee as a function of the ions present in water. This latter sentence is based on the well-known, but still poorly understood, Hofmeister series, whose predictions indicate that calcium and magnesium ions in the water used to brew coffee should enhance the solubility of important molecules in coffee, trigonelline included. This subject is still in its infancy as very little is known about the best water composition, namely identity and relative amount of dissolved ions, resulting in the best coffee [8-9].

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Detection of Gram(-) endotoxins: a study on the biorecognition-target interaction by means of Neutron Reflectometry

Alessandro Cangiano [1,2], Noemi Gallucci [1,2], Luke A. Clifton [3], Alba Silipo [1], Luigi Paduano [1,2], Giuseppe Vitiello [4,2]

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Gram(-) bacteria are pathogenic microorganism which outer membrane of the external envelope is composed by complex molecules, such as lipopolysaccharides (LPS), consisting of three structural domains: lipid A, the core oligosaccharide and the O antigen, endotoxins related to the infections induced by pathogens and so they represent a suitable target for a selective detection.
Among biorecognition molecules, aptamers are very appealing. They are single-stranded DNA or RNA with a high affinity and specificity toward specific analytes.
Recently, a small aptamer, LA27, has been identified for the LPS selective recognition. Now, the portion of the LPS interacting with LA27 is not well-understood yet, preliminary studies suggest an affinity with lipid A, as well as the affinity of the LA27 to LPS molecules deriving from different kind of Gram(-). In this context, we performed a biophysical investigation on the interaction of LA27 with asymmetric supported lipid bilayers prepared by Langmuir-Blodgett method: the outer leaflet was composed by DPPC while three LPS deriving from different Gram(-): *Akkermansia, Flavobacterium* and *Paenalcaligenes hominis* were used for the outer leaflet. For each of this sample, the interaction with LA27 at 25 and 37 °C was investigated performing Neutron Reflectometry experiments. This analysis gave us information about the aptamer positioning within the bilayer regions so that we shed light on the binding affinity of LA27 with a specific portion of LPS.

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Ancient Egypt bronze coffins investigation by Neutron Imaging

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In the context of an interdisciplinary project of Museo Egizio di Torino, that aims at studying *votive coffins for animal mummies* [1], eight bronze artefacts from Museo Egizio were investigated by Neutron Imaging and Neutron Activation at the TU Delft Reactor Institute. The study of metal artefacts of historical and artistic interest is based on the knowledge of the constituent materials and their methods of production. Since the traditional investigation of metal artefacts often relies on destructive sampling, it is mandatory to have diagnostic investigations capable of providing the maximum amount of information with a minimum level of invasiveness. Here we present some results related to two bronze votive statuettes suspected of hosting mummies of the animals they represent. The goal of this study was twofold: to respond to some technological and conservation issues (such as evaluating the possible spread of cracks inside the statues, identifying repairing parts of the statues, characterize the alloy microstructure, obtain clues about the casting process) and identify and try to reconstruct, if present, faunal remains. Neutron Imaging has already proved to be a powerful probe for the study of metallic artefacts in the field of Cultural Heritage [2], but in this study we demonstrate its effectiveness also for the investigation of faunal remains sealed inside bronze votive coffins, allowing with a totally non-invasive technique, to obtain a complete characterization of both the bronze and the contents of the mummy bundle.

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The GNeuS project, 19 post-doc positions in neutron sciences

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Taking into consideration tremendous changes in the European neutron landscape and assuming responsibility for sustainability, the neutron community is nowadays facing an important task to ensure long-term perspectives, that essentially depend on its ability to create a new generation of innovative highly skilled researchers. To tackle this challenge, Forschungszentrum Jülich (FZJ), Technical University Munich (TUM) and Helmholtz-Zentrum Hereon (Hereon), partners at the Heinz-Maier-Leibnitz Zentrum (MLZ), are running the Marie-Skłodowska Curie Action (MSCA) COFUND project "Global Neutron Scientists" GNeuS https://GNeuS.eu that trains young neutron scientists through the establishment of a well-structured post-doctoral research programme with a strong interdisciplinary and intersectoral approach and global outreach. Within GNeuS, Post-Doc grants are offered to solving the grand challenges facing mankind in areas such as environment, energy, key technologies, and life science as well as improving the existing instrumentation and the ancillary equipments and developing new sources or optimizing the existing ones. During the GNeuS Call N. 3, the 3 MLZ Partners offer more than 15 fellowships each with a duration of 24 months. The GNeuS Call N. 3 will open on November 1st, 2023, and the applications shall be submitted within on January 17th, 2024, at 18:00 CET, on the https://my.gneus.eu portal. Despite predefined topics for your research are available, any applicant is welcome to submit her/his own research plan. Questions can be addressed to GNeuS Management Office (gneus@mlz-garching.de).

On the structural organization of functionalized nanoparticles through Small-Angle Neutron Scattering

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Interest in nanoparticles (NPs) has exploded in the past decades primarily due to their novel or enhanced physical and chemical properties compared to bulk material. These extraordinary properties have created a multitude of innovative applications in the fields of medicine, sensing, agriculture, catalysis, food industry, and many others. Among the different NPs, the hybrid ones, capable of combining the properties of different inorganic or inorganic/organic materials, are the most interesting. The properties of such systems can be further modulated by driving the type of structure in which they are assembled.
Here, we present how it is possible to characterize through Small-Angle Neutron Scattering (SANS) the self-assembly of hybrid and/or coated NPs. Passing from single functionalized inorganic NPs, such as magnetite NPs coated with oleylamine and oleic acid. Systems in which single NPs coated with an organic double layer coexist with disordered aggregates, such as magnetite coated with oleylamine, oleic acid, and 18LPC or cerium oxide coated with oleylamine and oleic acid. Up to nanocomposites, in which nanoparticles are dispersed in a polymer, such as magnetite in HEUR polymer; or nanoparticles functionalized with human serum albumin and human transferrin to obtain nanoplatforms for multimodal imaging and theranostics.

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[4] Luchini A. et al. *Colloids and Surface B: Biointerfaces*, **2018**, *168*, 2

The role of phonons in magnetic relaxation of molecular nanomagnets unravelled by inelastic neutron scattering

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Molecular Nanomagnets (MNMs), molecules containing interacting spins, are characterized by many accessible low-energy levels that can be exploited to store and process quantum information. However, these applications are undermined by molecular vibrations and spin-phonon interactions, playing an important role in magnetic relaxation, and determining the coherence times of superpositions of states. Despite this, very limited experimental investigations on phonons and vibrations in MNMs were performed so far. This motivated a series of Inelastic Neutron Scattering (INS) experiments that we performed in the last years with the aim to directly access, for the first time, phonon dispersions and density of states (DOS) in MNMs.
In an innovative and challenging experiment, we exploited 4-dimensional INS to directly investigate phonon dispersions and polarisation vectors in a molecular qubit [1], by measuring the 4D scattering function in large portions of the reciprocal space. Both these quantities are in fact necessary for a quantitative modelling of the relaxation dynamics in MNMs. We also exploited INS to measure the DOS of Dy-based SMMs [2]. These INS experiments highlighted the critical role played by low-energy non-dispersive phonon modes, which undermine relaxation and coherence times in molecular qubits and make Raman mechanisms more efficient in SMMs, also providing new hints for the design of new and better-performing systems.
Our latest works also involve the study of phonons with INS in applied hydrostatic pressure, with the aim to disentangle the role played by specific lattice and molecular vibrations in the dominating relaxation mechanisms, and the exploitation of complementary techniques like Inelastic X-ray Scattering [3].

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A spectrometric transfer instrument for neutron metrology

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Secondary Standard Dosimetry Laboratories (SSDL) that use radionuclide neutron sources need to establish the traceability of their calibrations to Primary Standard Dosimetry Laboratories (PSDL). This can be done by using neutron sources whose emission rates were measured at PSDL or a transfer instrument calibrated at PSDL. These methods do not provide information on the energy distribution of the field. This may have an impact on reference fields based on alpha emitters, such as Americium-Beryllium, being their spectra slightly dependent on the size of the source and the amount of active material. Bonner Spheres (BS) are a valid spectrometric transfer instrument but are very time-consuming. In the last decade, a new class of single-moderator neutron spectrometers (SMNS) was developed. These devices condense the functionality of BS in a single moderator with specific geometry, embedding multiple solid-state thermal neutron detectors in previously optimized positions. SMNS are BS in terms of operation and performance but require only one exposure to determine the whole neutron spectrum. NWES (Neutron wide Energy Spectrometer) is a SMNS with a directional response based on a collimated cylinder. Being insensitive to the scattered field, NWES could be conveniently used as a spectrometric transfer instrument for neutron metrology. This work presents the spectrometer design and the calibration measurements performed in reference neutron fields, including monoenergetic neutrons.

Dynamic personality of proteins and effect of the molecular environment

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A long debated question in biophysics is on the role played by the molecular environment on affecting the protein internal dynamics, as the coupling between thebiomolecule and the solvent may have a crucial effect on both the biological functionality and stability. Here we address the impact of three different molecular environments, water, glycerol and glucose, that form progressively more viscous matrices around the protein surface. The protein dynamics in the sub-nanosecond timescale is investigated in a wide temperature range by incoherent neutron scattering. Three model proteins, belonging to three significantly different families are taken into account: the mesophilic lysozyme, the thermophilic thermolysin and the intrinsically disordered protein β-casein. By comparing the different trend of their thermal fluctuations, we find that the thermolysin internal dynamics is less sensitive to the impact of the environment than β-casein and lysozyme. The protein internal dynamics results from the delicate balance of the effect of the coupling with the environment and the specific intrinsic dynamics of the protein related to its thermal stability. Quite interestingly, when rescaling the mean squared displacements of lysozyme and thermolysin in all the molecular environments by the respective melting temperature measured by calorimetry, a critical common protein flexibility is found. This result suggests that the initiation of thermal unfolding in the protein requires a specific critical threshold for the amplitude of structural fluctuation, regardless of the coupling between the biomolecule and its environment or the protein "dynamic personality".

Structure and stability in self-assembled multidomain peptide fibres

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In this work[1] we investigate a family of peptides that form -sheet nanofibres and present an exceptional physical stability even after attachment of poly(ethylene glycol) (PEG). Using small-angle scattering techniques in combination with molecular dynamics simulations to probe the nanostructure, stability and molecular exchange, we show that fibres formed by $K_xW(QL)_yK_z$ multi-domain peptides are extraordinarily stable. These findings show that robust nanostructures with little susceptibility to physical and chemical perturbations can be engineered by using relatively short -sheet-forming peptides. Through a balance of hydrophobic interaction and hydrogen bonds, these peptide assemblies achieve superior stability as compared to regular amphiphiles. Our results clearly highlight the nanostructural stability that can be achieved by peptide assembly and further exploited in biomedical applications.

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The Neutron Resonance Transmission Imaging technique for elemental characterization of crucibles coming from brass workshops of the ancient Roman Mediolanum

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We present recent advances in Neutron Resonance Transmission Imaging (NRTI) at the Italian Neutron Experimental Station (INES) beamline of the ISIS spallation neutron source, and an application of this innovative method in the Heritage Science field. The NRTI technique relies on the measurement of the beam attenuation caused by resonant absorption of epithermal neutrons by material nuclei. Resonance structures in neutron-induced reaction cross-sections enable the identification and quantification of isotopes. NRTI allows the localization of isotope and element distributions within 2D (and potentially 3D) maps of the object bulk, enhancing the contrast between isotopes with similar attenuation coefficients.

NRTI is a promising technique for characterizing inhomogeneous samples and non-destructively examining archaeological objects. Therefore, we applied NRTI to Roman Italy's crucible fragments (I-II AD) used for bronze and brass production in antiquity. These terracotta pots, coated with refractory clay, may contain metallic inclusions on their surfaces but also in their bulk; therefore, X-rays or ion beam measurements need to be integrated with neutron investigations to disclose brass traces and composition inside these artefacts. NRTI analysis identified the qualitative elemental composition of the fragments, detecting brass, bronze, arsenic, antimony, silver, and lead in their bulk. These archaeological samples exemplify the utility of NRTI for investigating inhomogeneous objects by visualizing element and isotope distribution within the bulk.

IN13+: more flux, more science

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IN13 is a backscattering spectrometer working with thermal neutrons with wavelength 2.23 Å corresponding to energy of 16.45 meV. The energy resolution is of the order of 8 µeV and the energy window is ± 100 µeV. In addition, the value of the incident energy gives the availability of high momentum transfers ($Q < 4.9$ Å^{-1}), much larger than obtainable with currently worldwide available spectrometers. The instrument fills the energy gap between IN6-SHARP or IN16B and IN5 at ILL, IRIS and OSIRIS at the Rutherford-Appleton laboratory (RAL) in United-Kingdom, BASIS at ORNL or HFBS-NCNR at NIST in the US, and DNA at J-Parc in Japan.

The major drawback of IN13 being the low neutron flux on the sample, implying long acquisition times that put limits on the experimental data obtainable and requires important sample masses, a major upgrade was undertaken during the last 2 years. This included the guide refurbishment, the design of a new monochromator, a new deflector, and further additional minor improvements.

The instrument has been dismounted in late 2021 and recently remounted. Preliminary tests were done before summer and first official experiments are planned from September on. I will report here the concept of the upgrade and very first results.

In-solution and interface study on biological membranes and their interaction with Prohibitin

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Prohibitins (PhB) are highly conserved heterodimer proteins composed of two subunits PhB1 and PhB2 arranged to make a multimeric ring at the inner of the mitochondrial membrane (IMM). Each PhB subunit has an N-terminal region that anchors the prohibitin complex to the membrane (NT-PhB). PhB complex plays a crucial role in premature cellular ageing, apoptosis and maintaining mitochondrial homeostasis. The formation of the Prohibitin complex is affected by cardiolipin (CL), which is mostly present in the IMM and is responsible for maintaining the shape and curvature of the mitochondrial membrane. Despite the essential role of the PhB complex, little is known regarding its structure.
Two of the aims of this project are: (i) to characterize the interaction between the NT-PhB with the membrane and establish a possible synergy of the two PhB homologues, and (ii) to understand the role of CL in this interaction. These questions were addressed by employing simplified membrane models with *in-solution* techniques such as Small-Angle X-ray and Neutron Scattering (SAXS-SANS). To implement these techniques we employed interface techniques, such as Quartz-Crystal Microbalance with Dissipation Monitoring (QCM-D) and Neutron Reflectometry (NR). Our results revealed that the N-terminal PHB peptides disrupt the membrane microstructure. The presence of CL and/or phosphatidylethanolamine enhances the effect of the peptides on membranes and induces a modification of the membrane microstructure.

Status of the SORGENTINA-RF project

Antonino Pietropaolo[1] for the SRF-Collaboration

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The SORGENTINA-RF project aims at developing an accelerator-driven 14 MeV neutron fusion source.
The main scope is the production of medical radioisotopes, but a series of experimental activities and numerical simulations are carried out to study the possibility of obtaining thermalized neutron fields for different applications.
In this contribution, an update of the status of the project is presented in relation to two key components:

1. The mockup of the rotating target
2. The ion source and accelerator

Together with the update on the two components, an experimental study on deuterium implantation on Titanium will be briefly discussed in relation to the operation mechanism of the SORGENTINA's rotating target and ion source.

Attività del Laboratorio di Metrologia dei neutroni dell'INMRI-ENEA

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Il Laboratorio di Metrologia dei neutroni dell'Istituto Nazionale di Metrologia delle Radiazioni Ionizzanti (INMRI) dell'ENEA, operativo nel C.R. Casaccia, sviluppa e mantiene i campioni nazionali di rateo di emissione neutronica, E_n, e di densità di flusso neutronico termico, $\dot{\Phi}_n$. Il primo si basa sulla tecnica del bagno a solfato di manganese ($MnSO_4$), con cui si misura, in modo diretto e con incertezza $\leq$2% (*k=1*), il rateo di emissione neutronica, nell'intervallo 10^5-10^7 s^{-1}, da sorgenti sigillate di ^{241}Am-Be, ^{241}Am-Li, ^{241}Am-B, ^{241}Am-F e ^{252}Cf.
Il secondo si basa su una pila termica con nucleo moderatore in polietilene e riflettore in grafite costituita da sei sorgenti di ^{241}Am-Be (E_n~2.3 10^6 s^{-1}), posizionate in modo complanare a 60° l'una dall'altra, tali da produrre un valore di $\dot{\Phi}_n$ nella pila pari a 1,15 10^4 cm^{-2} s^{-1} (incertezza di 2% (*k=1*)).
I campioni vengono validati da periodici confronti, organizzati a livello internazionale nell'ambito del CCRI-III[1] del BIPM, a cui il Laboratorio partecipa con altri Istituti Primari di Metrologia.
Un servizio di taratura, svolto secondo normativa ISO-8529, viene garantito sia utilizzando le sorgenti neutroniche a E_n noto, sia grazie alla presenza nel Laboratorio di un contatore lungo, modello De Pangher, tarato anch'esso con le sorgenti di cui sopra, che funge da campione di trasferimento di E_n. In tal modo è possibile effettuare tarature, in condizioni di riferimento, di strumenti di neutroni usati presso reattori, acceleratori e/o in radioprotezione con le sorgenti di cui sopra ovvero utilizzare il contatore lungo per eseguire misure in situ presso impianti nucleari.
I codici Monte Carlo MCNP e Fluka vengono anche utilizzati a supporto delle attività sperimentali.

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Tecniche di Luce di Sincrotrone per la Scienza dei Beni Archeologici

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The use of synchrotron radiation (SR) for the analysis of archaeological samples has been increasing over the past years, and experiments related to cultural heritage (CH) study have been performed at many beamlines of Elettra, the Italian SR facility.
TwinMic, the Soft X-ray Microscope, integrates the advantages of complementary scanning and full-field imaging modes into a single instrument.
X-Ray Fluorescence is a highly versatile beamline, optically designed for spectroscopy as well as for microscopy.
The flexible design of the MCX beamline allows a wide range of diffraction experiments relevant for the CH, from phase identification to atomic structural studies.
SYRMEP, the X-ray microtomography station, is a highly flexible beamline allowing analysis in both absorption and phase contrast mode.
The XAFS beamline provides microscopic structural information through the analysis of a sample X-ray absorption spectrum.
UV resonant Raman spectroscopy performed at IUVS beamline is a non-destructive powerful tool for obtaining a detailed compositional characterization of pigments in artworks.
Infrared Microscopy techniques at SISSI beamline offer the possibility to correlate the sample morphological features with its vibrational local pattern at diffraction limited spatial resolution.
The SPEM hosted at the ESCAmicroscopy beamline allows to combine chemically surface sensitive measurements with high spatial resolution.

Abstract dei poster

Amorphous-amorphous transformation induced in glasses by intense x-ray beams

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The first measurements on oxide glasses by means of X-ray Photon Correlation Spectroscopy have revealed a striking fast relaxation time even in the deep glassy state [1]. The technique used to probe the glasses atomic scale dynamics is the X-ray based version of Photon Correlation Spectroscopy (PCS). The fast relaxation has been observed in oxide and metallic glasses. In the case of network forming glasses, the intense X-ray flux generates an artificial dynamics relaxing with a decay time inversely proportional to the dose rate of radiation [2]. The interaction of the X-ray beam with matter generates several photoelectrons that stimulate a subsequent cascade of secondary electrons. The ones with lower energy localise on self-trapped excitons that distort the glass network. At this stage, the breakage of some atomic bonds is stimulated with the consequent motion of the nearby atoms [3]. The artificial dynamics shows a correlation curve with a faster-than-exponential shape which is at odds with the typical stretched exponential relaxations of supercooled liquids. Those compressed exponential functions are due to an excess of stress present in the material, which gives rise to intermittent dynamics and is released via atomic rearrangements [4]. The investigations reported so far have been limited to absorbed doses of a few gigagray in which the phenomenon Is reversible and the structure is barely affected. In the limit of high delivered doses, we have observed that the initial glass is transformed in a new amorphous state which is stable under irradiation [5]. The new phase continues to rearrange under the beam with a stretched exponential relaxation analogous to the one found by macroscopic measurements of supercooled liquids. This suggests that X-ray radiation pumps the glass towards a higher minimum in the potential energy landscape (PEL). We show how this new amorphous state and its dynamics correlates well with the variation in connectivity of different glasses, precisely in a boron oxide glass and a set of silica based glasses with different level of sodium insertion.

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SAXS characterization of gel nanocomposite containing fluorine doped zinc oxide nanoparticles

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The project aims to design and characterize nanocomposite materials composed of hydroxypropyl cellulose (HPC), the most well-known cellulose derivatives and inorganic Fluorine doped ZnO nanoparticles. Nanocomposite hydrogels have been proposed for the functional implementation of conventional hydrogels. Hydroxypropylcellulose (HPC) has the most interesting property of thermoresponsivity upon temperature increase (around 42 °C, lower critical solution temperature, LCST) forms aggregates. The incorporation of suitably nanoparticles with physico-chemical properties produce a hybrid nanocomposite material with peculiar properties for potential application in several fields such as electronic, electrochemical and biomedical devices.

Here we present a structural characterization of hydroxypropyl cellulose containing fluorine-doped zinc oxide nanoparticles through techniques mainly small-angle X-ray scattering (SAXS) with temperature increases, dynamic light scattering (DLS) and Raman measurements. The small angle X-ray scattering was used to study the effect on hydroxypropyl cellulose clustering with varying amount of doped zinc oxide NPs upon temperature. In the case of just HPC the cluster formation was observed only after 45°C, while with varying the HPC to NPs ratio considerably change in the shape and slope of the curves was noted, that according to Raman measurements could be due to the interaction of the NPS with the polymer chain. The effect is much clear when we have a higher ratio of NPs to HPC which also effect the clustering nature of the gel formation. Those results were further cross checked with the dynamic light scattering (DLS) and Raman measurements. Fluorescence measurements were also collected in parallel to evaluate the effect of nanoparticle clustering during polysaccharide gel formation. The preliminary results suggest that the nanoparticles interact with the HPC chains and that play a crucial effect in ruling the structural organization of the gel.

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GO/silica nanocomposites for white light sources

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The aim of this work is to obtain graphene oxide-based materials that are capable of emitting white light if excited under certain conditions. The emission of white light from nanostructured carbon forms differs from conventional white LEDs. As it was found, graphene oxide exhibits a bright white-light emission when they are excited with laser light in the near infrared region. In the visible range the emitted spectrum fits better to the sun spectrum than that of conventional white light sources (blue LED-based), which emit a combination of spectral lines approaching a white-light impression. However, in comparison to a standard black body emitter, it does not emit considerable intensity also in the infrared region, which fits this source for many specific applications [1-5].

Here, the synthesis of nanocomposites based on graphene oxide (GO) and silica was performed by sol-gel method, whereby the hydrolysis and condensation of silica takes place in the presence of exfoliated GO in powder or in aqueous dispersion. Several samples were synthetized modifying the experimental parameters such as the GO amount and the thickness of the glass. The obtained glassy nanocomposites were investigated by Raman Spectroscopy to verify the effect of silica matrix on the GO structural properties. The emission in the visible range, induced by the above laser, was evaluated.

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Sonobioreactor:
a novel platform to study ultrasounds-induced bioeffects

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Ultrasound-based technologies have gathered much interest as a bioprocess optimization tool. Indeed, ultrasounds were shown to increase the rate of transport of mass transfer throughout the cell, furthermore, they can induce the removal of inhibitory feedback metabolites from the cell's surface [1]. The combination of these effects can result in an acceleration of cell metabolism. However, the challenge of realizing engineering tools to fully exploit the potential of ultrasound is full of pitfalls, and their widespread use in laboratory tests is still limited. For this it is crucial to have a fully characterized and modulable platform to induce ultrasounds without affecting routine culturing conditions [2,3]. A novel platform has been manufactured and presented here, based on the stimulation of ultrasound sources. To study the response of the liquid under the acoustic pressure field the wave amplitude and the frequency in different positions were recorded with a hydrophone and simulations with COMSOL Multiphysics were implemented.

The device was applied into two different settings to the culture of green microalgae, as Desmodesmus sp and Chlorella vulgaris, and of yeasts, as Saccharomyces cerevisae. Experiments showed the ability of a fine-tuned

mechanical cycle to induce an optimization in terms of biomass productivity and of bioprocess duration. This promising device is now under customization for other bioprocesses, so that the sonobioreactor can be proposed as a novel tool for sustainable cell culture.

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Title, Arial 14 pts

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High-performance instrumentation projects rely on high-performance neutron guide infrastructure. During the extended reactor outage (2021 – 2023) we have replaced the H1-H2 beam-tube, in-pile optics and three new guides with innovative geometries to provide intense neutron beams to new or upgraded instrumentation.

The upgraded IN5 (2019) time-of-flight spectrometer and its new elliptically focussing H16 cold-neutron guide demonstrates the best-use of phase-space and boasts huge gains in intensity, in particular at shorter wavelengths, while focussing onto much smaller samples.

The new H24 thermal-guide uses a rather elegant concept of a common-curved-trumpet exploiting two radii of curvature to naturally diverge and expand the guide to be split into two distinct branches with four dedicate end-of-guide positions for instrumentation.

The new H15 cold- guide has a rather complex opposing-curved expanding section, referred to as 'the trumpet' serving two important purposes: The first is to spatially expand the neutron guide allowing the guide to be split into multiple individual guide branches and dedicated end-of-guide beam positions. The second is that the opposing curve leaves a 'fingerprint' correlation between the divergence profile and spatial position at the end of the trumpet. Importantly, this allows guide branches to be more widely separated in angle therefore allowing space for substantially more instrumentation down-stream.

Development of drug delivery systems for hydrophobic metastatic melanoma inhibitors

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Over the last years, melanoma treatment strategies have significantly improved patient survival, but there are still unresolved issues in current therapies. New drug combinations are needed to target non-responsive or relapsing patients, and kinases are nowadays established therapeutic targets in the design of novel drugs against cancer [1]. Recently, an in vivo screening demonstrated that the dual targeting of Aurora kinase A and MEK by using the combination of drug inhibitors alisertib and trametinib is highly effective against metastatic melanoma tumors derived from patients [2]. This synergy has already outperformed the standard-of-care therapy in in vitro and in vivo models, nevertheless, aiming at clinical trials, improved drug bioavailability, cellular uptake and tumor accumulation are needed. In this work, we firstly study the inhibitor drugs at the molecular level, from a chemical and crystallographic point of view, with the aim of unravelling their internal interaction profile. This information is fundamental to design novel pharmaceutical co-crystals and salts of studied inhibitors, thus increasing their solubility in biological media. Finally, novel inhibitor loaded nanoformulations are designed with the aim of overcoming the yet unresolved toxicity and efficacy issues in therapy, also providing an increased tumor accumulation via nanoparticle surface functionalization.

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Purification And Characterization of Iron Oxide Nanoparticles (IONs) and Their Potential Use as Drug Delivery Vectors

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Iron oxide Nanoparticles (IONPs) are an important tool in drug delivery for the treatment of wide spectrum of cancer diseases and it is important to investigate the features of these systems in order to develop an appropriate drug delivery system. An innovative approach to obtain IONPs is the use of naturally synthesized NPs derived from magnetotactic bacteria. In this work we used Magnetospirillum gryphiswaldense (MSR-1) to obtain natural IONPs called Magnetosomes (MS). MS are composed by a core of iron oxide coated with a protein rich lipid bilayer. The biosynthesis of these NPs carried out inside MSR-1 by a set of proteins which bring iron ions from outside the cell, crystallize them in the form of iron oxide particles that mature into chains of magnetosomes. The bilayer around the iron core provides a large surface area for the interaction with bioactive molecules and the polarized amino groups on MS membrane increase the negative charge of the surface facilitating electrostatic interaction with bioactive molecules. We show the results of the characterization of naturally MS by means of Dynamic Light Scattering (DLS), Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and X-Ray Diffraction (XRD).
Small Angle X-Ray and Neutron Scattering (SAXS/SANS) was carried out to investigate internal structure of iron oxide core and the properties of the MS membrane.

Characterization of 3D micro-structured TIMEPIX detectors for neutron imaging

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Neutron imaging provides additional information to X-ray imaging and can be used in many applications, for example nuclear engineering, non-industrial diagnostics and homeland security. This paper presents a new 3D structured pixel detector for thermal neutron detection and imaging. It is based on Timepix read-out chip technology (256x256 pixels of 55x55 μm^2 size). The detector, without converted materials, was initially tested in the laboratory with a 241Am source, to simulate events that are induced by reaction products of active material in the silicon bulk, for example $^{6}Li(n,\alpha)^{3}H$ in the case where the holes are filled with ^{6}Li, with positive results. The signals generated by alpha particles and noise signals were discriminated thanks to the analysis of the size of event clusters and energy deposited. In addition to the use of an alpha source, we tested the detector with different gamma sources, to evaluate the gamma rejection ratio, as, in the presence of an intense thermal neutron field, an intense flux of gamma rays may be generated by induced reactions.
These results can be useful as a starting point for future experiments, where neutron beam test will be used, after filling the cavities with active materials, such as LiF. In this paper the results of the characterization and a comparison between experimental data and Monte Carlo simulations will be shown.

PEG-based biomolecular sensors

Margherita Recanatini, Paolo Moretti, Paolo Mariani and Yuri Gerelli

The global impact of the SARS-CoV-2 pandemic has underscored the pressing need for innovative diagnostic assays that are rapid, sensitive, and reliable. While numerous analytical tools have been harnessed to combat the pandemic, many are grounded in conventional methodologies that either necessitate centralized laboratories or, when expedited, compromise sensitivity. Remarkably, a critical gap persists: the absence of effective means for swift and precise quantification of intact, infectious viral particles in respiratory and environmental samples. To bridge this gap, our project is dedicated to enabling ultrasensitive detection of model virion nanoparticles.

Quartz Crystal Microbalance with Dissipation (QCM-D) offers real-time insights into alterations in mass and viscoelastic properties of a thin solid surface film. By evaluating the frequency and dissipation of oscillations in a quartz crystal, the absorption of materials can be quantified, shedding light on the efficacy of surface modifications. Moreover, this technique provides invaluable comprehension of the interaction between the modified surface and target particles, a cornerstone of sensing applications.

The primary objective of this project is to develop optimized surface functionalization protocols using gold surfaces as templates. By investigating key parameters such as PEG grafting density, PEG chain lengths, and the relative amount of active and passive moieties, we aim to achieve a delicate balance that promotes effective binding to target nanoparticles and macromolecules while reducing non-specific interactions. In this contribution we describe the preliminary results obtained by using short active and passive PEG molecules together with test proteins to determine the binding efficiency.

Purification and SAXS analysis of the Nucleocapsid Protein of the SARS-CoV 2 virus

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With the Covid-19 outbreak, great attention has been paid to the mechanism of the SARS-CoV 2 virus infection to develop new therapies. In particular, the nucleocapsid (N) protein has gained immense interest as it is structurally associated with the RNA of the coronavirus and therefore represents a potential molecular target. In recent studies, the ability of the N protein to phase-separate in the presence of viral RNA has been reported to play a key role in the viral replication process. However, the mechanism through which this occurs is not yet understood. Our purpose is to study the structural features of the nucleocapsid protein and to understand the mechanistic basis for the nucleocapsid-mediated RNA packaging. In this work, we focused on the study of the structural features of the N protein using Small-Angle X-ray Scattering (SAXS). For this purpose, we first purified the recombinant full-length N protein using the expression vector R619-X67-527 (Addgene plasmid # 170204), transformed into BL21DE3pLys *Escherichia coli* cells. SAXS experiment was carried out at ID02 beamline, at the European Synchrotron, Grenoble, France. Our preliminary results show that the protein appears to have an elongated conformation and complex supramolecular structures, probably in the form of fibril-like structures.

Laboratorio di Metrologia dei neutroni dell'INMRI-ENEA: Simulazioni a supporto delle attività sperimentali

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Il Laboratorio di Metrologia dei neutroni dell'Istituto Nazionale di Metrologia delle Radiazioni Ionizzanti (INMRI) dell'ENEA, operativo nel C.R. Casaccia, si avvale dell'utilizzo di codici di calcolo per il supporto delle attività sperimentali.
Tali codici sono basati su metodi Montecarlo che consentono lo studio del trasporto dei neutroni all'interno di sistemi che presentano una geometria complessa. Vengono pertanto utilizzati con lo scopo di modellare nel dettaglio le configurazioni sperimentali (sorgenti, strumentazione e ambienti di lavoro) e costituiscono attualmente uno strumento essenziale nella caratterizzazione e taratura di rivelatori di neutroni. Le simulazioni sono utilizzate per la determinazione accurata di fattori correttivi necessari nelle misurazioni, al fine di ridurre le incertezze di misura.
Modelli sono stati sviluppati mediante il codice FLUKA, di alcuni dei principali metodi di misura e di alcune delle sorgenti di riferimento all'interno del laboratorio stesso.
Nello specifico sono stati simulati i seguenti dispositivi:
- il bagno al solfato di manganese (sistema primario per il campione della grandezza "rateo di emissione neutronica");
- long counter (sistema secondario di trasferimento per la grandezza "rateo di emissione neutronica") costituito da un contatore modello De Pangher;
- pozzetto termico (sistema primario per il campione di densità di flusso di neutroni termici), costituito da una pila termica con un valore di flusso neutronico termico di $1{,}15 \cdot 10^{4}$ $cm^{-2}s^{-1}$.
Il poster descrive come sono state predisposte le simulazioni effettuate, con particolare riferimento alla descrizione delle configurazioni sperimentali.

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