Società Italiana di
Spettroscopia Neutronica

XXXIII
Congresso Annuale della Società Italiana di Spettroscopia Neutronica

Milano, 14-16 Settembre 2022

XXXIII Congresso Annuale SISN
Milano, 14-16 Settembre 2022

Questo Congresso è dedicato
alla nostra amica e collega

Laura Cantù

Hai fortemente voluto
questo congresso a Milano
e hai continuato a lavorare
alla sua realizzazione
fino a quando le forze
te lo hanno permesso.

Grazie!

In ricordo di Laura

Nella mattina del 5 agosto 2022 è mancata la Prof.ssa Laura Cantù, professore ordinario di Fisica Applicata del Dipartimento di Biotecnologie Mediche e Medicina Traslazionale della Facoltà di Medicina e Chirurgia all'Università degli Studi di Milano. Laura si è laureata in Fisica nel 1983. La sua ricerca ha riguardato diversi aspetti della Fisica applicata negli ambiti della materia condensata.

Nel campo della spettroscopia neutronica, Laura si è dedicata allo studio delle proprietà chimico-fisiche e dell'auto aggregazione di sistemi colloidali, tensioattivi e soprattutto macromolecole biologiche. Ha condotto studi sulle proprietà strutturali e dinamiche di sistemi lipidici, dalle micelle a modelli di membrana, a differenti livelli di scala temporale e spaziale, utilizzando tecniche di scattering a basso e alto angolo, riflettometria, scattering elastico incoerente, scattering quasi elastico.

Laura ha voluto fin dall'inizio inserirsi in un dipartimento di scienze della vita, avviando collaborazioni interdisciplinari e aprendo la ricerca sperimentale in fisica applicata e in particolare la spettroscopia (visibile, neutroni e raggi-x) a nuovi ambiti, come la biofisica, la biologia e la biochimica, fino alla medicina e alla farmaceutica, istaurando nel tempo anche proficue collaborazioni interdisciplinari. Importanti sono i risultati ottenuti nello studio del ruolo dei gangliosidi nella modulazione delle proprietà strutturali di aggregati biomimetici di crescente complessità, nei meccanismi molecolari alla base di patologie degenerative e nella caratterizzazione di nuovi approcci terapeutici.

Anche recentemente Laura si è dedicata a nuovi temi, come lo sviluppo di nuove matrici di bio-polimeri per la rigenerazione dei tessuti e ha partecipato alla squadra di Anna Moroni e Gerard Thiel coordinatori del progetto ERC "noMAGIC", Noninvasive Manipulation of Gating in Ion Channels, appena concluso.

Laura è stata molto attiva anche all'interno della Società Italiana di Spettroscopia Neutronica, ricoprendo diverse cariche e partecipando con impegno, dedizione e generosità alle attività della Società. Basti ricordare l'entusiasmo contagioso con il quale ha organizzato il XXXIII Congresso della SISN. Dalla sessione sulle attività formative in collaborazione con la Società Italiana di Fisica alla cena sociale presso una pizzeria gestita da ragazzi autistici e laboratorio di inclusione sociale, Laura è stata una fucina di idee e proposte, portate avanti senza risparmiarsi con quel suo coinvolgente sorriso.

Fabio Bruni e i soci della SISN

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Programma del XXXIII Congresso Annuale SISN

Invited talk

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Microscopic collective dynamics in liquid neon-deuterium mixtures: neutron scattering and quantum simulations

Daniele Colognesi
IFAC – CNR, Sesto Fiorentino (FI), Italy

In this talk a combined neutron scattering and quantum simulation study of the collective dynamics in liquid neon-deuterium mixtures, at a temperature of T=30 K and in the wave-vector transfer range 4 $nm^{-1} < q < 51$ nm^{-1}, is presented. Two deuterium concentrations are investigated, one close to 25% molar and the other close to 50% molar, together with pure neon. The dynamic structure factor for the centers of mass of the two molecular species is extracted from the neutron scattering data and subsequently compared with that obtained from three different quantum simulation methods, such as *Ring Polymer Molecular Dynamics* and two slightly different versions of the Feynman-Kleinert approach. A general agreement is found, even though some discrepancies both among simulations, and between simulations and experimental data, can be observed. In order to clarify the physical meaning of the present spectroscopic results, an analysis of the longitudinal current spectral maxima is carried out showing the peculiarities of the deuterium center-of-mass dynamics in these mixtures. A comparison with the centroid molecular dynamics results obtained for the deuterium center-of-mass self-dynamics in the same liquid mixtures is finally proposed.

Co-authors: Dr. Ubaldo BAFILE (IFAC-CNR, Italy); Dr. Eleonora GUARINI (Dipartimento di Fisica e Astronomia, Università di Firenze, Italy); Prof. Martin NEUMANN (Fakultät für Physik der Universität Wien, Austria); Dr. Tatiana GUIDI (ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Science and Technology Facilities Council, UK).

Oxygen ion diffusion mechanisms in non-stoichiometric oxides explored by neutron scattering

Monica Ceretti
ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier

Understanding fundamental mechanisms of oxygen ion conduction in solid oxides at moderate temperatures is today an important issue for the development of a variety of technological devices, such as oxygen membranes, electrolytes for sensors or membranes in SOFCs. Two structure types, both perovskite-derivatives, show oxygen-ion conductivity at moderate temperatures or even at ambient: the Ruddlesden-Popper K_2NiF_4 type structure, and the brownmillerite-type structure. Both types are non-stoichiometric and are able to accommodate an important amount of oxygen on interstitial or regular lattice sites, filling up the 1D oxygen vacancy channels.

We report here a combination of neutron diffraction, inelastic neutron scattering and ab initio lattice dynamics calculations, to evidence that this oxygen mobility is related to low energy phonon modes, underlying their importance to trigger low temperature oxygen mobility $(Nd/Pr)_2NiO_{4+\delta}$ with K_2NiF_4 type structure.[1-3]

In particular, neutron powder diffraction revealed a complex phase diagram of unprecedented complexity, involving a series of highly organized 3D modulated phases related to oxygen ordering.[4, 5] All phase transitions involve translational periodicities exceeding 100 A, and were all found, with fast ordering kinetics. The structural correlations induced by the presence of interstitial oxygen atoms thus suggest a collective phason-like oxygen diffusion mechanism together with dynamical contributions from the aperiodical lattice creating shallow diffusion pathways, down to room temperature.

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The mechanism of interaction of spike protein and fusion peptides with model membranes

Giovanna Fragneto
Institut Laue-Langevin, 71 avenue des Martyrs, 38042 Grenoble

Model biological membranes from synthetic and natural lipids were used to study the mechanism of fusion of the spike protein as well as fusion peptides from SARS-CoV-2 with cells. Neutron scattering techniques were used to determine the structural and dynamical modifications in an effort that has seen several ILL scientists and external collaborators involved. Only the structural studies from neutron reflectivity and SANS measurements will be detailed here.

Lipid stripping was observed in the study of the interaction of the soluble spike with ACE2 receptors in the membranes [1]. The peptides had different modalities of interaction with the membrane which allowed to suggest a possible mechanism of fusion [2]. The effect of cholesterol was also investigated.

The importance of using natural lipid extracts produced at the L-Lab facility (www.ill.eu/L-Lab) to produce the membranes will be highlighted.

The talk is dedicated to Laura Cantù, and will acknowledge our precious collaboration in lipid research. In memory of our friendship, her passion for neutrons and contagious smile.

[1] Luchini A., Micciulla S., Corucci G., Batchu K.C., Santamaria A., Laux V., Darwish T., Russell R.A., Thépaut M., Bally I., Fieschi F., Fragneto G.* - Lipid bilayer degradation induced by SARS-CoV-2 spike protein as revealed by neutron reflectometry - Scientific Reports 11, 14867-1-14867-11 (2021)

[2] Santamaria A., Batchu K. C. , Matsarskaia O., Prévost S. F., Russo D., Natali F. , Seydel T., Hoffmann I., Laux V., Haertlein M., Darwish T. A. ,Russell R. A., Corucci G., Fragneto G. , Maestro A.*, and Zaccai N. R.* - Strikingly Different Roles of SARS-CoV-2 Fusion Peptides Uncoveredby Neutron Scattering - Journal of the American Chemical Society 2022, 144(7)

Recent advancements in neutron imaging

Nikolay Kardjilov, Ingo Manke, André Hilger, Tobias Arlt, John Banhart
Helmholtz Centre Berlin for Materials and Energy (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The material characterization by neutron imaging reached a new level after developing innovative techniques using different contrast mechanisms than the common beam attenuation. In this way properties of materials and complex systems can be resolved by position sensitive mapping of diffraction, small-angle scattering and refraction signals. In addition the improved spatial and time resolution of the detector systems allow for micro tomography studies and 3D dynamic investigations. Applications related to 2D and 3D visualization of material phase heterogeneities, texture, fluid dynamics, magnetic structures and phase transitions in applied materials will be presented and analysed.

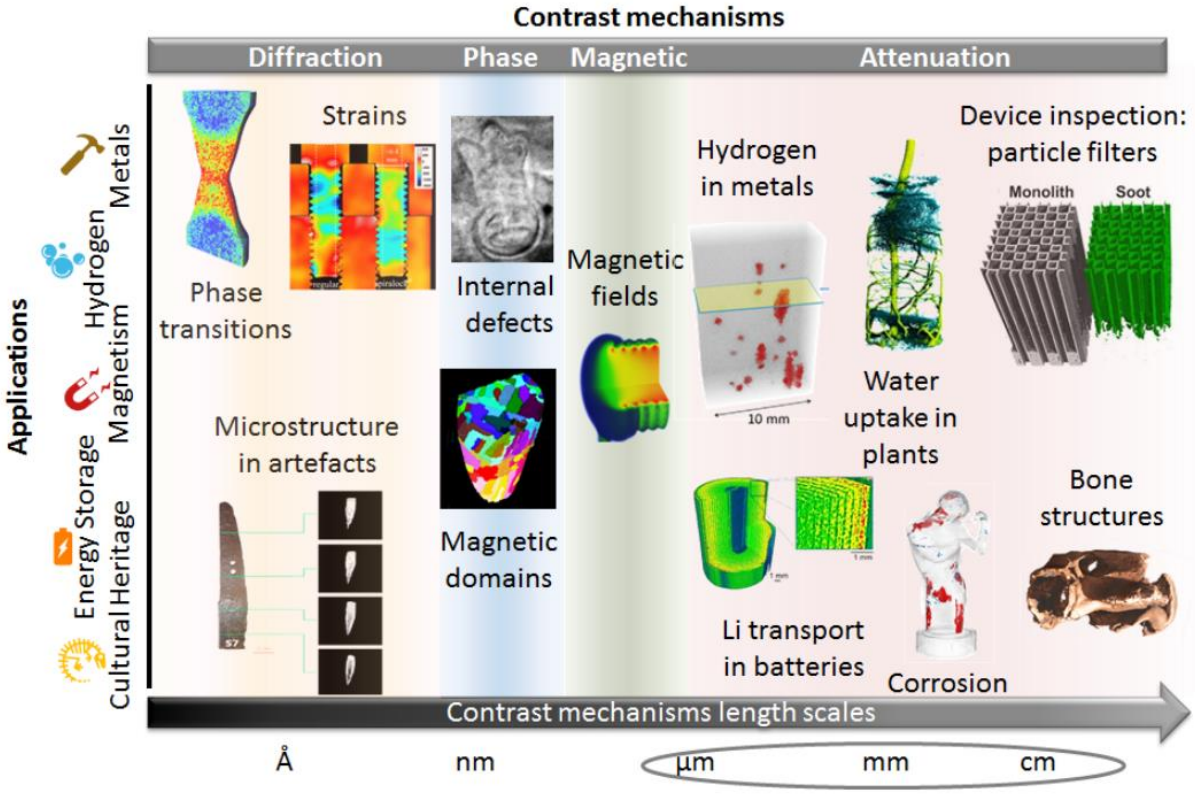

Figure 1: Different contrast mechanisms can be used to explore various length scales in materials and to study their properties and related processes. The relation between contrast mechanisms and different application fields is presented. The length scale presented on the lower axis relates to the corresponding contrast mechanism specified on the upper axis. For the attenuation based image techniques the large length scale was emphasized by grouping the scales from µm to cm.[1]

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The ILL - Perspectives and opportunities for science and innovation in the next decade for scientists from Italy

Mark Johnson

Institut Laue-Langevin, 71 avenue des Martyrs, 38042 Grenoble

Talk

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Extended range Bonner Sphere Spectrometer per misure neutroniche in alta quota

A. Calamida [1], A. Fontanilla [1], A. I. Castro Campoy [1], C. Cantone [1], A. Pietropaolo [1,2], J. M. Gomez-Ros [1,3], V. Monti.[4], E. Mafucci [4,5], S. Vernetto [4,5], A. Pola [6], D. Bortot [6], R. Bedogni [1].

1. *INFN, Laboratori Nazionali di Frascati, via Enrico Fermi 40, 00044, Frascati, Italy*
2. *ENEA Dept. Fusion and Technologies for Nuclear Safety and Security, Frascati, Italy*
3. *CIEMAT, Av. Complutense 40 - 28040, Madrid, Spain*
4. *Università degli Studi di Torino, via P. Giuria 1, 10125, Torino, Italy*
5. *INFN, Sezione di Torino, via P. Giuria 1, 10125, Torino, Italy*
6. *Politecnico di Milano, Dipartimento di Energia, via La Masa 34, 20156 Milano, Italy*

Al fine di misurare lo spettro cosmico neutronico al alte altitudini è stato progettato, nell'ambito del progetto SAMADHA (*South Atlantic Magnetic Anomaly Dosimetry at High Altitude*) dell'INFN, un *Extended Range Bonner Sphere Spectrometer* (EBSS). Lo spettrometro consiste di otto sfere moderatrici, 6 di polietilene ad alta densità (HDPE) e 2 di HDPE più un inserto di materiale ad alta densità. Ogni sfera ha un contatore proporzionale cilindrico di elio-3 al suo interno pressurizzato a 10 bar. La matrice di risposta per ogni sfera è stata calcolata usando il codice Monte Carlo (MC) MCNP6. A causa dei bassi tassi di conteggi aspettati nell'*environnement* sperimentale, sono stati adottati dei particolari criteri di design per prevenire l'insorgere di segnali spuri non neutronici. Lo spettrometro è stato esposto in un campo neutronico di riferimento impiegando una sorgente di ^{241}Am-Be presso il Politecnico di Milano. Si è potuto così validare la matrice di risposta ottenuta dalle simulazioni MC con un'incertezza complessiva di circa ± 2 %.

Non-destructive diagnostic of the manufacturing process of the Porta Sud of Battistero di Firenze by Andrea Pisano through neutron techniques

F. Cantini [1-3], F. Grazzi [2, 3], R. Filardi [4], B. Agostini [4], S. Agnoletti, [5], A. Brini [5], M. Baruffetti [5], M. Galeotti [5], A. Cagnini [5], S. Porcinai [5], A. Scherillo [6], A. Fedrigo [6], A. Hillier [6], L. Speranza [5].

1. *Università degli Studi di Firenze, Dipartimento di Fisica e Astronomia, Sesto Fiorentino, FI (Italy)*
2. *Consiglio Nazionale delle Ricerche, Istituto di Fisica Applicata Nello Carrara, Sesto Fiorentino (Italy)*
3. *Istituto Nazionale di Fisica Nucleare, Laboratorio di Tecniche Nucleari per i Beni Culturali, Sesto Fiorentino (Italy)*
4. *Opera di Santa Maria del Fiore, Firenze (Italy)*
5. *Opificio delle Pietre Dure, Firenze (Italy)*
6. *Science and technology Facility Council, ISIS Neutron and Muon Source, OX110QX (UK)*

The Porta Sud of Battistero di Firenze is a 5 meters high bronze artifact designed by Andrea Pisano and cast by Lorenzo D'Avanzo and co-workers between 1329 and 1336. It is one of the oldest Middle Ages bronze gates in existence in Europe. It has two shutters, each decorated by 14 quatrefoil scene relief panels, 24 lion heads (located at the corner of the panels), and 37 decorative friezes with all made in a quaternary alloy of copper, zinc, tin and lead with copper and zinc as main elements. All the components were separately cast, gilded and mechanically embedded into the shutter frames. The gate was recently dismounted from its location on the south side of Battistero to be restored in the metal conservation department of Opificio delle Pietre Dure (OPD) in Firenze.

During the restoration 5 elements were detached from the gate (two of them felt down during the Florence flood in 1966): a relief decorated panel (Formella), a lion head, a decorative frieze and two back disks which were transported to the ISIS neutron and muon source in Oxfordshire (UK) to be analyzed with different non-destructive neutron techniques such as neutron imaging, neutron diffraction and nuclear resonance capture analysis. The combination of this methods allowed us to characterize the alloy of the 5 detached elements, to obtain morphological, compositional, microstructural details of each element, and to perform a high accuracy technological investigation of the casting manufacturing procedures.

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Uso di sorgenti di neutroni a spallazione per l'irraggiamento della microelettronica

C. Cazzaniga [1], M. Kastriotou [1] and Frost D.[1]

1. *ISIS Neutron and Muon source, STFC-UKRI, Rutherford Appleton Laboratory*

La microelettronica ha visto di recente un continuo aumento in potenza di calcolo e complessità, accompagnato da un crescente uso in settori dove l'affidabilità e' critica, come l'avionica, l'automazione dei veicoli, applicazioni mediche e infrastrutture di comunicazione. Per questo motivo industria e accademia fanno un crescente utilizzo di sorgenti di neutroni con spettro atmosferico, allo scopo di testare gli effetti della radiazione su dispositivi e sistemi.

I neutroni atmosferici vengono prodotti in laboratorio da reazioni a spallazione, quando un fascio di protoni a energia elevata > 500 MeV collide su un bersaglio composto da un metallo pesante. In nord America, a LANSCE (USA) e TRIUMF (Canada), dei bersagli sono dedicati esclusivamente alla produzione di neutroni veloci. Ad ISIS (UK) per la prima volta si e' integrata una linea di neutroni atmosferici, ChipIR, in un'infrastruttura dedicata alla produzione di neutroni termici, da usarsi principalmente per studi di diffrazione. ChipIR ha una linea di vista progettata per estrarre i neutroni veloci dal bersaglio di tungsteno. Un simile concetto e' stato ora riproposto anche a CSNS (Cina).

Anche i neutroni termici possono causare effetti sulla microelettronica. In sistemi commerciali, le impurità di boro possono causare un'alta probabilità di fallimento per la cattura di neutroni termici. Per questo motive anche una linea di neutroni termici, EMMA, e' usata ad ISIS per studi di irraggiamento. Infine, due sorgenti di neutroni monoenergetici, 14 MeV e 2.5 MeV, completano il parco di fasci di neutroni che ad ISIS sono dedicati a studi di microelettronica.

Effect of chemical and structural modifications on the phonon-induced magnetization dynamics of Single-Molecule Magnets

S. Chicco[1], E. Garlatti [1,2], T. Guidi [4], P. Bonfà [1], I. J. Onuorah [1], A. Mavromagoulos [5], A. B. Canaj [6], J. Skelton [3], D. Mills [3], P. Santini [1,2], N. Chilton [3], M. Murrie [5] and S. Carretta [1,2].

1. *Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, I-43124 Parma, (IT) and UdR Parma, INSTM, Parma, (IT)*
2. *INFN, Sezione di Milano-Bicocca, gruppo collegato di Parma, I-43124, (IT).*
3. *Department of Chemistry, The University of Manchester, Oxford Road, Manchester M139PL (UK).*
4. *Physics Division, School of Science and Technology, University of Camerino, Camerino (MC) I-62032, (IT)*
5. *School of Chemistry, University of Glasgow, Glasgow G12 8QQ Scotland, (UK)*
6. *EaStCHEM School of Chemistry, The University of Edinburgh, David Brewster Road, Edinburgh, EH9 3FJ, Scotland, (UK)*

Single-Molecule Magnets (SMMs) are promising candidates for the miniaturization of data storage devices. [1] Indeed, SMMs possess a bi-stable ground state and display slow relaxation of the magnetization. Mononuclear Dy-based SMMs are promising candidates for this application, and recently a record blocking temperature (60-80 K) have been reported for dysprosocenium compounds [2]. The high anisotropy barrier is not the only factor influencing the blocking temperature. Indeed, 4f-based molecules with similarly high barriers can display very different relaxation dynamics. Therefore, it is fundamental to understand the role of phonons in the relaxation dynamics of SMMs and how they are affected by the chemical structure and its deformations. Here we present two works focusing on how phonon spectra in Dy-based SMMs are modified by structural deformation induced by applied pressure, or by chemical modifications of surrounding ligands and/or counter-ions. We measured the phonon density of state of several Dy-based compounds by inelastic neutron scattering (INS), on the spectrometers IN8 (in applied pressure) and IN1 at the ILL. The INS data are then compared with density functional theory (DFT) calculations of phonon modes, with an optimal agreement. DFT-calculated phonon energies and polarization vectors are indeed the starting point for the modelling of the relaxation dynamics of SMMs. These results allow us to gain an unprecedented insight on the origin of high-blocking temperatures in SMMs, beneficial for improving their performances.

This work has received funding from the European Union's Horizon 2020 Research and Innovation Programme (FET-OPEN project FATMOLS) under grant agreement No. 862893. The computational work was supported by the SUPER, Action 1.5.1, POR-FESR 2014–2020 Emilia Romagna project, by CINECA IsB20_PRISM and IsC71_DMSPER Grants, by the Royal Society University Research Fellowship and ERC StG, and ERC CoG and EPSRC Standard Grant.

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[3] A. Chiesa, F. Cugini, R. Hussain, E. Macaluso, G. Allodi, E. Garlatti, M. J. Giansiracusa, C. A. P. Goodwin, F. Ortu, D. Reta, J. M. Skelton, T. Guidi, P. Santini, M. Solzi, R. De Renzi, D. P. Mills, N. F. Chilton, and S. Carretta, Phys. Rev. B 101, 174402 (2020).

Understanding phonon-mediated relaxation in Rare-Earth Single Molecule Magnets: insights from INS

A. Chiesa [1,2,3,] E. Garlatti [1,2,3], P. Bonfà [1], E. Macaluso [1,2,3], I. J. Onuorah [1], V. S. Parmar [4], Y. S. Ding [5], Y. Z. Zheng [5], M. J. Giansiracusa [4], D. Reta [4], E. Pavarini [6], T. Guidi [7], D. P. Mills [4], N. F. Chilton [4], R. E.P. Winpenny [4], P. Santini [1,2,3] and S. Carretta[1,2,3]

1. *Università di Parma, Dipartimento di Scienze Matematiche, Fisiche e Informatiche, 43124 Parma, Italy*
2. *INFN*
3. *UdR Parma, INSTM, I-43124 Parma, Italy*
4. *Department of Chemistry, The University of Manchester, Manchester, U.K.;*
5. *Frontier Institute of Science and Technology, Xi'an Jiaotong University, 710054 Xi'an, Shaanxi, China*
6. *Institute for Advanced Simulations, Forschungszentrum Juelich and JARA High-Performance Computing, RWTH Aachen University, Aachen, Germany*
7. *ISIS Facility, Rutherford Appleton Laboratory, Didcot, U.K.*

Single-ion magnets are emerging as one of the most promising platforms for high-density information storage, with some Dy-based complexes showing slow relaxation of the magnetization up to 80 K [1]. To further improve their performance by proper design, a deep understanding of magnetic relaxation is mandatory.

Here we present a cost-effective approach describing the peculiar behavior of these compounds based on different phonon-mediated mechanisms. To derive our model, we start from inelastic neutron scattering measurements of the phonon density of states and we combine it with ab-initio calculations of the crystal-field states and of local vibrations, finally explaining a broad range of Ac and DC magnetization and nuclear magnetic resonance experiments.

We apply our approach to some paradigmatic molecules all containing a single Dy ion, but showing very different relaxation [2,3]. We clearly explain such behaviors based on the different crystal-field symmetries and different phonon modes observed by INS and computed ab-initio, arising from different arrangements of the ligands. Our model allows us to disentangle the different mechanisms at play, to identify the crucial ingredients behind slow relaxation and to derive a general recipe to design high-blocking-temperature rare-earth single-ion magnets.

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[2] A. Chiesa et al., Phys. Rev. B 101, 174402 (2020).
[3] E. Garlatti et al., J. Phys. Chem. Lett. 12, 8826-8832 (2021).

Carbohydrates role in bioprotection: their interaction with model polypeptides in aqueous solution

M. Di Gioacchino [1], F. Bruni [1], O. Alderman [2], S. Imberti [2], M.A. Ricci [1]

1. *Dipartimento di Scienze, Università degli Studi Roma Tre, via della Vasca Navale 84, 00146 Roma, Italy*
2. *UKRI-STFC, ISIS neutron and muon source, Rutherford Appleton Laboratory, Harwell Campus, Chilton, Didcot, OX11 0QX, United Kingdom*

The issue of the interaction of carbohydrates with a biomolecule is of great interest, as these interactions are responsible for the biomolecule protection against environmental stresses, such as dehydration and osmotic pressure [1]. This phenomenon is tackled by investigating at the atomic scale the interaction of carbohydrates (glucose and trehalose) with aqueous solution of two model peptides, namely N-methylacetamide (NMA) [2] and Glycyl-L-prolyl-glycinamide-HCl (GPG) [3]. These studies, performed by neutron diffraction with isotopic substitution augmented by Monte Carlo simulation analysis [4], evidences clear differences between the behaviour of two carbohydrates. While trehalose confines water within the hydration shell of the solute [5,6], glucose enters this shell in competition with water molecules [7]. As a result, the peptide functional structure in aqueous solution is deformed in presence of glucose, while it remains unperturbed in presence of trehalose. These observations may be the key to distinguish the protection mechanism against drought from that against osmotic pressure [7].

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Lung surfactants: effect of composition on the physicochemical properties of biomimicking membranes

N. Gallucci[1,2], A. Cangiano[1], A. Santamaria[3,4], G. Pompea, G. Del Vecchio[1], L. Cavalcanti[5], G. Vitiello[2,6], L. Paduano[1,2]

1. *Department of Chemical Sciences, University Federico II, Naples, Italy*
2. *CSGI, Center for Colloid and Surface Science, Sesto Fiorentino, Italy*
3. *Institut Laue-Langevin, Grenoble, France*
4. *Departamento de Quimica Fisica, Universidad Complutense de Madrid, Madrid, Spain.*
5. *ISIS Neutron and Muon Source, STFC, Didcot, UK*
6. *Department of Chemical, Materials and Production Engineering, University Federico II, Naples, Italy*

The last pandemic disease highlights the importance to know the interaction between virus and eukaryotic membrane.[1] Membrane model systems, such as liposomes, are widely studied, however, our knowledge about the interaction between natural systems, such as viruses, with synthetic and natural interfaces are far from fully understood. This gap limits the ability to leverage this understanding to push the next level of selectivity, efficiency, and targeting. Lung surfactant is a complex with a unique phospholipid and protein composition. It is present as a thin film lining the alveolar surface of the lung with an essential function of lowering the surface tension and the energy for breathing. It also prevents alveolar collapse.[2,3] For these reasons, it seemed appropriate to understand first how lipid part of the lung membranes affected the physicochemical properties of the systems itself. This was done by studying the thermodynamic quantities, the properties at the interface, and the mechanical properties of pulmonary surfactants, combing different techniques, such as DSC, DLS, SANS, and Langmuir Adsorption Isotherm. Understanding how the phospholipids affect the physicochemical properties of the membrane can benefit the development of new strategies to contrast the proliferation of new disease.

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The CHNet_NICHE experiment of INFN.
The construction and performances of a new neutron imaging station at Laboratorio Nazionale di Fisica Nucleare in Pavia

F. Grazzi[1,2], N. Gelli[1], and the CHNet_NICHE collaboration[1,3,4,5,6]

1. *Istituto Nazionale di Fisica Nucleare, Sezione di Firenze*
2. *Consiglio Nazionale delle Ricerche, Istituto di Fisica Applicata "Nello Carrara", Sesto Fiorentino (FI)*
3. *Istituto Nazionale di Fisica Nucleare, Sezione di Pavia*
4. *Istituto Nazionale di Fisica Nucleare, Sezione di Milano Bicocca*
5. *Istituto Nazionale di Fisica Nucleare, Sezione di Bologna*
6. *Istituto Nazionale di Fisica Nucleare, Sezione di Torino*

The INFN Cultural Heritage Network (CHNet) of INFN represents one of the most important collaboration networks in Cultural Heritage diagnostic in Italy. It consists of a network of more than 15 laboratories all over Italy, equipped with portable and laboratory analytical instrumentation. The Neutron Imaging for Cultural Heritage Experiment (NICHE) represents the first step of CHNet towards the development and application of neutron methods in Cultural Heritage within the Italian territory. The possibility to have an operational neutron imaging station in Italy makes possible to perform neutron radiography and tomography measurements on several historical and archaeological artefacts since the administration and safety procedures to move samples within Italy are much easier than transporting them abroad making neutron imaging affordable for small Museums and Restoration Centers. The station is located on the thermal beam port of the TRIGA MARK II 250 kW reactor of Laboratorio di Energia Nucleare Applicata, jointly operated by INFN and Università di Pavia.
The NICHE experiment is three years long (expires in December 2022) and consists in the installation, characterization and CH-related sample measurements. The results of such activity will be shown in this presentation.

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Characteristics and Internalization Mechanism of Extracellular Vesicles

S. Helmy[1,2], P. Brocca[1], P. Parisse[3,4], L. Casalis[4], and V. Rondelli[1]

1. *Department of Medical Biotechnology and Translational Medicine, Università degli Studi di Milano, Segrate, Italy*
2. *Biophysics Group, Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt*
3. *Istituto Officina dei Materiali-National Research Council (CNR-IOM), Area Science Park, Trieste, Italy*
4. *Elettra Sincrotrone Trieste, Area Science Park, Trieste, Italy*

Extracellular Vesicles (EVs) secreted into the extracellular space, proved their role in mediating the intercellular communication between close and far tissues. Yet, how they internalize into target cells is still an unanswered question. We are employing integrative techniques for correlating the structure-function properties of EVs extracted from Neuroblastoma cells (Ctrl EVs) and comparing them to EVs (Oligo EVs) isolated from the same cells treated with the OligoGM1 oligosaccharide, known for its neurotrophic and neuroprotective functions on neuronal cells1. These EVs were characterized by diverse biochemical and physical techniques. While their interaction with model membranes was investigated by atomic force microscopy (AFM), differential scanning calorimetry (DSC), Fourier transform infrared spectroscopy (FT-IR) and neutron reflectometry (NR) which was applied to monitor the structural effects brought by EVs to different simple and complex model membranes to clarify perceptions on EVs' membrane internalization mechanism. It was noted that these EVs, were different from one another regarding their chemico-physical characteristics and their interaction with target model membranes, and also distinct from different origin EVs2,3. A peculiar internalization mechanism of EVs into the model membranes was observed. Thus, our results prove the distinctiveness of EVs from different origin cells and the importance of integrated experimental approaches4 in this uprising hot field.

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Room temperature multiferroicity in γ-$BaFe_2O_4$

F. Mezzadri[1,2], F. Orlandi[3], D. Delmonte[1], G. Calestani[2], E. Cavalli[2], E. Gilioli[1], V. V. Shvartsman [4], P. Graziosi [5], S. Rampino [2], G. Spaggiari [1,6], M. Solzi [6], M. Casappa[1,2].

1. *IMEM-CNR, Parco Area delle Scienze 37/A, 43124 Parma, Italy*
2. *Department of Chemistry, Life Sciences and Environmental Sustainability, University of Parma, Parco Area delle Scienze 17/A, 43124 Parma, Italy*
3. *ISIS Facility, Rutherford Appleton Laboratory, Harwell Campus, Didcot OX110QX, United Kingdom*
4. *Institute for Materials Science and Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Universitätsstrasse 15, 45141 Essen, Germany*
5. *CNR-ISMN, Via P. Gobetti 101, 40129 Bologna, Italy*
6. *Department of Mathematical, Physical and Computer Sciences, University of Parma, Parco Area delle Scienze 7/A, Parma*

Multiferroics are promising materials for the design of new multifunctional devices, in particular when coupling of ferroelectricity (FE) and long range magnetism is involved. However, most of the known multiferroics are not ordered at RT, so the discovery of new materials is crucial for the development of the field, as well as the thorough study of both their nuclear and magnetic structures, allowing the modelling of the coupling mechanisms and possibly addressing suitable chemical subtitutions aimed at fine-tuning of the physical properties. γ-$BaFe_2O_4$ is a “stuffed trydimite” with reported weak ferromagnetic behavior and mild photocatalytic activity. Our single crystal X-ray diffraction studies point out the polar nature of the compound at RT, giving rise to FE properties, fully characterized by electrical and piezo force microscopy measurements. On the other hand, neutron powder diffraction reveals a G-type antifferomagnetic (AFM) spin structure with T_N=890K. No detectable canting of the atomic moments is present, in agreement with SQuID measurements carried out on phase pure thin films. This result suggests the weak ferromagnetic component previously reported in bulk samples to be ascribed to traces of spurious phases, not detected by other techniques. Within this framework, neutron diffraction behaves as a phase-sensitive technique, not affected by the presence of impurities masking the AFM signal in magnetometric measurements.

Neutrons help the study of innovative nanomaterials for curative and preventive wood deacidification treatments.

A. G. Taglieri[1], R. Schweins[2], S.Zorzi[3], Gilles Chaumat[4] and C. Mondelli[5]

1. *Dept. of Industrial and Information Engineering and Economics, University of L'Aquila, Monteluco di Rojo, 67100 L'Aquila, IT.*
2. *Institut Laue Langevin, 71, Avenue des Martyrs Cedex 9 38042 Grenoble, FR.*
3. *Dept. of Molecular Science and Nanosystems, University Ca' Foscari Venezia, Via Torino, 155/b ETA, 30172 Venezia-Mestre, IT.*
4. *ARC-Nucleart CEA, 17, Avenue des Martyrs, Cedex 9, 38042 Grenoble, FR.*
5. *CNR-IOM-OGG, Institut Laue Langevin, 71, Avenue des Martyrs Cedex 9 38042 Grenoble, FR.*

Waterlogged wooden artifacts represent an important historical legacy of our past. They are very fragile, especially due to the severe phenomenon of acidification that may occur in the presence of acid precursors when they are brought to land. The immersion of the wooden artifacts in a solution of PEG to replace the water in the structure and prevent cracking as the wood dries out it is not effective to stop the acidification that can emerge on the wood years after the treatment. To date, a satisfactory solution for the deacidification of ancient wood on a large scale has still not been found. In this paper, we propose, for the first time, eco-friendly curative and preventive treatments using nanoparticles (NPs) of earth alkaline hydroxides dispersed in water and produced on a large scale. We present the characterization of the NPs in particular with small-angle neutron scattering, together with the study of the deacidification efficiency of the treatments on a 2000 years old Gallo-Roman barge at the Lugdunum Museum (Lyon, France, on loan from ARC-Nucleart (Grenoble, France). We demonstrate that all our treatments are very effective for both curative and preventive aims, able to assure an almost neutral or slightly alkaline pH of the treated woods. [!] Furthermore, the use of water as a solvent paves the way for large-scale and eco-friendly applications, which avoid substances that are harmful for the environment and for human health.

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Structural and Thermodynamic Analysis of Prefibrillar WT α Synuclein and Its Mutants by a Combination of Small-Angle Scattering and Variational Bayesian Weighting

P. Moretti[1], P. Mariani[1], M. G. Ortore[1], N. Plotegher[2], L. Bubacco[2], M. Beltramini[2] and F. Spinozzi[1].

1. *Università Politecnica delle Marche,Department of Life and Environmental Science (DiSVA), Ancona, Italy*
2. *Department of Biology University of Padova, Padova, Italy*

The small-angle X-ray scattering SAXS technique was used to study α-synuclein (α-syn) [1], the intrinsically disordered protein (IDP) involved to Parkinson's disease. SAXS experiments were performed as a function of temperature and concentration on the wild type (WT) and on the three different pathogenic mutants (G51D, E46K and A53T). SAXS curves were analyzed using a new variational Bayesian weighting method (VBWSAS) based on a set of conformers, including unfolded monomers, trimers and tetramers. The aim of this new methodology is to identify the conformers which populate WT α-syn and the pathogenic mutants under prefibrillar conditions. The VBWSAS method takes into account the effects of temperature and concentration using a thermodynamic scheme and considers long-range protein-protein interactions in the framework of random phase approximation [2]. Simultaneous analysis of the entire dataset indicates that WT α-syn is mostly present as unfolded monomers and trimers, but not tetramers, as previously derived from several studies. On the contrary, different combinations of conformers characterize the mutants. The derived conformational behavior therefore suggests a different availability of species prone to aggregation, depending on the mutation, temperature and concentration of the α-syn variants. The VBWSAS approach can be of fundamental importance to describe the conformational and aggregative properties of other IDPs and could also be applied in Small Angle Neutron Scattering.

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The SORGENTINA-RF project

A. Pietropaolo[1] for the SRF Collaboration

1. *ENEA- Dept. Fusion and Technologies for Nuclear safety and Security*

The SORGENTINA-RF project is presented in terms of general structure and description of the main tasks and activities to be carried out.
The project is devoted to the design and development of a medium power 14 MeV fusion neutron source relying on a rotating target and a deuterium/tritium ion accelerator.
The main focus of the neutron facility is the production of radiopharmaceutical precursors, in particular ^{99}Mo as precursor of ^{99m}Tc, a radio-tracer used in single photon emission computed tomography. The nuclear reaction involved in the production of ^{99}Mo is the inelastic reaction ^{100}Mo(n,2n)^{99}Mo.The facility will assess the chain that starts with the irradiation of the natural molybdenum (where ^{100}Mo has an isotopic abundance of about 10%) up to the production of the so-called mother solution, a liquid solution named sodium molybdate.
The facility is supposed to provide also fast and thermal neutron beams for studies on innovative medical radioisotopes as well as materials.

Synthesis and investigation of PNIPAM homo- and block- co- polymers: from linear chains to self-assembled micelles

B. P. Rosi[1], J. Allgaier[1], M. Kruteva[1], S. Förster[1].

1. *Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1: Neutron Scattering and Biological Matter)*

Poly(N-isopropylacrylamide) (PNIPAM) is a thermoresponsive polymer well known for having a lower critical solution temperature (LCST) around 32°C in water, at which a coil-to-globule transition occurs. The thermoresponsive character makes PNIPAM attractive for both technological applications and fundamental studies, in particular, it has been exploited to draw simple but predictive models for protein structure and dynamics [1].
The versatility of PNIPAM has prompted the synthesis of PNIPAM-based thermoresponsive materials with specific architectures [2]. A great interest has been raised toward PNIPAM-based block copolymers. When the other blocks are persistently hydrophobic, as in the case of polystyrene (PS), PNIPAM-containing block copolymers can form thermoresponsive micelles and micellar gels, which are attractive for temperature-regulated loading and release applications. Moreover, the intrinsic complexity of these systems compared to "classical" micelles makes them more suitable to reproduce the sophisticated behaviour of biological membranes [3]. The composition of PS-PNIPAM copolymers affects the micellar structure, which in turn strongly influences the thermal response of the system. Structural properties are also found to impact on the local dynamics on the PNIPAM shell, as well as on the global diffusion of the micelles [4]. For a deeper understanding, systematic studies of both structural and dynamical properties of PS-PNIPAM diblocks are required.

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Neutron capture and neutron diffraction techniques in the characterisation of stony meteorites

R. Rossini[1,2], T. Agoro[3], M. Cataldo[1,2,3], M. Clemenza[1,2], G. Gorini[1,2], A. Hillier[3], M. Laubenstein[4], G. Marcucci[1,2], M. Musa[1], M.P. Riccardi[5,6], A. Scherillo[3], D. Di Martino[1,2]

1. *Università degli Studi di Milano-Bicocca, Milan, Italy*
2. *INFN section of Milano-Bicocca, Milan, Italy*
3. *STFC, ISIS Neutron and Muon Source, Didcot, United Kingdom*
4. *INFN Laboratori Nazionali del Gran Sasso (LNGS), L'Aquila, Italy*
5. *Università degli Studi di Pavia, Pavia, Italy*
6. *Arvedi Laboratory, CISRiC, Pavia, Italy*

The study and non-destructive characterisation of meteorites is an important task in modern science. In fact, meteorites can unveil important information about the origin of the Solar System and the Cosmogenesis. However, meteorites can also be samples with a historical-cultural value and they should be handled with care, avoiding destructive measurements when possible.

In this framework, we developed a new multidisciplinary non-destructive protocol to perform this characterisation, where the key point is the use of neutron-based techniques for elemental and mineralogical analysis. We carried out all the neutron measurements at the INES beamline of the ISIS Neutron and Muon Source, in the United Kingdom.

In particular, Time-of-Flight Neutron Diffraction (ToF-ND) was carried out and analysed with Rietveld refinement. In this way, one can extract information about the mineralogical phases content, presence of strains and elemental substitutions.

Neutron-capture techniques such as Neutron Resonant Capture Analysis (NRCA) and space-resolved Neutron Resonant Transmission Imaging (NRTI) enabled the analysis of the presence and the localisation of certain elements within the sample.

The protocol, which also entails gamma spectroscopy and muon-based measurements, has been validated through an extensive study on a thin section by means of micro-Raman spectroscopy and scanning electron microscopy, returning confident results.

Endocytosis across scales: from molecular structures to a functional process

A. Santamaria[1,2], A. Maestro[1,3,4], N. R. Zaccai [5], E. Guzmán[2]

1. *Institut Laue-Langevin, Grenoble, France.*
2. *Universidad Complutense de Madrid, Spain.*
3. *Centro de Física de Materiales - Materials Physics Center, San Sebastián, Spain.*
4. *IKERBASQUE-Basque Foundation for Science, Bilbao, Spain.*
5. *University of Cambridge, England*

Clathrin-mediated endocytosis is the main mechanism by which eukaryotic cells internalize and recycle membrane proteins. It is driven by different proteins (such as CALM) that solely interact with the cell membrane inner leaflet. This interaction relies on the presence of negatively charged lipids in the plasma membrane, such as phosphatidyl-inositol-4,5-biphosphate (PIP_2), whose hydrophilic headgroup contains an inositol ring phosphorylated in position 4 and 5. By exploiting interfacial techniques such as ellipsometry, surface pressure-area isotherms, Brewster angle microscopy (BAM) and neutron reflectometry (NR), PIP_2-containing model membranes in the form of lipid monolayers have been investigated: the structure in the direction orthogonal to the membrane plane has been described, and correlated with the in-plane lipid organization. BAM proved the formation of PIP_2 clusters, and NR allowed determining the inositol ring orientation. Moreover, PIP_2-containing model membranes in the form of monolayers, solid supported bilayers and liposomes, have been exploited to study the binding with CALM. Interfacial and bulk techniques, such as surface pressure-area isotherms, quartz crystal microbalance with dissipation monitoring (QCM-D), NR, dynamic light scattering (DLS) and small-angle neutron scattering (SANS), were used. Importantly, NR allowed determining the insertion of the protein in the membrane as well as unravelling its three-dimensional orientation upon lipid binding.

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New set-up for Neutron Resonance Transmission Imaging (NRTI) at the Italian Neutron Experimental Station INES@ISIS

A. Scherillo[1], G. Marcucci [1,2], A. Fedrigo[1], D. Raspino[1]

1. *ISIS neutron and muon source, STFC, United Kingdom*
2. *Università Milano-Bicocca, and INFN Milano Bicocca, Italy*

The Italian Neutron Experimental Station INES, located at the ISIS neutron and muon source (U.K.), is a general-purpose neutron diffractometer with main research topic in the domain of cultural heritage and material science. Thanks to the high penetration power of neutrons, measurements performed through neutron diffraction provide quantitative bulk information on the samples in a non-destructive way, in particular regarding phase analysis and microstructure. Complementary to phase analysis and micreostruture, neutrons can provide elemental and isotope analysis, if neutrons of energy in the eV range are available. In particular, Neutron Resonance Capture Analysis (NRCA), and Neutron Resonance Transmission Imaging (NRTI) can be used to determine, the presence of isotopes and their spatial distribution within the samples under investigation. The techniques are isotopically selective. Recently, a new detector based on GEM technology has been used on INES for transmission measurements, to obtain bi-dimensional maps of calibration standards and archaeological artefacts, aiming to extend its use to other application like reactor waste, batteries, superconductors etc..

Glasses, supercooled liquids and stability: probing the crystallization kinetics with neutrons

M. Zanatta[1], F. Sacchetti[2], and C. Petrillo[2]

1. *Dipartimento di Fisica, Università di Trento*
2. *Dipartimento di Fisica e Geologia, Università di Perugia*

Glasses are so ubiquitous in everyday life and technology that we could consider our days as the glass age. However, developments are based on a try and error approach since the fundamental comprehension of this material is far from being satisfactory. One of the main open issues concerns the glass stability. Indeed, glasses and their parental supercooled liquids are metastable states and their ultimate fate is to crystallize. The crystallization time and the kinematics of the process are both a limit to glassy application as well as a potential advantage. This is the case of the fast-crystallizing phase-change materials used as bit for permanent memories.

In this talk, I will show the results of a neutron diffraction investigation of the isothermal crystallization process in GeO2, a protypical strong glassformer. Experimental data allows to observe the real-time evolution of the process, showing the continuous reorganization of the amorphous structure towards a crystalline phase. In a timescale of days, the final material becomes composed by crystalline domains plunged into a low-density, residual amorphous matrix. We developed an empirical model to provide a description of the experimental data. This approach identifies a predator-prey-like interplay between crystal and amorphous, where the density variation acts as a blocking barrier. A straightforward application could be the description of the viscoelastic properties of volcanic magmas that ultimately control their eruptive style and thus the associated risks.

Poster

Collective dynamics of liquid silver by Brillouin neutron scattering and *ab-initio* MD simulations

G. Aroldi[1], E. Guarini[1]

1. *Dipartimento di Fisica e Astronomia, Università degli Studi di Firenze,via G. Sansone 1, I-50019 Sesto Fiorentino, Italy*

This work concerns a thorough investigation of the collective dynamics of liquid silver (l-Ag), exploiting neutron Brillouin scattering (NBS) measurements in combination with \textit{ab initio} molecular dynamics (AIMD) simulations, thanks to a cooperation among researcher's groups of Florence (Italy) and Valladolid (Spain) universities. The main purpose of this work is not only to provide experimental data for the dynamic structure factor $S(Q,\omega)$ of this liquid in the range 4 nm^{-1}< Q < 16 nm^{-1}, but also to investigate about the scarce detectability of shear waves seemingly involving the IB group elements, unlike other metals. In fact, as for the case of liquid gold (l-Au), the experimental determination of $S(Q,\omega)$ doesn't allow to establish a clear indication of the existence of transverse-like excitations even in the case of l-Ag, despite the high quality of the measured spectra on the BRISP spectrometer hosted at the ILL, Grenoble, and the accurate analysis of the collected neutron data. However, the remarkable agreement between data and simulations allowed a careful analysis of the simulations in a range of wave vectors Q overlapping the experimental one and extending it up to almost 50 nm^{-1}. A multi-modal representation based on the theory of exponential expansion of time correlation functions has been found to provide excellent description of simulation data for l-Ag, thus allowing a reliable determination of both transverse and longitudinal acoustic branches of the dispersion curve for this metallic liquid. The comparison with the apparently different dynamic behavior of liquid gold (where low-frequency excitations were not observed even by analyzing simulation data) is also commented throughout the work.

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Physical methods for the investigation of medieval trade networks: the case of *pietra ollare*

F. Brugnara[1], E. Maccadanza[2], F. Saggioro[2], F. Santaniello[3], L. Tubiana[1], M. Zanatta[1]

1. *Dipartimento di Fisica, Università di Trento*
2. *Dipartimento di Cultura e Civiltà, Università di Verona*
3. *Dipartimento di Lettere e Filosofia, Università di Trento*

The Middle Ages are commonly depicted as a dark period marked by an economic, intellectual, and cultural decline compared to the classical era. However, archaeology is showing the limitations of this widespread belief. Indeed, new methodologies to analyze archaeological findings provide strong evidence of complex and well-structured long-range trade networks, even for ordinary consumer goods, like pots and food containers. This is the case of the *pietra ollare* industry that blossomed during the Middle Ages. *Pietra ollare* defines a group of rocks common in the Alps with different mineralogical compositions strongly dependent on their provenance. This specificity can be used as a fingerprint to map commercial interconnections that extended up to Southern Italy and Greece.

This investigation involves many specimens and requires multiscale measurements, including a rapid screening and more time-consuming mineralogical analysis. To achieve this goal, we are developing a procedure based on X-ray fluorescence and Raman spectroscopy joined by a machine learning-based analysis. Here we focus on the XRF fast screening, showing that comparing the elemental composition of archeological findings and samples from outcrops gives a first insight into the raw material exploitation, if not even into the commercial routes, of the time.

Advanced neutron imaging at the SINQ (Paul Scherrer Institut)

M. Busi[1]

1. *Paul Scherrer Institute Forschungsstrasse 1115232 Villigen PSI Switzerland*

An overview of the neutron imaging capabilities and methodologies at the SINQ of the Paul Scherrer Institut (Switzerland) will be presented. This will include a short panoramic of the BOA, ICON and NEUTRA cold and thermal beamlines for the neutron imaging user program. Besides the conventional attenuation contrast imaging mode, current options for wavelength-selective, time-of-flight, polarization and grating interferometry neutron imaging modalities will be discussed.

Bi2CuMnO6: a new born from HP/HT synthesis

C. Coppi[1,3], F. Mezzadri[3], M. Solzi[2], F. Cugini[2], R. Cabassi[1], E. Gilioli[1], D. Delmonte[1]

1. *Institute of Materials for Electronics and Magnetism, National Research Council (IMEM-CNR), Parco Area delle Scienze 37/A, I-43124, Parma (Italy)*
2. *Department of Mathematical, Physical and Computer Sciences, University of Parma, Parco Area delle Scienze 7/A, I-43124, Parma (Italy)*
3. *Department of Chemical Sciences, Life and Environmental Sustainability, University of Parma, Parco Area delle Scienze 17/A, I-43124, Parma (Italy)*

Magnetoelectric multiferroics (MEMs) are materials that exhibit the coexistence of magnetic and ferroelectric order which requires strict and specific symmetry conditions, stratified by just 13 Shubnikov space groups on 122. Because ferroelectricity and ferromagnetism are usually competing and complementary phenomena, more constraints are needed and the mutual coexistence and correlation is driven by different mechanisms, like charge ordering, magnetic interactions, geometrical distortions or the presence of electronic lone pairs.

Bi-based double perovskites (Bi2BB'O6) represent a large group of studied systems showing multiferroics properties. The insertion of Bi3+ ion on A site allows the inclusion of a transition metal with a partially filled d-shell, inducing the magnetic behaviour. Because of the great tolerance to chemical substitutions and structural distortions of the perovskite structure, it is possible to change the ion (Cr, Mn, Fe, Co, Ni, Cu) on the B site tuning the final properties.

High Pressure/High Temperature (HP/HT) techniques are a powerful tool to synthesize and stabilize unusual crystallographic symmetries, oxidation states and increase coordination numbers for cations, as for Bi2FeMnO61, BiMnO32 and Bi2FeCrO63.

This work reports the successful HP/HT synthesis with a multianvil apparatus of Bi2CuMnO6, a promising new magnetoelectric multiferroic materials with a FM behaviour at room temperature. We have investigated the reaction yield, obtaining the best synthesis conditions varying pressure, temperature, and duration. The purer system crystallizes in an I-centered orthorhombic cell, with parameters a≈2asp, b≈c≈$\sqrt{2}$asp respect to the ideal cubic perovskite. In addition, we report electrical and magnetic characterizations, resumable in a resistive behaviour and a very sharp ferrimagnetic transition at 320 K.

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chiara.coppi@imem.cnr.it

Bioorthogonal chemistry promoted by metal and photo catalysis

C. D'Avino[1], S. Gutiérrez[1], M. Tomás-Gamasa[1], J. Luis Mascareñas[1]

7. *Department of Organic Chemistry, Centro de Investigaciones en Química Biolóxica y Materiais Moleculares (CiQUS) University of Santiago de Compostela - Santiago de Compostela (Spain).*

The study of biomolecules in their natural environment has attracted the interest of scientists over the years. However, the complexity of the cellular systems makes it extremely difficult to work in this field. In this sense, bioorthogonal chemistry was born as a research area that revolves around chemical reactions that do not generate adverse effects in biological systems.[1]

Recent work has shown that synthetically powerful organic transformations are compatible with water. However, fulfilling bioorthogonality remains a critical challenge. Herein, we demonstrate the possibility to develop bioorthogonal reaction using very straightforward and small molecules under mild conditions. Specifically, we report two different strategies:

- the use of transition metal catalysts.[2]
- the use of photocatalysis by visible light.[3]

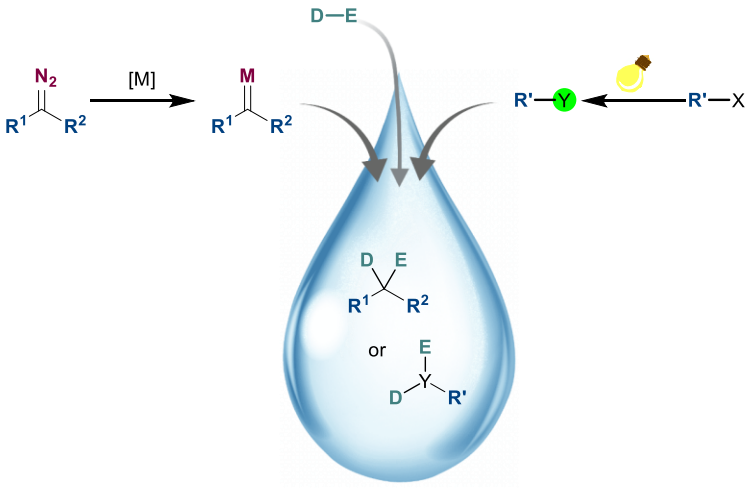

Figure 1. Schematic representation of the reaction's strategies

Finally, we investigate and optimize the two types of synthesis trying to overcome the difficulties of a cellular system to obtain a bioorthogonal reaction.

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Vibrational dynamics of ultra-stable and conventional glasses

I. Festi[1], E. Alfinelli[1], F. Caporaletti[2], A.I. Chumakov[3], D. Bessas[3], J. Rodriguez- Viejo[4,5], M. Gonzalez-Silveira[4,5], M. A. Ramos[6], G. Baldi[1].

1. *Department of Physics, University of Trento, I-38123, Povo, Trento, Italy.*
2. *Faculty of Science, University of Amsterdam, 1090 GL, Amsterdam, The Netherlands.*
3. *European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France*
4. *Departament de Física. Facultat de Ciències, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain.*
5. *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain.*
6. *Departamento de Física de la Materia Condensada, Condensed Matter Physics Center (IFIMAC), and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Madrid, Spain.*

The aim of my work is to measure the density of vibrational states (DOS) at low frequencies of an ultra-stable glass and to compare it with that of the corresponding conventional glass. At low temperature, the thermodynamic properties of glasses are remarkably different from that of the crystalline counterparts. For T<1 K, the specific heat of glasses depends linearly on temperature, in contrast to crystals, where the behavior of C_p is well described by the Debye's law: this anomaly is associated with an excess of vibrational states in glasses. Ultra-stable glasses instead exhibit the absence of this peculiarity, due to their high stability reached through the physical vapor deposition. The DOS allows us to have direct information on the density of these additional vibrations. The DOS measurements were carried out on samples of TPD, both ultra-stable and conventional, at the ID18 of the ESRF, in Grenoble. By exploiting the inelastic X-ray scattering with nuclear resonance analysis, it was possible to reach an energy resolution of 0.2 meV. In addition, Raman measurements were performed on these samples. The data analysis shows that the DOS of ultra-stable glass is lower than that of the conventional one, as expected. Furthermore, the specific heat found starting from the DOS data is compatible with that measured with calorimetry experiments. Instead, the Raman spectra do not present appreciable differences between the ultra-stable and the conventional glass at low frequencies.

Studio di reperti archeologici del territorio delle Marche mediante tecniche neutroniche

F. Fiori[1], Massimo Rogante[2]

1. *Università Politecnica delle Marche, Di.S.C.O., Via Brecce Bianche, 60131 Ancona, Italia*
2. *Studio d'Ingegneria Rogante, Contrada San Michele 61, 62012 Civitanova Marche (MC), Italia*

Vengono presentati i risultati di alcuni studi, eseguiti presso il Budapest Neutron Center mediante tecniche quali PGAA, PIXE, Diffrazione Neutronica e Radiografia Neutronica, per lo studio di reperti archeologici provenienti dal territorio della Regione Marche. In particolare, gli esperimenti hanno riguardato:

i) manufatti bronzei della Civiltà Picena, provenienti dalla necropoli del sito di Matelica (MC), risalenti al VII secolo a.C. Diversi frammenti sono stati analizzati, insieme ad un frammento dell'area archeologica di Fabriano (AN), aggiunto per comparazione;
ii) reperti metallici provenienti dall'area di *Tifernum Mataurense* a Sant'Angelo in Vado (PU), databili archeologicamente tra il primo e il tardo impero. Uno degli scopi principali è il confronto dei dati ottenuti relativi agli elementi leganti Cu, Sn e Pb con quelli acquisiti mediante PGAA sui bronzi piceni delle necropoli di Matelica;
iii) reperti metallici appartenenti alla collezione dell' *Academia Georgica Treiensis* di Treia (MC), risalenti al IX-IV secolo a.C., anch'essi presumibilmente rinvenuti nelle Marche. L'obiettivo principale di questo studio è stato quello di favorire la corretta descrizione dei reperti dal punto di vista tecnologico e dei materiali, anche nell'ottica di una comparazione con reperti provenienti da altri siti della regione.

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XXXIII Congresso Annuale SISN
Milano, 14-16 Settembre 2022

pH-dependent charge and structural properties of transfection lipid layers for RNA delivery

M. Grava[1], I. Mohd[2], J. Pusterla[1], N. Schwierz[2,3], E. Schneck[1]

1. *Institute for Condensed Matter Physics, Department of Physics, Technische Universität Darmstadt, Darmstadt, Germany*
2. *Department of Theoretical Biophysics, Max-Planck-Institute of Biophysics, Frankfurt am Main, Germany*
3. *Institute of Physics, University of Augsburg, Germany*

Cationic lipid-based delivery systems for messenger RNA (mRNA) are the basis of some of the most promising technologies for many biomedical applications, such as patient-specific cancer treatments and vaccines. The efficiency of the delivery process depends on the physicochemical properties of the involved molecules, specifically on structure, charge and pH.

In order to determine their pH-dependent structural properties, pH-induced changes in internal molecular organization, and the protonation degree of monolayers of positively chargeable transfection lipid mixtures, we combine synchrotron-based X-ray scattering and X-ray fluorescence [1, 2] with atomistic molecular dynamics simulations [3].

The experiments yield electron density profiles and surface charge densities, while the molecular dynamics simulations yield the area per molecule, the conformation of different lipid species, and the counter-ion distributions. The self-consistent analysis of experimental and simulation data provides unambiguous and detailed information on the transfection lipid layer characteristics.

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Sound propagation in vitreous silica studied via extreme ultraviolet transient grating spectroscopy

L. Maestri[1], E. Alfinelli[1], F. Bencivenga[2], F. Caporaletti[3], F. Capotondi[2], D. De Angelis[2], D. Fainozzi[2], L. Foglia[2], A. Martinelli[4], C. Masciovecchio[2], A. A. Maznev[5], R. Mincigrucci[2], G. Monaco[4], E. Pedersoli[2], M. Zanatta[1], G. Baldi[1].

1. *Department of Physics, University of Trento, I-38123, Povo, Trento, Italy.*
2. *Elettra-Sincrotrone Trieste, I-34149, Basovizza, Trieste, Italy.*
3. *Faculty of Science, University of Amsterdam, 1090 GL, Amsterdam, The Netherlands.*
4. *Department of Physics and Astronomy, University of Padova, I-35122, Padova, Italy.*
5. *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.*

The experiment carried out at the TIMER beamline of the FERMI FEL, in Trieste, consists in a spectroscopic investigation of sound propagation in vitreous silica via extreme ultraviolet transient grating. It can be considered as the second part of a previous experience of TG technique on silica. In the new experiment, the parameters of the setup are chosen in order to have a transient grating on the sample with wavevector Q above 0.3 nm^{-1}, reaching a previously unexplored frequency range. Laser-induced transient grating is a spectroscopic technique used in Condensed Matter studies. Two beams (pump) of the same wavelength (λ_{ex}) are overlapped on the sample to create a periodic intensity pattern, which leads to a periodic profile in temperature over the exposed zone of the sample. A third time-delayed laser beam is used as probe and the light diffracted by the transient grating is focused on a CCD camera, from which the signal is obtained. The sample is investigated both at room and low temperature (nominal T = 52 K). The model function, used to fit the transient grating signal, takes into account the phonons decay time (τ), the thermal grating decay time (τ_{th}) and the frequency oscillations of the acoustic waves (ω_0 and $2\omega_0$). Moreover, the sound velocity in vitreous silica can be obtained from the parameter ω_0 and the transient grating wavevector Q, using the formula $v = \omega_0/Q$. The results are compared with the vast literature on sound attenuation and propagation in silica.

Asymmetric supercapacitor with graphene-based electrodes

A. Morenghi[1], G. Magnani[1], S. Scaravonati[1], M. Sidoli[1], M.Riccò[1], G. Bertoni[2], L. Aversa[3], R. Verucchi[3], D. Pontiroli[1]

1. *Nanocarbon Laboratory & Dipartimento di Scienze Matematiche, Fisiche e Informatiche dell'Università di Parma, Parma, Italy.*
2. *CNR – Istituto di Nanoscienze, Modena, Italy.*
3. *IMEM-CNR, Povo (TN), Italy.*

Supercapacitors (SCs) are able to store electrochemical energy with higher power density and longer cycle life than batteries. The major SCs issue is the poor energy density, due to the physical origin of their capacitance. Graphene-based porous materials are remarkable candidates as SCs electrodes, thanks to high graphene specific surface area and superior electronic conductivity [1]. Graphene decoration with transition oxide nanoparticles is expected to further enhance capacitance by introducing red-ox reactions [2]. Then, the voltage working window can ben further enlarged coupling two electrodes with different potential ranges [3]. In this study, thermal exfoliated graphite oxide (TEGO), having a specific surface area of 500 m^2/g, has been employed as active material in SCs electrodes, displaying a capacitance of 105 F/g at 10 mV/s. Moreover, owning a great amount of defects, TEGO is able of anchoring Ni nanoparticles (NPs) [4]. During the early voltammetric cycles in KOH 3.5 M electrolyte, metal Ni-NPs converted in $Ni(OH)_2$, reaching a high reversible specific capacitance of 1340 F/g at 10 mV/s. Coupling an electrode of pure TEGO with another of TEGO decorated with Ni-NPs we made an asymmetric supercapacitor which reached an extended voltage window of 1.6V in KOH 3.5 M aqueous electrolyte [5].

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Dynamic cluster formation, viscosity and diffusion in monoclonal antibody solutions

I. Mosca [1], K. Pounot [1,2], C. Beck [1,2], C. Grapentin [3],O. Matsarskaia [1,2], T. Seydel [1,2] and F. Schreiber [1]

1. *Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen, Germany*
2. *Institut Max von Laue - Paul Langevin, 71 Avenue des Martyrs, 38042 Grenoble Cedex 9, France*
3. *Lonza Group Ltd – Drug Product and Services, Hochbergerstrasse 60G, 4057 Basel, Switzerland*

Antibodies play an essential role in the immune response of mammals. Monoclonal antibodies (mAbs) are particularly relevant for therapeutic approaches due to their high specificity and versatility. The pharmaceutical challenge is to formulate highly concentrated antibody solutions to achieve a significant therapeutic effect, while minimizing their viscosity and keeping it under the subcutaneous injectability limit [1], thus rendering the drug administration to patients less difficult and painful. Since the understanding of macroscopic viscosity requires an in-depth knowledge on protein diffusion and dynamic cluster formation [2,3], we study the self-diffusion of five mAbs of the IgG1 subtype (produced and characterized at Lonza AG) in aqueous solution as a function of the type of antibody and of their concentration, by quasi-elastic neutron scattering (QENS). QENS allows to determine unambiguously the hydrodynamic mAb cluster size [4] and to gain information on the internal mAb dynamics. A subset of those mAbs has been also investigated using small angle neutron scattering (SANS) to obtain information on sample structure and on the nature of interactions occuring among mAb molecules. Complementary information is provided by molecular dynamics (MD) simulations and rheology measurements.
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mosca@ill.fr

Combined capacitive and electrochemical charge storage mechanism in high performance graphene-based lithium-ion batteries

S. Scaravonati[1], M. Sidoli[1], G. Magnani[1], A. Morenghi[1], M. Canova[2], Jung-Hyun Kim[2], M. Riccò[1], D. Pontiroli[1].

1. *Nanocarbon Laboratory, INSTM & Department of Mathematical, Physical and Computer Sciences, University of Parma, Parco Area delleScienze 7/A, 43124, Parma, Italy;*
2. *Center for Automotive Research, The Ohio State University, 930 Kinnear Road, 43212, Columbus, Ohio, USA.*

Improvements in Li-ion battery technology can be achieved by developing novel, high-performance electrode materials. Graphene appears to be a good candidate as an anode material for Li-ion batteries thanks to the similarity with graphite, the good electrical conductivity, the ability to achieve fast charge and discharge cycles, and the higher capability to host lithium ions. Our previous studies demonstrate the capability of intercalating lithium in graphene-based electrodes with a high specific capacity of 500 mA h g^{-1} at C/5 current. In this study, graphene, synthesized through scalable thermal exfoliation of graphite oxide, and hydrogenated graphene is employed to assemble optimized Li-ion half-cells, which are systematically characterized by means of electrochemical measurements. Hydrogenated graphene boasts an impressive reversible specific capacity with fast charge/discharge capabilities, exceeding 370 mA h g^{-1} even at 25C-rate. Diffusion mechanisms of lithium is haracterized at different states of intercalation by means of electrochemical impedance spectroscopy. In addition, a novel combined electrostatic and electrochemical charge storage mechanism of lithium ions in graphene-based electrodes is proposed, based on three-electrode cyclic voltammetry investigation. Furthermore, graphene and hydrogenated graphene anodes are paired with commercial cathode materials, to study the feasibility of their application to full-cells.

A preliminary study of Cu-based alloys and artificial corrosion patinas by neutron imaging analysis

L. Vigorelli[1,2,3], A. Vietti[1,3], S. Grassini[3,4], L. Guidorzi[2], M. Magalini[2,3], A. Re[2,3], A. Lo Giudice[2,3], F. Grazzi[5,6], N. Gelli[6]

1. *Dip. di Elettronica e Telecomunicazioni, Politecnico di Torino*
2. *Dip. di Fisica, Università degli Studi di Torino*
3. *INFN, Sezione di Torino*
4. *Dip. di Scienza Applicata e Tecnologia, Politecnico di Torino*
5. *Consiglio Nazionale delle Ricerche, Firenze*
6. *INFN, Sezione di Firenze*

When archeological copper-based artifacts are buried in soil for a long time, the result is a corrosion patina characterised by complex chemical and metallurgical structures [1]. The study of this finds requires several analytical techniques to characterise the material and the corrosion products [2]. Non-destructive studying methods represent an important tool for conservators to obtain valuable information about works of art in a non-invasive way. In the last decades, neutron imaging techniques have gained great importance in the Cultural Heritage field thanks to the results obtained [3]. In this study, several Cu-based alloys with composition like archaeological ones were prepared, some of them also artificially patinated. The samples were analysed with thermal neutrons at the L.E.N.A. Centre in Pavia, where a new facility for imaging studies has been recently developed in the framework of the CHNet-NICHE project and is currently under optimisation. The aim of the analysis is providing a reference for this specific beamline, estimating the attenuation coefficient values and its spatial distribution in the samples by means of digital radiography and to distinguishing between the alloy (inner part) and the patina (external part) with computed tomography. The goal is to determine the nature and properties of archaeological artefacts of unknown structure using the data obtained by analysing the Cu-based reference alloys.

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XXXIII Congresso Annuale SISN
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Inside the synergistic effect of W-O-Ru and oxygen vacancies in boosting water splitting reaction

S. Zorzi[1], T. A. Shifa[1], E. Moretti[1] A. Vomiero[1,2], and E. Cattaruzza[1]

1. *Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Via Torino 155, 30172 Venezia, Italy*
2. *Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University of Technology, 97187 Luleå, Sweden.*

Hydrogen is considered as a promising green carbon-neutral fuel to solve the energy crisis moving decarbonising the planet. Electrochemical water splitting is nowadays one of the widely used methods to produce hydrogen. However, the outstanding catalytic properties of noble metals are hindered by their low availability and very high price. There is an urgent request to develop highly active and stable electrodes with reduced amounts of noble metals [1].

Recently the dominant role of Ru in hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), in which Ru atoms play an important role due to its appropriate H* adsorption strength, has been explored [2].

On the other hand, WO_3 has emerged as a promising catalyst in water splitting owing to its remarkable activity as a current collector. Atom controllable doping of Ru in WO_3 will bring about intriguing feature from the basis of perturbed electronic environment/unsaturated sites near the metal atoms to create thermodynamically suitable platform for catalysis.[3] In this work, we describe a facile and easily scalable method for the synthesis of oxygen vacant Ru-WO_{3-x} nanotrees electrode material, grown on nickel foam. The doped material exhibits higher electrochemical activity, (with respect to the undoped electrode) and generate an extremely high current during OER, resulting in high O_2 production, which can match the requirements for future industrial applications.

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Sessione congiunta SIF-SISN sulla formazione nel campo della scienza con i neutroni

The Training on Neutron Techniques Schools

R. Magli[1]
renato.magli@unimi.it

1. *Dipartimento di Scienze Biomediche Chirurgiche e Odontoiatriche, Università degli Studi di Milano*

SISN organizes a three-year program of Specialized Summer Schools called Training on Neutron Techniques (TNT), open to Graduate and PhD students and to Post-Docs working in scientific disciplines as Biology, Chemistry, Earth Sciences, Material Sciences, Physics, Sciences for Cultural Heritage Conservation, and similar. The physical bases of neutron sources and of neutron scattering techniques for the study of condensed matter are presented and discussed, with examples and applications in various scientific fields. Specific attention is paid to recent developments and to those in progress and expected for the current decade. The scientific potentialities of the experimental methods are discussed for instruments accessible both at reactor-based facilities and at spallation sources, also in view of the European ESS project (the future European Neutron Scattering facility). The 2022 edition focuses on Diffraction and Structural Imaging, while the topic of 2023 will be Inelastic Scattering and in 2024 Small Angle Scattering and Reflectometry will be dealt with.

Training on Neutron Techniques (TNT): Neutron Diffraction and Structural Imaging

R. Magli[1], M Ceretti[2], F. Formisano[3], F. Grazzi[4], A. Pietropaolo[5]
renato.magli@unimi.it

2. *Dipartimento di Scienze Biomediche Chirurgiche e Odontoiatriche, Università degli Studi di Milano*
3. *ICGM, CNRS Montpellier*
4. *CNR-IOM, Grenoble*
5. *CNR-IFAC, Sesto Fiorentino, INFN-CHNet*
6. *ENEA, Frascati*

The first edition of the TNT Summer Schools, focused on Neutron Diffraction and Structural Imaging, took place from 11 to 19 June 2022 in S. Giovanni (BZ). The School has been attended by 25 students coming from Asian and European laboratory. The physical basis of the neutron sources (both reactors and spallation sources) and of the instrumentation needed for structural studies have been introduced and discussed. Then neutron diffraction with crystals, powder and disordered systems has been discussed with examples and tutorials ranging from single crystal applications to magnetic scattering, to materials science, to cultural heritage conservation, etc. The second part of the school has been devoted to Structural Imaging. After introductory lectures on the theory of neutron imaging and on the related instrumentation, several applicative seminars and tutorials have presented and discussed imaging techniques, as energy selective, phase contrast, polarized imaging, grating interferometry, neutron resonance imaging.

Le Advanced Summer Schools della SISN
Edizione 2018

L. Del Rosso[1], A. De Francesco[2], E Guarini[2]
l.delrosso@ifac.cnr.it

1. *1CNR-IFAC, Sesto Fiorentino, Italia*
2. *2CNR-IOM c/o Institut Laue Langevin, Grenoble, France*
3. *3Dipartimento di Fisica e Astronomia, Università di Firenze, Sesto Fiorentino, Italia*

La scuola del 2018, più specialistica rispetto alla tradizionale offerta didattica della SISN, è stata la prima a carattere internazionale e ad essere dedicata non solo a dottorandi e postdoc ma anche a ricercatori, esperti di scattering di neutroni, interessati ad approfondire le conoscenze sui metodi statistici e computazionali utili nell'analisi e interpretazione dei dati. La gestione dei dati, le procedure di correzione, i principali programmi, i modelli di fit più generali e le tecniche di simulazione sono stati trattati per le diverse tecniche (ND, QENS, INS, SANS) allo scopo di affrontare le tipiche difficoltà che si presentano dopo una misura. La scuola si proponeva di trattare i tanti aspetti relativi ad un'accurata analisi e i modi per verificare l'affidabilità dei risultati, sia tramite il confronto con simulazioni, sia attraverso controlli statistici basati sull'inferenza Bayesiana. Docenti e studenti, a volte volutamente scambiati nei loro ruoli - dando vita a un Simposio più che ad una scuola tradizionale - provenivano da Europa, Asia, Stati Uniti, Sud America. Dai questionari è emerso un grande apprezzamento per il tipo di formazione e per l'organizzazione generale.

Neutrons and Muons for Magnetism: The 2019 edition of the SISN Advanced School

S. Chicco[1], T. Guidi[2,3], R. Caciuffo[1,4,5], E. Moneta[5]
simone.chicco@unipr.it

1. *Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma,Italia*
2. *ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Harwell Oxford,United Kingdom*
3. *Scuola di Scienze e Tecnologie, Sezione di Fisica, Università di Camerino, Italia*
4. *Istituto Nazionale di Fisica Nucleare, Via Dodecaneso 33, IT-16146 Genova, Italia*
5. *Joint Research Centre, Karlsruhe, Germany*

L'edizione 2019 dell'Advanced Summer School SISN è stata dedicata alle applicazioni di neutroni e muoni allo studio del magnetismo. La Scuola, organizzata dalla SISN in collaborazione con il Joint Research Centre (JRC) della Commissione Europea, si è svolta dal 2 al 6 Settembre 2019 presso il centro di ricerca del JRC situato ad Ispra (Varese), sulla riva lombarda del Lago Maggiore. La Scuola ha ricevuto 42 domande di partecipazione e sulla base delle motivazioni espresse nelle lettere di candidature, sono stati ammessi 21 studenti, provenienti da 10 diverse nazioni. La Scuola si è articolata in una serie di lezioni sulle principali tecniche d'interesse per lo studio dei fenomeni e dei materiali magnetici, seguite da esercitazioni pratiche sull'uso di programmi di calcolo per la visualizzazione dei dati e per la loro interpretazione. Tre lezioni, dettate da docenti di assoluto prestigio scientifico, quali Claudia Felser, Stuart Parkin and Vincent Cros, sono state dedicate ad argomenti non direttamente collegati alle tecniche sperimentali oggetto della scuola, ma molto innovativi e di elevato interesse scientifico.

Le Giornate Didattiche SISN: dal 2004 al 2022 la fucina dei giovani neutronisti italiani

F. Spinozzi[1], D. Noferini[2], M. Zanatta[3]
f.spinozzi@univpm.it , marco.zanatta@unitn.it , daria.noferini@ess.eu

1. *Università Politecnica delle Marche, Dipartimento di Scienze della Vita e dell'Ambiente*
2. *European Spallation Source ERIC, Lund (Svezia)*
3. *Università di Trento, Dipartimento di Fisica*

La formazione dei giovani ricercatori è una delle principali finalità della Società Italiana di Spettroscopia Neutronica (SISN). A tale scopo, dal 2004 la SISN organizza le Giornate Didattiche (GD), una scuola introduttiva allo scattering di neutroni con forte connotazione interdisciplinare. Le GD sono infatti pensate per studenti, dottorandi e giovani ricercatori provenienti da diverse aree: Fisica, Chimica, Biologia, Geologia, Scienza dei Materiali, Conservazione dei Beni Culturali... Nella prima parte delle GD vengono introdotti i fondamenti dello scattering di neutroni e delle varie tecniche; nella seconda gli studenti applicano quanto appreso conducendo veri esperimenti, dal 2007 presso l'Institut Laue-Langevin (Francia). Post pandemia, le GD riprendono nel 2022 con una seconda sessione basata su esperimenti virtuali (causa temporaneo shutdown di molte sorgenti europee) svolti da gruppi di studenti con supervisione di un tutor. Come nel caso reale, gli studenti approfondiranno un caso scientifico, valuteranno i parametri strumentali, analizzeranno dataset reali e presenteranno i risultati con un seminario. Nel corso degli anni, le GD hanno formato centinaia di giovani ricercatori, molti dei quali hanno proseguito la loro avventura nella
neutronica. Oltre alla storia delle GD, i direttori presenteranno dati sulla loro efficacia per la formazione.

L’esperienza delle Giornate Didattiche SISN 2022: gli esperimenti virtuali

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Dinamica di protoni in elettroliti solidi per celle a combustibile di nuova generazione

D. Noferini [1], B.P. Rosi.[2]
e gli studenti delle GD2022
daria.noferini@ess.eu
b.rosi@fz-juelich.de

1. *European Spallation Source ERIC, Lund (Svezia)*
2. *Jüelich Center for Neutron Science JCNS, Jüelich (Germania)*

Gli zirconati di bario drogati sono al centro di grande attenzione per le possibili applicazioni come elettroliti solidi in celle a combustibile di nuova generazione. Sebbene la presenza del dopante sia necessaria per la conduzione dei protoni, non è ancora stato del tutto delucidato il legame fra le modifiche alla struttura locale dovute al dopante e la dinamica dei protoni. Anche i dettagli del
meccanismo della conduzione dei protoni sono ancora dibattuti. Lo scattering inelastico di neutroni permette di investigare con grande efficacia la dinamica dei protoni in questi materiali, grazie all'elevata cross section di scattering incoerente dell'idrogeno. Durante l'esercitazione gli studenti possono confrontarsi con dati acquisiti con uno spettrometro di neutroni su campioni di zirconato di bario drogati. In particolare possono seguire la trasformazione dei dati da intensità misurata a fattore di struttura dinamico e la susseguente analisi volta ad identificare le caratteristiche della dinamica dei protoni.

Transizione di fase di un doppio strato lipidico studiata tramite riflettometria neutronica

Y. Gerelli[1] e gli studenti delle GD2022
y.gerelli@staff.univpm.it

1. *Università Politecnica delle Marche, Dipartimento di Scienze della Vita e dell'Ambiente*

Il doppio strato lipidico è un paradigma per studi biologici e tecnologici, ad esempio per l'indagine delle interazioni e dei processi molecolari coinvolti nella funzione cellulare, nelle malattie e per lo sviluppo di biosensori. Inoltre, è uno dei prototipi di sistemi naturali autoassemblanti. Grazie a questa capacità, la struttura di doppi strati lipidici è in grado di variare spontaneamente in risposta a stimoli esterni, cambi di composizione e interazioni con molecole ospiti. La riflettometria neutronica è una tecnica non invasiva capace di fornire una descrizione su scala nanometrica della struttura di doppi strati lipidici depositati su superfici planari. In questo esperimento è stata applicata per caratterizzare la variazione di struttura di doppi strati lipidici in funzione della temperatura. In particolare, la tecnica ha permesso di identificare variazioni di densità all'interno del doppio strato lipidico, i.e. in una regione inaccessibile da altre tecniche di microscopia.

XXXIII Congresso Annuale SISN
Milano, 14-16 Settembre 2022

Interazioni tra membrane lipidiche e proteine studiate tramite diffusione a piccolo angolo dei neutroni (SANS)

V. Rondelli[1] e gli studenti delle GD2022
valeria.rondelli@unimi.it

1. *Università degli studi di Milano "La statale", Dipartimento di Biotecnologie Mediche e Medicina Traslazionale*

Il design di un esperimento di scattering di neutroni a basso angolo (SANS) richiede di valutare accuratamente diversi aspetti. Una volta inquadrato il problema scientifico è fondamentale la conoscenza del campione e questo richiede, ove possibile, lo svolgimento di misure di caratterizzazione preliminari. Anche la scelta della facility dove richiedere tempo macchina e lo strumento specifico sono molto importanti e sono strettamente legati al problema scientifico, al
tipo di campione da studiare e alla quantità di campione disponibile. Talvolta può essere d'aiuto effettuare misure preliminari su strumenti meno performanti per poter poi richiedere accesso alle facilities più richieste con strumenti più performanti. Una volta raccolti i dati, l'analisi di questi per ottenere informazioni strutturali richiede lo sviluppo di modelli teorici per la loro interpretazione o, come spesso accade, può essere effettuata a mezzo di programmi di analisi già sviluppati a questo proposito. Durante l'esercitazione questi aspetti verranno declinati rispetto ad un caso scientifico di interazione membrana lipidica-proteina.

Dopo le giornate didattiche SISN: l'esperienza di due Alumni

XXXIII Congresso Annuale SISN
Milano, 14-16 Settembre 2022

Analisi dell'effetto della composizione lipidica sull'attività della fosfolipasi tipo A in sistemi di membrane modello

G. Corucci[1]
corucci@ill.fr

1. *Institut Laue-Langevin, Grenoble (Francia)*

Le fosfolipasi-A (PLA) appartengono al gruppo degli enzimi idrolitici (EC-3), e catalizzano l'idrolisi dei glicerofosfolipidi (GFL) in acidi grassi e liso-fosfolipidi (LFP). Le PLA possiedono una grande varietà di funzioni nelle cellule viventi, che spaziano dal rimodellamento delle membrane cellulari, fino al rilascio di molecole segnale (come l'acido arachidonico). Alcune di queste PLA sono di
rilevanza medica perché risultano coinvolte in malattie neuro-degenerative ed autoimmuni. Per questo motivo risulta importante la comprensione del meccanismo di azione, come primo passo verso la cura di queste patologie PLA-correlate. Ad oggi, i fattori che regolano la specificità enzima/substrato non sono del tutto compresi. Questo progetto tenta di elucidare la complessa interazione PLA/substrato, cercando di comprendere quali siano i fattori che spingono l'enzima a preferire un substrato rispetto ad un altro, delucidando il meccanismo di azione con il quale agiscono. Studi precedenti dimostrano che la reazione mediata dalle fosfolipasi avviene in due step: efflusso del GFL dalla membrana, dove il GFL lascia la membrana plasmatica per entrare nel sito attivo dell'enzima; e l'accomodazione, che indica il grado di assestamento del GFL nella tasca catalica. In questo progetto analizziamo in dettaglio questa teoria mediante l'utilizzo di scattering di neutroni e tecniche biofisiche complementari come QCM-D, ellissometria e spettrometria di massa.

Studio del confinamento dell'acqua in nanotubi di imogoliti

A.D'Angelo[1,2], E. Paineau[1], P. Launois[1], S. Rols[2]
arianna.dangelo@universite-paris-saclay.fr

1. *Laboratoire de Physique des Solides, CNRS-Université Paris Saclay, Orsay, France*
2. *Institut Laue-Langevin, Grenoble, France*

I nanotubi di imogoliti (INT) con stechiometria (OH)3Al2O3Si(OH) sono particolari materiali argillosi formati da fogli di gibbsite arrotolata con all'interno unità isolanti SiO3(OH). Gli INT possono essere sintetizzati con processi di chimica soft e gli atomi di silicio (SI-INTs) possono essere sostituiti da atomi di germanio (Ge-INTs). In entrambi i casi, il diametro interno di questi nanotubi idrofilici è realmente nanometrico, 1.5 nm per i Si-INTs e 3 nm per i Ge-INTs. Per questo motivo, le proprietà di superficie prevalgono e gli INTs sono ottimi sistemi modello per studiare il ruolo delle interfacce sul comportamento dell'acqua. Risultati recenti sui Ge-INTs hanno mostrato che i wetting-layer si stabilizzano a 300 K con una simmetria locale triangolare. Questo studio si concentra sulle Si-INTs e sul processo di assorbimento e diffusione dell'acqua nelle loro cavità interne. I risultati presentati sono stati ottenuti da esperimenti di scattering quasielastico, inelastico e spin-echo, combinati con simulazioni di dinamica molecolare (MD) ottenute con una parametrizzazione esistente per il potenziale di interazione acqua-imoglolite. Gli spettri QENS e la densità degli stati simulate dell'acqua assorbita in Si-INT saranno comparati con i Ge-INT e con i dati sperimentali ottenuti all'Institut Laue Langevin, sugli spettrometri IN6-SHARP

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