SOCIETÀ ITALIANA DI SPETTROSCOPIA NEUTRONICA

XXX CONGRESSO ANNUALE SISN

Roma
24-26 Giugno 2019

BOOK OF ABSTRACTS

Indice

Programma

Lunedì 24 Giugno 2019

Argiletum, Aula Urbano VIII
Dipartimento di Architettura, Università di Roma Tre
Via della Madonna dei Monti, 40

10.00

REGISTRAZIONE

10.45

APERTURA DEL XXX CONGRESSO ANNUALE SISN

SISTEMI BIOLOGICI E SOFT MATTER

Chair: Antonio Benedetto, Paolo Mariani, Ernesto Scoppola, Francesco Spinozzi

11.00
Structural characterization of Nanoparticles for drug delivery: tuning nanostructure and mucus interaction
Elena Del Favero

11.30
High-resolution neutron scattering data reveal the decoupling of proteins and water at the dynamical transition
Antonio Benedetto

11.50
Structural investigation on TEMPO-oxidized nanocellulose
Andrea Fiorati

12.10
Effect of membrane-protein interaction on lipid bilayers
Caterina Ricci

12.30
Structure of human telomere G-quadruplex in the presence of a model drug along the thermal unfolding pathway
Lucia Comez

13.00 - 14.30

PRANZO

14.30
Integrated motions of molecular machines and motors: from structure to mechanics
Giacomo Mariani

15.00
Protein-like dynamical transition in microgels: a molecular dynamics study
Letizia Tavagnacco

15.20
Study of membrane phase transition in bacterial vesicles
Angelo Sarra

15.40
Mucin thin layers: a model environment for mucosal delivery
Valeria Rondelli

16.00 - 16.30

COFFEE BREAK

MAGNETISMO

Chair: Stefano Carretta

16.30
Investigating molecular nanomagnets with four-dimensional inelastic neutron scattering: magnetism, spin dynamics and beyond
Elena Garlatti

17.00
Four-dimensional inelastic neutron scattering simulated on a quantum hardware
Alessandro Chiesa

17.20
Unveiling the role of phonons in reaching very high blocking temperatures in Dy-based single-molecule magnets
Emilio Macaluso

NEUTRONI PER LA FUSIONE

Chair: Antonino Pietropaolo

17.40
Conversione da MCNP a FLUKA del codice source della macchina FNG di Frascati e successivi sviluppi
Alessandro Calamida

17.55
Studio del processo di produzione di ^{99}Mo attraverso la reazione ^{100}Mo$(n, 2n)^{99}$Mo indotta da neutroni a 14 MeV per la fisica medica
Silvia Palomba

18.10
High temperature operation of CVD diamond detectors in current mode
Silvia Cesaroni

18.25
Caratterizzazione di Self Powered Neutron Detectors per neutroni veloci da utilizzare nella facility DONES
Flaminia Di Giambattista

18.40

CONCLUSIONE DEI LAVORI

Martedì 25 Giugno 2019

Argiletum, Aula Urbano VIII
Dipartimento di Architettura, Università di Roma Tre
Via della Madonna dei Monti, 40

LIQUIDI E LEGAME IDROGENO

Chair: Maria Antonietta Ricci

9.00
Ice clathrates and filled ices under pressure: neutron insights on planetology and gas storage
Livia Eleonora Bove

9.30
Tuning the fast dynamics of PNIPAM-based systems with biologically relevant solvents
Benedetta Petra Rosi

9.50
Diffusion dynamics in hydrated PNIPAM microgel powders through volume phase transition
Pietro Tozzi

10.10
Hydration and Aggregation of Glycine in Aqueous Solution
Michael Di Gioacchino

10.30
Ionic liquids for energy
Oriele Palumbo

11.00 - 11.30

COFFEE BREAK

METODI E STRUMENTAZIONE

Chair: Andrea Orecchini

11.30
New experimental opportunities at the ILL - Neutron Spin-Echo upgrades
Bela Farago

12.00
Structure of PANTHER: a thermal time of flight spectrometer at the ILL
Giuliana Manzin

12.30
Quasielastic Neutron Scattering - is there another way? The Elastic Scattering Spectroscopy route
Gordon J. Kearley

13.00 - 14.30

PRANZO

14.30
Overview and Progress of the ESS Instrument Suite
Andrew Jackson

15.00
Italian in-kind contribution to the accelerator of the European Spallation Source
Santo Gammino

15.30

ASSEMBLEA DEI SOCI SISN

All'interno dell'Assemblea saranno aperti i lavori
degli *Stati Generali della Neutronica*.

19.00

CONCLUSIONE DEI LAVORI

20.30

CENA SOCIALE

Mercoledì 26 Giugno 2019

Argiletum, Aula Urbano VIII
Dipartimento di Architettura, Università di Roma Tre
Via della Madonna dei Monti, 40

8.55

SALUTO DA PARTE DEL DIRETTORE DEL DIPARTIMENTO DI ARCHITETTURA DELL'UNIVERSITÀ DI ROMA TRE, PROF. ELISABETTA PALLOTTINO

BENI CULTURALI E APPLICAZIONI ALLA SCIENZA DEI MATERIALI

Chair: Francesco Grazzi e Armida Sodo

9.05
Diagnostiche di spettroscopia atomica con possibilità di stratigrafia sui Beni Culturali – Applicazioni nel progetto ADAMO
Roberta Fantoni

9.35
Oltre le parole: quello che i libri nascondono
Marina Bicchieri

10.05
Neutron diffraction investigations of seabed metal treasures
Francesco Armetta

10.25
Nanomateriali e la sfida conservativa delle architetture storiche: un sogno nel cassetto o una realtà prossima?
Ludovica Ruggiero

10.45
Effect of microstructure on mechanical properties and residual stresses in interpenetrating aluminum–alumina composites fabricated by squeeze casting
Fabrizio Fiori

11.15 - 11.45

COFFEE BREAK

11.45

150 ANNI DI TAVOLA PERIODICA

SALUTO DEL MAGNIFICO RETTORE DELL'UNIVERSITÀ DEGLI STUDI DI ROMA TRE,
PROF. LUCA PIETROMARCHI
INTRODUZIONE DA PARTE DEL PRESIDENTE SISN, PROF. FABIO BRUNI

LECTIO MAGISTRALIS

Primo Levi e il Sistema Periodico: chimica, letteratura, memoria

Luigi Dei

Magnifico Rettore dell'Università degli Studi di Firenze *La partecipazione alla*

lectio magistralis è libera.

13.00 - 14.30

PRANZO

UPDATE DA VESPA E T-REX

Chair: Fabio Bruni

14.30
The VESPA project: moving towards the detailed design
Leonardo del Rosso

14.50
T-REX
Andrea Orecchini

15.00

INFRASTRUTTURE DI RICERCA PER LA NEUTRONICA: QUALE FUTURO PER L'ITALIA?

Incontro e discussione tra la Comunità Neutronica e Corrado Spinella,
Direttore del Dipartimento Scienze Fisiche e Tecnologie della Materia del CNR

L'incontro organizzato dal DSFTM del CNR e dalla SISN,
la partecipazione è libera.

Abstract dei talk

NEUTRON DIFFRACTION INVESTIGATIONS OF SEABED METAL TREASURES

F. Armetta

Dipartimento Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche - STEBICEF, Università degli Studi di Palermo, Parco d'Orleans II, Viale delle Scienze pad. 17, I-90128, Palermo, Italy.

The research group of Palermo I work with is performing an extensive work in the field of cultural heritage. Between the other topics there is the study of archaeological metal objects. Different case studies have been addressed such as the orichalcum ingots [1-2] coming from Gela seabed and the Tremiti plates. The presentation will report one of two of the studies where neutron diffraction played an important role, providing a huge amount of information.

For each of this case an appropriate set-up of analysis was developed in order to answer the archaeologist questions, and help to reconstruct the history of the objects. The used multianalytical approaches allows to establish a network of national and international collaborations. Particularly, neutron investigations performed on INES beamline at ISIS Large Facility have been a powerful non-invasive means of studying the artifacts, by providing information about the nature and the processing of the alloys. The investigations of orichalcum ingots and plates, not only replied the archaeologist questions but also they have had huge media success, with a strong impact on the dissemination of the importance of chemical-physical investigations to the study of archaeological objects.

[1] E. Caponetti *et al.*, Microchemical Journal, **2017**, 135.

[2] E. Caponetti *et al.*, Mediterranean Archaeology and Archaeometry, **2017**, 17 2.

HIGH-RESOLUTION NEUTRON SCATTERING DATA REVEAL THE DECOUPLING OF PROTEINS AND WATER AT THE DYNAMICAL TRANSITION

A. Benedetto

Department of Sciences, Roma Tre University, Rome, Italy,
and School of Physics, University College Dublin, Dublin, Ireland.

The dynamics of a model protein (Lysozyme) and its hydration water have been investigated by neutron scattering at very high-energy resolutions, up to 3 times better than the best ones used until now (0.3 μeV versus 1 μeV). Because of this improvement, it was possible to measure the decoupling between water and protein dynamics in proximity of the protein dynamical transition [1]. This decoupling, never observed before, is a clear sign that the transition in the dynamic of hydration water does not directly drive a corresponding change in the dynamic of proteins. As a result, the scenario generally accepted during the last 30 years has eventually been challenged, and a new theory on the connection between these two dynamics and protein function has to be formulated.

[1] A. Benedetto, J. Phys. Chem. Lett. **8**, 4883-4886 (2017).

OLTRE LE PAROLE: QUELLO CHE I LIBRI NASCONDONO

M. Bicchieri

MiBAC, Istituto centrale restauro e conservazione patrimonio archivistico e librario, Laboratorio di chimica.

Un libro racchiude le emozioni trasmesse dalle parole e spesso si ritiene che sia importante solo per il testo che contiene, così come un'opera grafica lo sia per l'immagine. Ma le storie che un bene culturale racconta travalicano il mero valore testuale o visivo. Raccontano dei lunghi viaggi della carta, della pergamena, dei minerali, di rotte e scambi commerciali, di scoperte scientifiche e tecnologiche, della genialità degli inventori, dell'evoluzione del gusto e dei costumi. In breve, raccontano la nostra storia.

Per scoprire ciò che il libro nasconde, occorre guardarlo con occhi diversi, gli occhi della scienza.

A partire dalla semplice microscopia ottica fino ad arrivare a più sofisticate tecniche spettroscopiche, si darà una differente chiave di lettura dell'oggetto libro.

ICE CLATHRATES AND FILLED ICES UNDER PRESSURE: NEUTRON INSIGHTS ON PLANETOLOGY AND GAS STORAGE

L.E. Bove

IMPMC, CNRS-UMR 7590, Université Pierre & Marie Curie, 75252 Paris, France.
Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy.

Gas clathrates are inclusion compounds encaging gas molecules (such as CH_4 or H_2) in polyhedral cages of hydrogen bonded water molecules. They are considered as interesting materials as gas resource and for gas storage in the light of their high mass % gas content. Among the different clathrate hydrates, methane hydrate is the most widespread naturally occurring gas hydrate as it is present in large quantities in oceanic shelves sediments and in permafrost regions. It has attracted considerable attention for its potential as geo-organic fuel resource [1]. Exchanging the guests in existing methane hydrate deposits with CO_2 has also been indicated as a promising two-in-one approach of energy recovery and concomitant carbon dioxide mitigation. Methane hydrates are also believed to exist at depth in many water-rich objects populating our solar system and their destabilisation could be responsible for the observed anomalous gas enriching of some planetary atmospheres [2].

Hydrogen clathrates also show a remarkably high hydrogen mass content (5.3 mass % of molecular hydrogen), which increases even more (up to 18 mass %) under high pressure (above 2 GPa), when the clathrate cages shrink and reorganize into structures bearing some resemblance to ice phases, known as filled ices [1].

As a matter of fact, high-pressure phases of methane and hydrogen hydrates can only find practical applications for gas storage if their synthesis pressures can be decreased. This requires a complete understanding of the mechanisms of formation and stabilisation in which the guest molecule dynamics plays a crucial role. The characterization of their structural, dynamical and conductivity properties under high pressure is not only crucial to model planetary interiors, but is a fundamental piece of information to unravel the nature of the interaction between the guest gas molecule and the ice skeleton.

In this talk I will present our recent work on methane and hydrogen hydrates at high pressure performed by neutron diffraction and incoherent inelastic and quasielastic neutron scattering revealing unexpected dynamical phenomena in gas clathrates under pressure [3,5] and new remarkable properties of filled ices [4,6].

[1] W.L. Mao, Physics Today **60**, 42 (2007).

[2] I. De Pater and J.J. Lissauer, Planetary Sciences, Cambridge University Press (2004).

[3] U.L. Ranieri *et al.*, Nature Comm. **8**, 1076 (2017).

[4] S. Schaack *et al.*, J. Phys. Chem. C **122**, 11159 (2018).

[5] U.L. Ranieri, J. Phys. Chem. Lett. **123**, 1888 (2019).

[6] S. Schaack *et al.*, Proc. Natl. Acad. Sci. USA, submitted (2019).

INTEGRATED MOTIONS OF MOLECULAR MACHINES AND MOTORS: FROM STRUCTURE TO MECHANICS

A. Calamida[1,2], S. Fiore[1,2], M. Pillon[1], M. Angelone[1], F. Andreoli[1], G. Pagano[1], S. Loreti[1],
A. Pietropaolo[1], U. Besi[1]

[1]ENEA – Frascati.
[2]Sapienza Università di Roma.

IPer realizzare la fusione nucleare per produrre energia elettrica sono necessari molti studi, sia in ambito fisico che ingegneristico. In particolare è molto importante studiare il comportamento di diversi materiali coinvolti sotto irraggiamento neutronico.
Per questo tipo di studi è stata costruita la macchina FNG. Questa accelera ioni di deuterio che fa poi collidere su un bersaglio di titanio-trizio. In questo modo si ottengono reazioni di fusione nucleare DT con produzione di neutroni. La macchina può essere configurata anche per produrre reazioni di fusione DD.
Per studiare possibili upgrade sulla macchina sono necessarie delle simulazioni che ne verifichino l'attuabilità. Fino ad ora si era usato il software MCNP per queste, ma adesso si è deciso di passare a FLUKA.
Il mio primo lavoro, per tanto, è stato convertire la source per FNG da MCNP a FLUKA. Successivamente sono state fatte delle simulazioni per validare il nuovo codice che hanno dato esito positivo.
Il passo seguente è stata l'implementazione dell'emissione delle particelle alfa/elio-3 nella source. In seguito, questa è stata configurata per poter emettere due particelle contemporaneamente. Così sarà possibile studiare se le due particelle emesse mantengano una correlazione fra di loro. In questo modo è possibile studiare se si può implementare un sistema di *trigger* su FNG.

HIGH TEMPERATURE OPERATION OF CVD DIAMOND DETECTORS IN CURRENT MODE

S. Cesaroni[1], M. Angelone[2]

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[2]2. ENEA Dipartimento Fusione e Sicurezza Nucleare, CR Frascati, via E. Fermi 45, 00044 Frascati (RM).

In the last years there has been an increasing interest in diamond detectors operating in harsh environments characterized by high temperature and intense γ and neutron fluxes. Attempts to develop diamond detectors able to operate at high temperature were already reported in literature, but all of them refers to the detector operated in "pulse mode", that is feasible up to $\sim$ 500 K. The mentioned temperature limit is not sufficient for some applications, e.g. the use of the detector in the Tritium Breeding Module (TBM) of the ITER tokamak, where the operational temperature ranges from $\sim$ 575 K (cooler inlet) up to $\sim$ 800 K (cooler outlet). In my last work, the operational performances and limits of an artificial single crystal CVD diamond detector operating in "current mode" at high temperature (HT) are investigated. The current mode operation enables to monitor fundamental nuclear parameters over time, such as the neutron flux and the on-line tritium production in fusion reactors. The diamond detector response in terms of leakage current was first characterized versus the temperature and the biasing voltage (HV), then the detector was exposed to intense ^{60}Co γ-ray and 14 MeV neutron fluxes. Its response and time dependent behaviour were studied at temperatures ranging from 300 K (room temperature) up to 675 K. Saturation of the measured response both with the applied HV and γ-ray dose rate was observed for $T > 625$ K.

FOUR-DIMENSIONAL INELASTIC NEUTRON SCATTERING SIMULATED ON A QUANTUM HARDWARE

A. Chiesa[1], F. Tacchino[2], M. Grossi[3], P. Santini[1], I. Tavernelli[4], D. Gerace[2], S. Carretta[1]

[1]Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, Italy.
[2]Dipartimento di Fisica, Università di Pavia, Italy.
[1]IBM Italia s.p.a., Circonvallazione Idroscalo, Segrate, Italy.
[1]IBM Research, Zurich Research Laboratory, Zurich, Switzerland.

Molecular Nanomagnets are at the forefront of current research in condensed matter Physics. Four-dimensional Inelastic Neutron Scattering (INS) is the technique of choice to characterize their spin dynamics, enabling an atomic-scale characterization of their eigenstates [1,2]. However, measurements on many new compounds consisting of a large number of interacting ions cannot be interpreted on classical computers, due to the exponential scaling of the required resources.

Here we show that the calculation of dynamical spin correlation functions necessary to compute the INS cross-section can be efficiently performed using the forthcoming generation of quantum computers [3]. By thorough experiments on IBM quantum hardware we simulate, for the first time with a quantum computer, the magnetic neutron cross-section of prototypical finite spin systems. We identify the most important gate errors and highlight strategies to mitigate them by applying general properties of the extracted correlations, thus recovering the correct dynamics even in complex simulation algorithms. The synergy between advances in neutron scattering and quantum information technologies, (with the realization of improved devices containing up to dozens of qubits) will enable a deeper understanding of complex spin systems, whose spectra shall be efficiently interpreted thanks to the speed-up of quantum processors.

[1] M.L. Baker, T. Guidi, S. Carretta, J. Ollivier, H. Mutka, H. U. Güdel, G.A. Timco, E.J. L. McInnes, G. Amoretti, R.E.P. Winpenny and P. Santini, Nature Phys. **8**, 906 (2012).

[2] A. Chiesa, T. Guidi, S. Carretta, S. Ansbro, G.A. Timco, I. Victorica-Yrezabal, E. Garlatti, G. Amoretti, R.E.P. Winpenny, and P. Santini, Phys. Rev. Lett. **119**, 217202 (2017).

[3] A. Chiesa, F. Tacchino, M. Grossi, P. Santini, I. Tavernelli, D. Gerace and S. Carretta, Nature Phys. **15**, 455 (2019).

STRUCTURE OF HUMAN TELOMERE G-QUADRUPLEX IN THE PRESENCE OF A MODEL DRUG ALONG THE THERMAL UNFOLDING PATHWAY

L. Comez[1], F. Bianchi[2], R. Biehl[3], F. D'Amico[4], A. Gessini[4], M. Longo[5], C. Masciovecchio[4], C. Petrillo[2], A. Radulescu[5], B. Rossi[4], F. Sacchetti[2], F. Sebastiani[6], N. Violini[5], A. Paciaroni[2]

[1]Dipartimento di Fisica e Geologia, Università di Perugia, Perugia, Italy.
[2]IOM-CNR c/o Dipartimento di Fisica e Geologia, Università di Perugia, Perugia, Italy.
[3]JCNS & ICS, Forschungszentrum Jülich GmbH, Leo-Brandt Strasse, Jülich, Germany.
[4]Elettra-Sincrotrone Trieste, AREA Science Park, Basovizza, Trieste, Italy.
[5]JCNS Forschungszentrum Jülich GmbH at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany.
[6]Lehrstuhl für Physikalische Chemie 2, Ruhr-Universität Bochum, Bochum, Germany.

A multi-technique approach, combining circular dichroism spectroscopy, ultraviolet resonance Raman spectroscopy and small angle scattering techniques, has been deployed to elucidate how the structural features of the human telomeric G-quadruplex d[A(GGGTTA)3GGG] (Tel22) change upon thermal unfolding [1]. The system is studied both in the free form and when it is bound to Actinomycin D (ActD), an anticancer ligand with remarkable conformational flexibility. We find that at room temperature binding of Tel22 with ActD involves end-stacking upon the terminal G-tetrad. SANS provides structural evidence for drug-driven dimerization of a significant fraction of the G-quadruplexes is provided. When the temperature is raised, both free and bound Tel22 undergo melting through a multi-state process. We show that in the intermediate states of Tel22 the conformational equilibrium is shifted toward the (3+1) hybrid-type, while a parallel structure is promoted in the complex. The unfolded state of the free Tel22 is consistent with a self-avoiding random-coil conformation, whereas the high-temperature state of the complex is observed to assume a quite compact form. Such an unprecedented high-temperature arrangement is caused by the persistent interaction between Tel22 and ActD, which stabilizes compact conformations even in the presence of large thermal structural fluctuations.

[1] F. Bianchi *et al.*, Nucleic Acids Res. **46**, 11927-11938 (2018).

STRUCTURAL CHARACTERIZATION OF NANOPARTICLES FOR DRUG DELIVERY: TUNING NANOSTRUCTURE AND MUCUS INTERACTION

E. Del Favero[1], E. Di Cola[1], F. Sonvico[2], V. Rondelli[1], P. Brocca[1], L. Cantù[1]

[1]BIOMETRA Dept., University of Milan.
[2]Dipartimento di Scienze degli Alimenti e del Farmaco, University of Parma.

Nanoparticles and nanoemulsions composed by a hydrophobic core stabilized by physiological lipids or surfactants have been widely proposed as efficient vectors for mucosal drug delivery. Besides the optimal encapsulation, the design of the best vectors has to face key properties as the target achievement and the controlled release of the drug. According to the final target, the selected administration route, and the delivery strategy, mucoadhesive or mucopenetrating agents, like chitosan and PEGylated surfactants, can profitably modulate the residence time and the interaction of nanoparticles with the mucus barrier. We applied a complete structural characterization of different new nanovectors with non conventional association of chitosan for ophthalmic and nasal administration. Results were obtained with complementary techniques, scanning the nanoparticles on different lenghtscales. Neutron scattering (SANS), allowing the enhanced visibility of selected components, was paralleled by dynamic light scattering (DLS) and Differential Scanning Calorimetry. Combined results guided the realization of chitosan-associated formulations with the optimal structural properties and allowed for determining their propensity to interact with the mucin gel and their biodegradability by enzymes typical of the mucus layer, such as lysozyme. The accessibility of structural properties on different lenghtscales comes out to be fully functional to the description of complex interacting colloidal biosystems.

THE VESPA PROJECT: MOVING TOWARDS THE DETAILED DESIGN

L. del Rosso and D. Colognesi

Istituto di Fisica Applicata "Nello Carrara" - Consiglio Nazionale delle Ricerche, via Madonna del Piano 10, Sesto Fiorentino (FI) - Italia.

The neutron instrumental suite of the new European Spallation Source (ESS, Sweden) is currently composed of 16 approved beam-lines. Among these, VESPA (Vibrational Excitation Spectrometer with Pyrolitic-graphite Analysers) is the only one with an Italian institution (i.e. CNR) as leading partner. The instrument will be fully dedicated to Neutron Vibrational Spectroscopy (NVS) for chemical and material science applications. Thanks to the high resolution and flux in the energy range of the so-called "fingerprint region" (i.e. 60-220 meV), VESPA will produce world leading science in NVS field. Its concept design has been officially approved by the ESS Tool Gate 2 panel about one year ago, so allowing the project to move forward to the detailed design phase. Here we illustrate the progresses to date of the design work, underlining the joint effort of the scientific and engineering team to develop the best performance and contain the criticalities that inevitably occur in a budget-limited project.

CARATTERIZZAZIONE DI SELF POWERED NEUTRON DETECTORS PER NEUTRONI VELOCI DA UTILIZZARE NELLA FACILITY DONES

F. Di Giambattista[1,2], O. Aberle[3], M. Angelone[2], M. Calviani[3], M. Pillon[2], S. Fiore[2]

[1]Università degli Studi di Roma "Tor Vergata", Via Cracovia 50, 00133, Roma. [2]ENEA - Centro Ricerche Frascati, Via Enrico Fermi 45, 00044, Frascati, Roma. [3]European Organization for Nuclear Research (CERN), Geneva, Switzerland.

I materiali strutturali utilizzati nei futuri reattori a fusione saranno sottoposti ad elevati flussi di neutroni veloci, provocando danni da radiazione di entità attualmente sconosciuta. Con lo scopo di effettuare test su tali materiali verrà costruita la facility DONES, che ospiterà una sorgente di neutroni veloci ad alto flusso. Tale flusso dovrà essere monitorato con rivelatori adatti all'utilizzo in ambienti ostili: i Self Powered Neutron Detectors (SPND).

I SPND hanno una struttura coassiale, in cui l'elettrodo interno (emettitore) è costituito dal materiale attivo sensibile ai neutroni. Sono stati realizzati due prototipi di SPND con materiali sensibili ai neutroni veloci: uno con emettitore di rodio e uno con emettitore della lega di alluminio 4047A.

I prototipi di SPND sono stati sottoposti a test per studiarne la risposta presso due sorgenti di neutroni: GELINA (JRC, Geel, Belgio) e n_TOF (CERN, Ginevra, Svizzera). In entrambe le facility i rivelatori sono stati installati vicino al punto di produzione dei neutroni, dove non erano mai state effettuate misure precedentemente.

In questo contributo saranno presentati i dati sperimentali raccolti, i risultati ottenuti e le prospettive future.

HYDRATION AND AGGREGATION OF GLYCINE IN AQUEOUS SOLUTION

M. Di Gioacchino, M.A. Ricci, F. Bruni

Università degli studi Roma Tre, Dipartimento di Scienze, via della vasca navale 84,00146, Roma, Italia

Glycine (gly) is the simplest amino acid and has several applications in pharmaceutical industry. Its more stable form in aqueous solution is the zwitterionic one [1]. Gly hydration and aggregation proprieties have been widely investigated by using both experimental and computational methods. However these studies report conflicting results, e.g. as far as gly aggregation is concerned [2,3]. It has been shown that there is a critical temperature ($T^* = 333$ K) at which the hydration shell around the gly undergoes a dynamic transition [4], which could also imply a structural transition. In this context, we have performed a neutron diffraction experiment, with isotopic H/D substitution augmented by EPSR simulations, on a gly aqueous solution as a function of concentration (1:17 - 1:30, solute molecule: solvent molecules) and temperature (300 K - 353 K) to obtain information at atomic scale on these transitions. We have seen a strong gly hydration, influenced neither by concentration nor by temperature. However, the structure of water is sensitive to both concentration and temperature, which determine quite distinct changes of the water H-bond network. We have evidenced signatures of gly aggregation at both concentrations investigated: at high concentration (1:17), the preferred aggregates conformation is the cyclic dimer; at low concentration (1:30) linear chains are favored. These results help to better comprehend gly aggregates formation and possibly protein folding processes.

[1] M.G. Campo, J. Chem. Phys. **125**, 114511 (2006).

[2] S. Hamad *et al.*, J. Phys. Chem. B **112**, 7280–7288 (2008).

[3] A.S. Myerson *et al.*, J. Crystal Growth **110**, 26 – 33 (1991).

[4] F. D'Amico *et al.*, J. Chem. Phys. **139**, 015101 (2013).

DIAGNOSTICHE DI SPETTROSCOPIA ATOMICA CON POSSIBILITÀ DI STRATIGRAFIA SUI BENI CULTURALI – APPLICAZIONI NEL PROGETTO ADAMO

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Il progetto ADAMO (Analisi, Diagnostiche e Monitoraggio), condotto all'interno del DTC (Distretto Tecnologie per la Cultura) della Regione Lazio, prevede la dimostrazione in laboratorio ed in situ di tecniche innovative di analisi e diagnostica su Beni Culturali di interesse regionale. Le tecniche spettroscopiche offrono in generale potenzialità di determinare la composizione di superfici complesse in maniera non distruttiva o micro-distruttiva. Le tecniche che consentono di ottenere informazioni sulla composizione elementale e hanno anche potenzialità di stratigrafia comprendono la spettroscopia neutronica, la PIXE (Proton Induced Xray Emission), basata sull'emissione di raggi X indotta dall'assorbimento di protoni, e la LIBS (Laser Induced Breakdown Spectroscopy), basata sull'emissione UV-Visibile da parte del plasma di ablazione laser. Le potenzialità delle tre tecniche in termini di analisi sub-superficiale verranno confrontate per applicazioni specifiche nel settore, considerando specificatamente le capacità di penetrazione di ciascuna. In particolare verranno presentati risultati significativi ottenuti mediante PIXE e LIBS per l'analisi di superfici dipinte stratificate, nell'ambito del progetto ADAMO, valutando le possibilità di integrazione dei dati per ottenere risultati quantitativi, oltre al riconoscimento di pigmenti e leganti dall'analisi elementale.

NEW EXPERIMENTAL OPPORTUNITIES AT THE ILL - NEUTRON SPIN-ECHO UPGRADES

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A major upgrade of the IN15 high resolution Neutron Spin Echo Instrument has been recently completed and by now it has been reached a smooth routine operation. The upgrade aimed not only on improved resolution but also higher throughput. At some conditions this can be as high as a factor 10, thus sample environement had to follow. We will also report on the status of the construction of WASP, the high Q high resolution Spin Echo. It had its first neutrons the last week before the reactor shut down and hopefully by the time of this meeting we can report some more news.

STRUCTURAL INVESTIGATION ON TEMPO-OXIDIZED NANOCELLULOSE

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Cellulose nanofibers are versatile building blocks for several preparations. They can be easily obtained via selective oxidation of the primary alcoholic groups of cellulose backbone to the corresponding carboxylic groups, by means of TEMPO/NaBr/NaClO oxidizing system. Depending on their concentration, aqueous dispersions of TEMPO-oxidized cellulose nanofibers (TOCNFs) show different rheological properties, ranging from low viscous solutions to highly viscous gels. In spite of this "gel-like" character, the structure can be easily disrupted by high shear rate to form a liquid. Indeed, TOCNF-dispersions behavior can change reversibly from elastic-dominated to viscous-dominated regimes, a behavior typical of thixotropic materials. These specific properties make these dispersions interesting for different biomedical purposes, including injectable gels. Moreover, the addition of cationic electrolytes (e.g. $Mg_2{}^+$, $Ca_2{}^+$) into TOCNF dispersions enables to form homogeneous and stable hydrogels. We herein report the results on the in deep multi-technique characterization on these systems, realized thanks to the support of CERIC and ELETTRA actions, by crossing the data obtained by small angle neutron scattering (SANS) analysis, UV Raman technique, and Brillouin lights scattering measurements. Overall these data provide a comprehensive characterization of the nanocellulose hydrogels, laying the foundations for further applications.

Effect of microstructure on mechanical properties and residual stresses in interpenetrating aluminum–alumina composites fabricated by squeeze casting

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Aluminum-alumina composites with interpenetrating network structure are interesting structural materials due to their high resistance to elevated temperature and frictional wear, good heat conductivity, enhanced mechanical strength and fracture toughness. In this work aluminum-alumina bulk composites and FGMs are manufactured by pressure infiltration of porous alumina preforms with molten aluminum alloy. Influence of the inter-penetrating microstructure on the macroscopic bending strength, fracture toughness, hardness and heat conduction is examined. Special focus is on processing-induced thermal residual stresses in aluminum-alumina composites due to their potentially detri-mental effects on material performance in structural elements under in-service condi-tions. The residual stresses are measured experimentally in the ceramic phase by neu-tron diffraction and simulated numerically using a micro-CT based Finite Element model, which takes into account the actual interpenetrating microstructure of the composite. The model predictions for two different volume fractions of alumina agree fairly well with the neutron diffraction measurements.

OVERVIEW AND PROGRESS OF THE ESS INSTRUMENT SUITE

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Sin dagli anni Novanta la tematica dell'accelerazione di fasci intensi di protoni ha ricevuto una grande attenzione in Italia, a partire dal progetto TRASCO/ADS e attraverso vari programmi di R&S finanziati da fondi europei e dalla Commissione Scientifica Nazionale V dell'INFN. Il know-how derivato da queste attività è stato prezioso nella fase di Accelerator Design Update del Linac per la European Spallation Source (ESS) e ha consentito di giocare un ruolo decisivo nella redazione del progetto della macchina, riconosciuto con la leadership italiana della sezione "Normal Conducting Linac" e con la fornitura di componenti importanti dell'acceleratore come contributo in-kind italiano, massimizzando così i vantaggi per i tre Enti partecipanti (INFN, CNR, Elettra) e indirettamente per l'industria nazionale. In particolare l'Italia sta fornendo in-kind la maggior parte della sezione normal conducting (sorgente di protoni ad alta intensità, LEBT e Drift Tube Linac), una parte della sezione superconduttiva (Medium beta elliptical cavities), l'insieme delle stazioni a radiofrequenza per la sezione "spoke" (fornita dalla Francia), alimentatori, magneti ed elementi di diagnostica.

La presentazione descriverà lo stato di avanzamento di tale contributo, a partire dalla sorgente di protoni già in funzione a Lund, inaugurata nel novembre 2018 alla presenza del Presidente della Repubblica Mattarella e del Re di Svezia. Sarà infine analizzata sinteticamente la ricaduta industriale di tale collaborazione tra Enti di Ricerca, con caratteristiche originali rispetto a precedenti esperienze.

INVESTIGATING MOLECULAR NANOMAGNETS WITH FOUR-DIMENSIONAL INELASTIC NEUTRON SCATTERING: MAGNETISM, SPIN DYNAMICS AND BEYOND

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In the quest for quantum technologies, Molecular Magnetism is offering a variety of promising systems. Indeed, Molecular nanomagnets (MNMs) can either be exploited as classical bits in high-density magnetic memories or as qubits for quantum information processing. Inelastic neutron scattering (INS) is a powerful tool to investigate the properties of these systems and new possibilities have been opened by exploiting the new generation of time-of-flight spectrometers with large arrays of position-sensitive detectors, which enable to efficiently measure the neutron cross-sections as a function of energy and of the three components of the momentum transfer vector **Q** in vast portions of the reciprocal space. This 4D-INS technique allows one to obtain an unprecedented insight into the coherent spin dynamics of MNMs [1]. For instance, we can unambiguously characterize the molecular magnetic interactions [2,3] and we can quantify entanglement in dimers of molecular qubits [4]. In addition, this technique has recently allowed us to measure for the first time phonon dispersions in a MNM, a key-ingredient to understand magnetic relaxation in these systems and a further step towards their use in quantum technologies.

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OVERVIEW AND PROGRESS OF THE ESS INSTRUMENT SUITE

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Construction of the physical infrastructure of ESS is now nearing completion and efforts are now turning to the construction and installation of technical components. Here we present the plans and progress for the initial ESS neutron instrument suite, consisting of 15 experimental beamlines and a test beamline. In addition to the beamlines, progress on supporting activities such as laboratories and data management will be presented, along with some thoughts towards the future.

QUASIELASTIC NEUTRON SCATTERING – IS THERE ANOTHER WAY? THE ELASTIC SCATTERING SPECTROSCOPY ROUTE

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Incoherent diffusive-motion is usually measured using quasielastic neutron scattering (QENS). However, it is difficult to extract dynamical information directly from the experimental QENS energy-spectrum, $S(q, \omega)$, so either analytical or molecular-dynamics models are typically used to understand the measured dynamics in the time-domain, $I(q, t)$. Currently, only neutron spin-echo (NSE) can measure the decay of atomic position in the time-domain directly. In practice the measured polarisation in NSE remains on the elastic condition, and this bears a tantalizing similarity to the technique "resolution elastic neutron scattering" (RENS), which used the integrated elastic intensity versus the experimental resolution-time to probe the overall system relaxation time [1]. RENS results, however, are intractable for obtaining $I(q, t)$. We will present an instrument concept, based either on back-scattering or time-of-flight, that makes RENS-like scan, but overcomes the limitations above to measure dynamics in the time-domain that do provide straightforward access to $I(q, t)$ [2,3]. We will show that under these special conditions, at each resolution point (at t_{RES}) we measure the integral of $I(q, t)$ up to t_{RES}, so the experiment provides the travelling-integral of $I(q, t)$ [3]. Differentiation of this signal provides $I(q, t)$ and we will discuss practical ways of obtaining this derivative.

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UNVEILING THE ROLE OF PHONONS IN REACHING VERY HIGH BLOCKING TEMPERATURES IN DY-BASED SINGLE-MOLECULE MAGNETS

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Single-Molecule Magnets (SMMs) represent the frontier of miniaturization in magnetic information storage by taking the size of the magnetic unit to the single-molecule limit. Recently, SMMs containing a single lanthanide ion [1] displayed unprecedentedly high blocking temperatures (TB), achieving the ambitious goal of magnetic memory effects at temperatures higher than liquid nitrogen. However, a systematic study on Dy-based SMMs [2] showed that the energy barrier Ueff for the inversion of magnetization induced by magnetic anisotropy is not a good figure of merit for the performances of these compounds. Previous theoretical calculations hint that processes such as two-phonon Raman processes must be taken into account, but further experimental evidences are needed. Therefore, we performed INS experiments on three different Dy-based SMMs with similar Ueff but different TB. From the measured spectra we extracted the phonon density of states (DOS) for each sample in order to identify the main differences between the DOS of the three different compounds. Moreover, comparison of these results with *ab-initio* calculations of phonon DOS will allow a better understanding of spin-phonon relaxation dynamics and will help in identifying the key factors in improving the TB of such compounds.

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PANTHER: A THERMAL TIME OF FLIGHT SPECTROMETER AT THE ILL

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PANTHER (Polarization ANalysis on a THERmal time-of-flight) is a multi-purpose direct geometry thermal neutron time-of-flight (TOF) spectrometer optimized for studies of magnetism, single crystals, and small samples, currently under construction at the ILL at the IN4C position on the H12 beam tube. Once online, it will feature high neutron flux, medium resolution, large detector coverage, and wide span of incoming energies allowing for fast mapping of magnetic and structural excitations over a large range of wave-vector and energy transfers. PANTHER will allow for the use of complex sample environment, including the 10 Tesla "IN5" magnet. It will also be equipped with full longitudinal polarization analysis using a ^{3}He-filter device (PASTIS-3).

Compared to IN4C, the main upgrades are the use of large position-sensitive detectors (PSD), a flight chamber connected to a wide-diameter sample area with a common vacuum, both shielded with 30 cm of borated PEHD, fully double focusing monochromators, additional background choppers, and non-magnetic construction materials. The expected gain in flux is of about a factor of two, an increased solid area of a factor of three, and a reduced background by a factor of ten. The improved signal-to-noise ratio of 60 will be profitable for studies of magnetism, lattice dynamics, and vibrational spectroscopy in the incoming energy range 6-120 meV.

Panther is expected to see its first neutrons in June 2019.

INTEGRATED MOTIONS OF MOLECULAR MACHINES AND MOTORS: FROM STRUCTURE TO MECHANICS

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Switchable functional molecules producing mechanical work constitute an active focus in nanotechnologies as they can be used for molecular-based devices and materials. The coupling in space and time of these building units into larger structures has been a challenge over the last few years in order to transfer the controlled molecular motion to the macromolecular assemblies.1 Recently, we have designed and synthesized a polymer gel integrating light-driven rotary motors as mechanically active reticulation units.2 Due to properly designed topological entanglements, and when activated by light, the unidirectional rotation of the rotary motor starts coiling the polymer chains which transforms the nanoration event in a contraction event at higher scales. A macroscopic contraction up to the 80% of the initial size can be reached. Interestingly, this system can function (i) continuously out of equilibrium, (ii) using a single stimulus, (iii) in an isotropic medium subject to Brownian motion and (iv) by increasing its global free energy over time. In particular, this means that such materials can store energy from light in entangled polymer chains, predominantly by decreasing their entropy in twisted topologies.
In this contribution, we present the first mechanical study of the light-induced contraction process. The existence of an optimal concentration for gel preparation in order to achieve maximal contraction will be discussed. Lastly, mechanicals properties of this class of materials will be combined with the structural properties as observed by SANS and SAXS to define guidelines to design and potentially improve the efficiency of this first generation of motorized active soft gels.

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STUDIO DEL PROCESSO DI PRODUZIONE DI ^{99}MO ATTRAVERSO LA REAZIONE $^{100}\mathrm{Mo}(n, 2n)^{99}$MO INDOTTA DA NEUTRONI A 14 MEV PER LA FISICA MEDICA

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Il contesto di questo lavoro sperimentale è l'investigazione dei metodi di produzione del ^{99}Mo alternativi a quello basato sulla fissione del ^{235}U. In particolare, si è rivolta l'attenzione alla reazione $^{100}\mathrm{Mo}(n, 2n)^{99}\mathrm{Mo}$ indotta da neutroni da 14 MeV prodotti dalla reazione deuterio-trizio al Frascati Neutron Generator (FNG).
L'obiettivo principale è stato quello di determinare tipo e quantità di impurezze che vengono generate nei campioni irraggiati e come queste si trasportano in fase di processamento radiochimico per la produzione del radiofarmaco. Questo è stato fatto analizzando i risultati dell'irraggiamento sia di molibdeno naturale in forma di polvere metallica, che di un pellet sinterizzato di ^{100}Mo metallico. L'approccio metodologico si è basato su diverse fasi:

- simulazioni con il codice MCNP per determinare le condizioni ottimali dell'irraggiamento;
- calcoli deterministici con il codice FISPACT-II per la determinazione dei radionuclidi attivati post irraggiamento a differenti cooling times;
- irraggiamento con neutroni a 14 MeV, con tempi di esposizione dei campioni e ratei di emissione scelti in base alle simulazioni effettuate con MCNP;
- misure di attività mediante spettrometria gamma effettuate presso l'Istituto Nazionale di Metrologia delle Radiazioni Ionizzanti (INMRI) dell'ENEA, utilizzando un rivelatore al germanio iperpuro (HPGe).

In questo contributo verrà presentata l'attività sperimentale e verranno discussi i principali risultati e le prospettive future.

IONIC LIQUIDS FOR ENERGY

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Ionic liquids (ILs) are largely studied for their properties, such us an extremely low vapor pressure, a high ionic conductivity, a high stability and a good solvent capacity, which make them particularly relevant in energy storage and electrochemistry applications. Moreover, the charming properties of these materials lie in the possibility of tailoring them by means of a proper choice of either the cation or the anion or by mixing with other liquids, such as water, alcohols or different ILs. A deep understanding of their microscopic properties and of the interactions within the ions of mixed system is fundamental in order to master such possibility. We present several examples of protic ionic liquids and mixed systems of ionic liquids and water where vibrational spectroscopies combined with ab initio simulations provide information about the microscopic configurations, the phase transitions and the kind of interactions occurring in the system. We show the existence of inhomogeneities in water-ILs mixed systems and the presence in protic and ether functionalized liquids of a strong and directional hydrogen bonds between the cation and the anions, providing an evaluation of the difference in the average energy between the H-bonded and the dispersion-governed configurations. In this framework neutron scattering can provide structural information about the formation of different domains, and indeed the occurrence of mesoscopic structural organization has already been reported.

EFFECT OF MEMBRANE-PROTEIN INTERACTION ON LIPID BILAYERS

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Amyloid β-peptide (Aβ) is known to be connected to the onset of Alzheimer's disease, due to its interaction with cell membranes in the human brain. Hence, the understanding of Aβ influence on the structure [1], and on the dynamical features of membranes remains a crucial molecular challenge [2]. Here, the results of a neutron-scattering study on the interaction of large unilamellar vesicles, as cell membrane models, with both freshly dissolved Aβ and early toxic prefibrillar oligomers are presented [3]. Small Angle Neutron Scattering allowed to observe the membrane-protein systems and hereafter to obtain the structural features of model membranes in presence of Aβ species in different aggregation states. On the other side, Neutron Spin Echo provided the dynamical characterization of the same system. In addition, the effect of coincubating the Aβ-peptide with the chaperonin Hsp60, which is known to interfere with it in its aggregation pattern [4], has been analyzed. Indeed, membrane stiffness increases after Aβ oligomers are released in solution, while the presence of even very low amounts of Hsp60 maintains unaltered the elastic properties of the membrane bilayer. These results can shed new light on the mechanisms underlying the pathogenic interaction between the peptide and lipid bilayers and on the ability of the chaperonin to interfere with Aβ aggregation, by the specific recognition of an Aβ-reactive transient species, allowing the remodulation of the aggregation cascade and the consequent insult on the cellular membrane.

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MUCIN THIN LAYERS: A MODEL ENVIRONMENT FOR MUCOSAL DELIVERY

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The fate of macromolecules of biological or pharmacological interest that enter the mucus barrier is a current field of investigation. Mucus is a highly viscoelastic secretion, covering the epithelia surfaces of the gastrointestinal, pulmonary, oral, nasal and genital tracts. Its function and composition differ at different locations of our body, but the general task of mucus is to protect mucosal tissues from dehydration, mechanical stress, and to act as barrier against microorganisms and toxic substances. Mucus is mainly composed of water (up to 95%), lipids, small proteins and nucleic acids, but its mechanical and viscoelastic properties are due to the main presence of high molecular weight glycoproteins, identified as mucins (MW from 0.5 KDa to 200 MDa), highly glycosylated proteins where sugars can account for up to 80% of the MW. Mucin can establish adhesive interactions with particulates via electrostatic interactions, van der Waals forces, hydrophobic forces, hydrogen bonding, or chain entanglement. Therefore, the development of mucosal drug delivery vehicles is a great challenge because little is still known about the interactions between mucin and other macromolecules: they can either penetrate rapidly or establish prolonged contact with mucus, depending on their specific composition and structure. Studies of the interaction between mucins and molecules involved in topical transmucoidal drug or gene delivery, is a prerequisite for nanomedicine design. We studied the interaction of mucin with the bio-inspired arginine-derived amphoteric polymer D,L-ARGO7 by applying complementary techniques. Small angle x-ray scattering in bulk unveiled the formation of hundreds nanometer sized aggregates, phase separated from the mucin mesh. On the molecular scale, quartz crystal microbalance with dissipation and neutron reflectometry applied to thin mucin layer targeted by the polymer, highlighted polymer interaction with the mucin layer and showed induced instability of the deposition after rinsing. Of relevance we succeeded in building up a new significant model for epithelial tissues covered by mucus, obtaining the deposition of a mucin layer on top of a glycolipid enriched phospholipid single membrane, suitable to be investigated by neutron reflectometry. Since complexation between mucins and biomacromolecules takes place close to the cell membrane surface, the present model is potentially predictive of the fate of nanodrugs intended to cross mucus and enter epithelial cells.

TUNING THE FAST DYNAMICS OF PNIPAM-BASED SYSTEMS WITH BIOLOGICALLY RELEVANT SOLVENTS

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PNIPAM is a thermo-responsive "smart" material that undergoes to a coil-to-globule transition in correspondence of a Lower Critical Solution Temperature (LCST) around 305 K: below the LCST the polymer chain is in a hydrated, un-folded state, while above this temperature the chains collapse in a globular structure. PNIPAM-based systems are object of intense research, both for theoretical studies and for technological applications, in fields spanning from drug delivery to cell growth. In a recent work the picosecond dynamics of concentrated PNIPAM samples has been investigated for the first time through a neutron scattering experiment [1]. The Elastic Incoherent Neutron Scattering (EINS) intensities showed a discontinuous decrease at increasing temperature in correspondence of a critical temperature $\sim$ 250 K. This behaviour recalls the so-called protein dynamical transition (PDT), that is the onset of anharmonic motions in the fast dynamics of hydrated proteins above a critical temperature T_d. Activation of the anharmonic dynamics and protein biological functionality are strictly related. PDT strongly depends on the environment, and different solvent can act as plasticizers or stabilizers. We have recently investigated the effect of glycerol, a well known protein-stabilizer, on the fast dynamics of PNIPAM-concentrated samples. We found that, as in proteins, the dynamics of PNIPAM is largely dependent on the features of the solvent. [1] M. Zanatta *et al.*, Sci Adv **4**, eaat5895 (2018).

I NANOMATERIALI E LA SFIDA CONSERVATIVA DELLE ARCHITETTURE STORICHE: UN SOGNO NEL CASSETTO O UNA REALTÀ PROSSIMA?

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Gli elementi architettonici e non, esposti all'ambiente urbano, sono soggetti a fenomeni di degrado che ne pregiudicano lo stato conservativo. Oltre all'inquinamento, un altro fattore di rischio per le superfici lapidee è costituito dai microrganismi che ne alterano l'aspetto estetico e ne intaccano le proprietà chimico-fisiche.

Attualmente gli interventi di restauro prevedono l'utilizzo di materiali polimerici con funzioni protettive o consolidanti. I nanomateriali, aggiunti ai materiali tradizionali, permettono di ottenere una nuova generazione di prodotti multifunzionali con specifiche ben definite, ad esempio anti-inquinanti e anti-batteriche. Le nanoparticelle più studiate sono le nanoparticelle di biossido di titanio (TiO_2): grazie alle proprietà fotocatalitiche sono in grado di ridurre la quantità di inquinanti e conseguentemente di mantenere più pulite le superfici.

Oltre ai materiali autopulenti si sta lavorando per lo sviluppo di materiali con proprietà antivegetative a rilascio controllato. Le proprietà antivegetative di questi rivestimenti sono legate all'aggiunta di nanocontenitori in silice, caricati, in fase di sintesi, con il biocida. Questo approccio riduce la quantità di biocida impiegato e aumenta la durata nel tempo del trattamento.

In conclusione, i nanomateriali possono dotare di nuove funzionalità le superfici, implementare i benefici della manutenzione conservativa e «amplificare» il risultato in termini di durabilità ed efficacia nel tempo.

STUDY OF MEMBRANE PHASE TRANSITION IN BACTERIAL VESICLES

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In the last few years, it has been discovered that the majority of eukaryotic and prokaryotic cells release small lipid vesicles. These vesicles, generally called micro-vesicles or exosomes, are becoming the object of a great scientific interest, because of their role as carrier of information about progenitor cells, through their cargo of proteins and nucleic acids and the biochemical composition of their membrane [1]. Here we present a study of the temperature-induced phase transitions in the membrane of bacterial Outer-Membrane-Vesicles (OMVs). In particular, we study the OMVs produced by E.Coli which are considered a model system for biological studies. Indeed, as known from the literature [2], E.Coli membrane presents different temperature phase transitions due to structural changes in the organization of the lipid bilayer. We have analysed the thermotropic behaviour of the OMVs membrane by DLS [3] and SAXS measurements at varying temperature. The results showed that also OMVs present membrane phase transitions that are related to a thickness variation of lipid bilayer, as revealed by SAXS. To deeply analyse the membrane behaviour at the transition temperature, we are planning SANS measurements with D2O contrast variation method.

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PROTEIN-LIKE DYNAMICAL TRANSITION IN MICROGELS: A MOLECULAR DYNAMICS STUDY

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Hydrated proteins become biologically active above a temperature of about 220 K at which also a sudden increase of the protein mobility occurs. This molecular process, known as the protein dynamical transition, has been the subject of intensive research, but a deep understanding of its nature still remains elusive. Evidence of a protein-like dynamical transition was recently reported also for a non-biological system, such as poly(N-isopropylacrylamide), PNIPAM, microgels. [1] These micrometer particles, made of a cross-linked polymer network, share many features with proteins, because of their extended covalent connectivity and their amphipilic character. In this contribution we describe the molecular origin of the low temperature dynamical transition in microgels, as obtained from atomistic molecular dynamics simulations. [2] The study is based on a nanoscale model of microgel network in water which has been validated by a direct comparison with elastic incoherent neutron scattering experiments. [1] We show which molecular processes control the dynamics of both the macromolecule and water below the dynamical transition temperature. Through a comparison with the low temperature behavior of bulk water, we demonstrate that below the dynamical transition temperature water dynamics is mainly determined by the macromolecule-water hydrogen bonding interaction. Our findings suggest that the macromolecule-water coupling plays a driving role in the dynamical transition.

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DIFFUSION DYNAMICS IN HYDRATED PNIPAM MICROGEL POWDERS THROUGH VOLUME PHASE TRANSITION

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PNIPAM microgels are nanometer-sized hydrogel particles able to change their behaviour from soft to hard colloids, undergoing a fast and reversible volume phase transition (VPT) from a swollen hydrophilic state to a collapsed hydrophobic state upon increasing temperature. In diluted water solutions, the VPT occurs at about 32°C.

In order to study the diffusional dynamics in the ps regime, quasi-elastic neutron scattering measurements were carried out at the spectrometer IN5 at ILL (Grenoble, France). The sample was studied in solution with water at very high polymer concentrations (10%, 30%, 40%, and 50%). The measurement was performed at different temperatures through the volume phase transition in order to measure its effect both on the polymer and the hydration water. The analysis carried out has made possible to model the behavior of both the PNIPAM microgel and the solvent, whose hydration component can be separated from the bulk one.

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