

SOCIETÀ ITALIANA DI SPETTROSCOPIA NEUTRONICA



XXVI CONGRESSO ANNUALE

Roma e Frascati, 1-3 Luglio 2015

BOOK OF ABSTRACTS

In memoria di Marco Zoppi

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Programma

Mercoledì 1 Luglio

Sapienza Università di Roma
Dipartimento di Chimica
Edificio Cannizzaro – Aula C

Neutroni per la Scienza Sessione speciale del XXVI Congresso SISN

14.00

REGISTRAZIONE

15.00

BENVENUTO DEL PRESIDENTE DELLA SISN

Neutroni in Italia

Una panoramica della ricerca italiana che usa i neutroni

Chairman: Debora Berti

15.10

Neutron diffraction as tool for solving structural problems in lithium materials

Michele Catti

15.30

The manufacturing of Japanese swords: a non-destructive quantitative analysis of steel composition and microstructure through neutron diffraction and neutron imaging techniques

Francesco Grazzi

15.50

Looking for the secret of biomolecules' functionality with neutron scattering

Alessandro Paciaroni

16.10

Unravelling the Spin dynamics and Microscopic Properties of Molecular Nanomagnets by Neutron Scattering

Stefano Carretta

16.30 – 17.00

COFFEE BREAK

Keynote lecture

Chairman: Yuri Gerelli

17.00

Presentazione della Società Italiana di Spettroscopia Neutronica

Paolo Mariani

17.15

Molecules and materials seen by neutrons

Christiane Alba-Simionesco

La sessione Neutroni per la Scienza è proposta dalla Società Italiana di Spettroscopia Neutronica come momento per promuovere l'uso e le potenzialità delle tecniche di scattering neutronico nei diversi ambiti di ricerca. La partecipazione a questa sessione è libera e non richiede l'iscrizione al Congresso o alla Società.

Giovedì 2 Luglio

ENEA, Centro Ricerche di Frascati

8.30

REGISTRAZIONE

8.50

APERTURA DEL XXVI CONGRESSO ANNUALE SISN

Chairman: Antonino Pietropaolo

9.00

Neutrons: a tool for Plasma Diagnostics

Maurizio Angelone

9.20

Hydrogen self dynamics in liquid H₂-D₂ mixtures studied through inelastic neutron scattering

Daniele Colognesi

La ricerca con i neutroni

Prospettive per l'Italia e per l'Europa

Chairman: Paolo Mariani

9.40

European neutron scattering facilities: a chance, a threat and a revival?

Christiane Alba-Simionesco

10.00

Infrastrutture europee e CNR nella ricerca con neutroni

Corrado Spinella

10.20

Discussione

10.30 – 11.00

COFFEE BREAK

Chairman: Alessio De Francesco

11.00

Inelastic Neutron Scattering Study of Frustrated anti-ferromagnetic molecular rings: Cr₉ and Cr₈Mn

Alessandro Chiesa

11.15

Functionalized Iron Oxide Nanoparticles: Developing a Biocompatible System

Alessandra Luchini

11.30

Thermodynamics of protein–nanoparticle interactions. A SAXS and SANS study

Gabriele Campanella

11.45

Exploring cell biodiversity

Irina Piazza

12.00

New Sorgentina Fusion Source (NSFS) experimental facility supporting materials research

Patrizio Console Camprini

12.20

Una sorgente nazionale di neutroni: a cosa serve, a chi serve, quanto costa?

Fabio Bruni & Antonino Pietropaolo

12.30

PRANZO

Chairman: Alessandra Filabozzi

14.00

Flux and neutron spectrum measurements in fast neutron irradiation experiments

Marica Rebai

14.20

Hybrid Superconducting Neutron Detectors

Ivano Ottaviani

Lo stato dei progetti italiani per ESS

Chairman: Francesco Spinozzi

14.40

Overview della suite strumentale di ESS

Fabio Bruni

15.00

T-REX: A Time-of-flight Reciprocal space Explorer for the future European Spallation Source

Nicolò Violini

15.15

The VESPA spectrometer at ESS

Daniele Colognesi

15.30

ANIMA: il progetto di uno strumento multi-purpose per l'analisi di proprietà strutturali dall'Å al μm

Renato Magli

15.45

USANS for SANS instruments: the project OPUS for Loki@ESS

Claudia Mondelli

16.00

Development of GEM-based thermal neutron detectors

Gabriele Croci

16.15

BAND-GEM detectors for SANS measurements at the European Spallation Source

Giorgia Albani

16.30

Efficient Shielding for the European Spallation Source: Borated concrete and ceramic B₄C tiles

Francesco Grazi

16.35

Discussione

16.45 - 17.00

COFFEE BREAK

17.00 - 19.00

ASSEMBLEA DEI SOCI SISN

*L'Assemblea inizierà ricordando Marco Zoppi,
collega e amico recentemente scomparso.*

20.30

CENA SOCIALE

Venerdì 3 Luglio

ENEA, Centro Ricerche di Frascati

Chairman: Marco Maccarini

9.00

Neutron cross sections of the hydrogen liquids from first principle quantum calculations

Eleonora Guarini

9.20

Counter-ion Exchange in Guanosine Quadruplexes: A Contrast-Variation Neutron Diffraction Experiment in Condensed Hexagonal Phase

Silvia Moscatelli & Federica Carducci

9.40

The role of hydration in carbohydrates properties

Laura Maugeri

9.55

PVA-based microgels as carrier systems for industrial applications

Marco Perfetti

10.10

Local structure of temperature and pH-sensitive colloidal microgels

Valentina Nigro

10.25

Activities at the ENEA Casaccia Research Reactors

Mario Carta

10.45 - 11.15

COFFEE BREAK

11.15 - 12.30

L'IMPEGNO ITALIANO NELLE LSF EUROPEE PER LA NEUTRONICA

Tavola rotonda moderata da Paolo Mariani.

Partecipano: Ubaldo Bafile, Fabio Bruni, Giuseppe Gorini, Maria Antonietta Ricci, Alessandro Triolo e Cirino Vasi.

12.30

CONCLUSIONI E SALUTI

12.40

VISITA AI LABORATORI DEL CENTRO DI RICERCA ENEA DI FRASCATI

Abstract dei contributi

BAND-GEM DETECTORS FOR SANS MEASUREMENTS AT THE EUROPEAN SPALLATION SOURCE

G. Albani¹, J. Birch², X.X. Cai^{3,5}, C. Cazzaniga¹, G. Claps⁶, G. Croci¹, G. Gortini¹, G. Grosso⁷, R. Hall-Wilton^{2,3,4}, C. Höglund^{2,3}, L. Hultman², K. Kanaki³, I. Llamas Jansa^{3,5}, A. Muraro⁷, F. Murtas⁶, E. Perelli Cippo⁷, M. Rebai¹, M. Tardocchi⁷.

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The European Spallation Source (ESS) will be the most powerful neutron source, 30 times brighter than today's leading facilities.

Small Angle Neutron Scattering (SANS) will be among the first measurements to be performed at the ESS because of its broad range of applicability across material science, biology and soft matter research.

The expected high neutron fluxes, with associated high count rate requirements on the detectors, have been the main driver for developing a new type of neutron detector based on the Gas Electron Multiplier (GEM) technique. The GEM technique is well established for charged particle measurements in high energy physics applications at CERN and elsewhere. The new development concerns the neutron conversion to charged particles. It is well known that a single layer of ¹⁰B can provide an efficiency that is < 5% for thermal neutrons. In the BAND-GEM approach a 3D geometry for the neutron converter was developed that is expected to provide an average efficiency > 50% in the wavelength of interest for SANS measurements, while meeting all the requirements to have a good *Q* resolution for SANS.

In the presentation the BAND-GEM detection method will be described and the simulation results will be presented. First results based on counting rate tests with a BAND-GEM prototype and the comparison with ³He will be reported and approaches for optimizing the detector performance will be discussed.

NEUTRONS: A TOOL FOR PLASMA DIAGNOSTICS

M. Angelone

ENEA, Centro di Ricerche di Frascati, Frascati, Italy

Presently, the most investigated plasmas are formed by deuterium (D) ions or by mixture of D and tritium (T) ions. The D-D reactions produces 2.5 MeV neutrons through one of the two possible reaction channels (about 50% probability each) that is $D + D \rightarrow T + n$, while the D + T reaction produces 14 MeV neutrons through $D + T \rightarrow {}^4\text{He} + n$. Neutrons, being neutral, escape from the plasma carrying with them not only most of the energy produced by the plasma (about 80%) but also many useful information about the status and quality of the plasma (e.g. fusion power, plasma temperature, plasma shape etc.). The measurement of neutrons produced in a plasma is nowadays one of the main tools for investigating fusion plasma and the development of proper experimental tool devoted to neutron measurement represent one of the most important diagnostics activities for future tokamaks (e.g. ITER, DEMO).

In this lecture the plasma as a neutron source is first considered, then the most important physical information that can be extracted from the neutron emission are discussed and eventually some of the most important neutron diagnostics apparatus are presented (e.g. spectrometers, radial neutron camera, etc.).

THERMODYNAMICS OF PROTEIN–NANOPARTICLE INTERACTIONS. A SAXS AND SANS STUDY

G. Campanella¹, P. Ghigna², G. Ceccone³, C. Ferrero⁴ and F. Spinuzzi¹

¹DiSVA department, Marche Polytechnic University, Ancona, Italy

²Department of Chemistry, University of Pavia, Pavia, Italy

³Nanobiosciences Unit, Joint Research Centre, Ispra, Italy

⁴European Synchrotron Radiation Facility, Grenoble, France

The use of nanoparticles for biomedical purposes has been under investigation for many years. Important applications, such as drug delivery, disease diagnosis and treatment, require intravenous delivery and interaction of nanoparticles with blood. For this reason, the study of interactions of nanoparticles with biomolecules and especially with serum proteins has received particular attention. Despite the applicative importance of coated nanoparticles, there is a lack of information on the mechanisms and thermodynamics at work. We propose to take advantage of small angle scattering (SAS) techniques to directly inspect samples containing both proteins and nanoparticles without any manipulation, allowing physiological conditions to be used for investigating stoichiometry and thermodynamics of the protein–nanoparticle association. We have developed a thermodynamic model able to describe the interplay between a protein and one binding site on the surface of the nanoparticle in terms of an equilibrium association constant. This was the basis of a theoretical work in which we have inspected the sensitivity of SAS techniques to detect protein–nanoparticle association especially for gold nanoparticles of different sizes with bovine serum albumin (BSA). Results have clearly shown that SANS experiments in heavy water solvent allow to obtain the best conditions of scattering length densities contrasts to highlight the differences of the form factor of bound and unbound nanoparticles.

UNRAVELLING THE SPIN DYNAMICS AND MICROSCOPIC PROPERTIES OF MOLECULAR NANOMAGNETS BY NEUTRON SCATTERING

S. Carretta

Dipartimento di Fisica e Scienze della Terra, Università di Parma, Parma, Italy

Molecular nanomagnets (MNM)s are molecules containing a core of magnetic ions whose spins are strongly coupled by superexchange interactions. They form crystals which behave like ensembles of non-interacting magnetic units. Being among the first examples of finite-size spin systems, MNMs have been test beds for addressing several important quantum phenomena. Neutron scattering has played a key role in the understanding of the spin dynamics and of the microscopic properties of MNMs.

In this talk I review our recent investigations of MNMs by neutron scattering. I show that the determination of the four-dimensional inelastic-neutron scattering function in vast portions of the reciprocal space enables the spin dynamics to be determined directly [1], without the need of a model Hamiltonian. This allows us to determine how quantum fluctuations propagate along antiferromagnetic rings, to test the degree of validity of the Néel-vector-tunnelling framework and to investigate the presence of entanglement in a dimer of Cr₇Ni molecular qubits.

Finite spin chains are ultimate-size structures of great importance both for fundamental physics and applications. I report the quantitative study of their microscopic spin structure by polarized neutron diffraction [2]. The results reveal finite-size effects depending on the boundary condition and the parity of the chains.

[1] M. Baker et al, *Nature Physics* **8**, 906 (2012).

[2] T. Guidi et al., *Nature Communications* **6**, 7061 (2015).

ACTIVITIES AT THE ENEA CASACCIA RESEARCH REACTORS

M. Carta¹, G. Bianchini¹, L. De Dominicis², V. Fabrizio¹, L. Falconi¹, O. Fiorani¹,
M. Palomba¹, A. Santagata¹, E. Santoro¹, and M. Sepielli¹

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The ENEA (Italian National Agency for New Technologies, Energy and Sustainable Economic Development) Casaccia Research Centre is located about 25 kilometres (15 miles) northwest of Rome. The Centre hosts most of the ENEA programmatic Units operating in several fields like: bio-technologies, renewable energy sources, innovative energy cycles, environment, technological applications of research nuclear reactors, etc.. Research activities in the nuclear field are mainly linked to the presence of 2 research reactors in Casaccia: TRIGA RC-1 and TAPIRO.

TRIGA (Training Research Isotopes General Atomic) RC-1 is a pool thermal reactor operating since 1967, it has a maximum thermal power of 1 MW and it is equipped with several neutron channels available for materials irradiation with various neutron flux and spectra (maximum neutron flux in the core center around 2.7×10^{13} n/s/cm²). Even if TRIGA RC-1 is a thermal reactor, in many positions inside the core it is possible to perform material irradiations with not negligible epithermal and fast energy neutron flux components (for some positions Cadmium Ratio can reach values around 1.7). Currently the facility is mainly used for irradiations for medical applications, Neutron Activation Analysis (NAA) and it plays an important role in the frame of 7 EU Framework Programme EDEN (End-user driven DEmo for cbrNE) focused on enhancing the management of CBRNE (Chemical, Biological, Radiological, Nuclear and Explosives) incidents related events, especially cross-borders ones. As a vocation the facility is also used for reactor operators training and University students teaching.

TAPIRO (TAratura PIlta Rapida a Potenza 0) is a fast neutron source reactor. It was licensed in 1971 with a maximum power of 5 kW. The project, entirely developed by ENEA's staff, is based on the general concept of AFSR (Argonne Fast Source Reactor - Idaho Falls). This is certainly a facility unique in Europe, maybe all over the world, because the high quality of characterization of its neutronic field (TAPIRO can be considered as a "standard" fast neutron field, ideal for instruments calibration purposes). The reactor, made of a compact cylindrical homogeneous HEU (High Enriched Uranium) Mo-U core with a copper reflector and a spherical borated concrete shielding, has several experimental channels with different dimensions and different neutron spectra. At the maximum power of 5 kW the highest flux in the core center is around 3×10^{12} n/s/cm² (8×10^{11} n/s/cm² with $E > 1.35$ MeV). Currently the facility is mainly used for irradiations supporting the F4E (Fusion for Energy) programs and LHC (Large Hadron Collider) instruments testing. The facility is presently candidate to support NEA (Nuclear Energy Agency) supported research fields in the domain of basic nuclear data improvement for Minor Actinide issues management (closure of nuclear power plants fuel cycle and long-lived wastes management).

NEUTRON DIFFRACTION AS TOOL FOR SOLVING STRUCTURAL PROBLEMS IN LITHIUM MATERIALS

M. Catti

Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Milano, Italy

Important physical and/or chemical properties of crystalline materials often depend on a specific subset of the full structural features. A typical example are framework structures hosting guest atoms/ions/molecules, which possess the wanted property in connection with their configuration. However, just these cases very often present challenging problems for a structural characterization, due to (i) too large scattering contrast between host and guest atoms, and (ii) disorder of the guest species. The issue of contrast, particularly severe for hydrogen and lithium materials, can be addressed by use of powder neutron diffraction in both the constant wavelength and time-of-flight versions.

Applications of this approach will be discussed in the important case of lithium materials, where Li^+ ions are intercalated species in the framework structure of a transition metal oxide. A large diffusivity of lithium is required in these systems to achieve good performance either as ionic conductors (solid electrolytes) or as electrodes in rechargeable batteries. To understand the structural conditions which make Li ions diffuse fast, their location in the equilibrium structure have to be determined accurately. The methodological problems and the main results on a number of materials of interest for application to lithium batteries will be reviewed and discussed.

INELASTIC NEUTRON SCATTERING STUDY OF FRUSTRATED ANTI-FERROMAGNETIC MOLECULAR RINGS: Cr_9 AND Cr_8Mn

A. Chiesa¹, S. Carretta¹, T. Guidi², M. Baker³, R.J. Woolfson³, G. Amoretti¹, C. Barker³, D. Collison³, E.J.L. McInnes³, H. Mutka⁴, J. Ollivier⁴, G.A. Timco³, R.E.P. Winpenny³ and P. Santini¹

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³School of Chemistry and Photon Science Institute, The University of Manchester, Manchester, UK

⁴Institut Laue-Langevin, Grenoble, France

The spin dynamics of large odd-numbered anti-ferromagnetic (AF) molecular rings is investigated by inelastic neutron scattering techniques (INS) on powder samples. Odd membered AF rings are of great interest due to the presence of competing AF exchange interactions that result in frustrated spin ground states. To characterize spin frustration a sound microscopic model is required. Hence, we have investigated the low energy dynamics of the recently synthesized Cr_8Mn and Cr_9 wheels by INS. A microscopic spin Hamiltonian (SH) is adopted, accurately reproducing INS and magnetometry results. The model is then exploited to investigate the internal spin structure of the ground state, via the analysis of spin pair correlations and spin chirality.

Both compounds are characterized by a $S = 1/2$ ground multiplet, resulting from competing AF interactions. While in Cr_8Mn the ideal C_9 symmetry is broken by the Mn, the investigated Cr_9 variant is close to a regular enneagon. In this picture, perfect translational symmetry of the Cr-Cr interactions produces a frustrated, four-fold degenerate ground state. High-resolution INS measurements show a peak at only 0.1 meV resulting from a slight distortion of the ideal enneagon which produces a splitting of the two ground doublets. We have accurately modelled the experimental results by means of a SH with only two different exchange constants. This classifies Cr_9 as one of the large molecular rings closest to be an "ideally frustrated" system.

HYDROGEN SELF DYNAMICS IN LIQUID H₂-D₂ MIXTURES STUDIED THROUGH INELASTIC NEUTRON SCATTERING

D. Colognesi¹, M. Celli¹, U. Bafile¹, M. Neumann², A. Orecchini^{3,4}

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⁴Institut Laue-Langevin, Grenoble, France

We have measured the dynamic structure factor of liquid para-hydrogen mixed with normal deuterium ($T = 20$ K) at two different concentration levels using incoherent inelastic neutron scattering. This choice has been made since the presence of D₂ modifies the self dynamics of H₂ in a highly non-trivial way, acting both on its pseudo-phononic and its diffusive parts in a tunable way. After an accurate data reduction, recorded neutron spectra were studied through the modified Young and Koppel model and the H₂ center-of-mass self dynamic structure factor was finally extracted for the two mixtures. Some physical quantities (i.e. self diffusion coefficient and mean kinetic energy) were determined and compared with accurate quantum Monte Carlo calculations, which, in addition, also provided estimates of the velocity auto-correlation function for the H₂ centers of mass. These estimates, in conjunction with the Gaussian approximation, were used to simulate the H₂ center-of-mass self dynamic structure factor in the same range as the experimental one. The agreement between measured and calculated spectra was globally good, but some discrepancies proved the unquestionable breakdown of the Gaussian approximation in these semi-quantum systems at a level comparable to that already observed in pure liquid para-hydrogen.

THE VESPA SPECTROMETER AT ESS

M. Zoppi¹, **D. Colognesi**¹, A. Fedrigo^{1,2,3}, M. Hartl², U. Bafile¹, M. Celli¹, F. Grazzi¹,
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²European Spallation Source, Lund, Sweden

³Niels Bohr Institute, Copenhagen, Denmark

VESPA (Vibrational Excitation Spectroscopy with Pyrolytic-Graphite Analysers) will be the best resolution broad-band inelastic neutron scattering spectrometer in the world. It will be also the world's first high-intensity inelastic neutron scattering instrument. VESPA is an indirect-geometry spectrometer designed to study the vibrational dynamics of atoms in molecules and solids and, by including a series of diffraction banks, it will also provide their structural patterns. The instrument represents the neutron analogue of an infrared or Raman spectrometer. It is optimised to characterise molecular vibrations over a wide energy range (up to 500 meV), while simultaneously recording structural variations using diffraction detectors. It is equipped with triple blind-chopper system that allows selecting the desired neutrons flux by relaxing or improving the instrumental energy resolution. The overall counting rate for the inelastic signal will be more than one order of magnitude (up to 200 meV) larger than that of the best similar spectrometer currently available, i.e. VISION at SNS. VESPA will give unique insights in materials science not only by telling us "how atoms move" with spectroscopy but also "where atoms stay" with diffraction. Envisaged applications include energy materials, functional chemistry, nanotechnology, surface science, catalysis, biochemistry, geochemistry, condensed matter physics etc. VESPA will allow studying non-hydrogenous materials, as well as tiny high-pressure samples, routinely with inelastic neutron scattering.

NEW SORGENTINA FUSION SOURCE (NSFS) EXPERIMENTAL FACILITY SUPPORTING MATERIALS RESEARCH

**P. Console Camprini¹, P. Agostini¹, D. Bernardi¹, M. Angelone², M. Frisoni³,
A. Pietropaolo², M. Pillon², A. Pizzuto²**

¹ENEA Brasimone Research Center, Camugnano, Bologna, Italy ²ENEA Frascati Research Center,
Frascati, Roma, Italy ³ENEA Bologna, Bologna, Italy

Within the framework of fusion technology research and development, a neutron source has long been considered a key facility to perform irradiation tests aiming at populating materials engineering database - supporting DEMO reactor design and licensing. New Sorgentina Fusion Source (NSFS) has been proposed taking advantage of well-established D-T neutron generators technology, scaled in order to attain a bright source of about 10^{15} n/s. The provision of an actual 14 MeV neutron spectrum, resembling that of a D-T fusion machined, is a relevant feature. In this contribution, the main facility characteristics are provided, together with a brief discussion on target thermal and mechanical issues.

DEVELOPMENT OF GEM-BASED THERMAL NEUTRON DETECTORS

G. Croci^{1,7,8}, A. Muraro⁷, G. Albani¹, E. Perelli Cippo⁷, J. Birch², X. Cai^{3,5}, C. Cazzaniga¹, G. Claps⁶, G. Gorini^{1,8}, G. Grosso⁷, R. Hall-Wilton^{2,3,4}, C. Höglund^{2,3}, L. Hultman², K. Kanaki³, I. Llamas Jansa^{3,5}, F. Murtas⁶, L. Robinson³, M. Rebai¹, M. Tardocchi⁷

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³European Spallation Source ESS AB, Lund, Sweden

⁴Mid-Sweden University, Sundsvall, Sweden

⁵Institute for Energy Technology (IFE), Kjeller, Norway

⁶INFN - Laboratori Nazionali di Frascati, Frascati, Italy

⁷Istituto di Fisica del Plasma (IFP-CNR), Milano, Italy

⁸INFN - Sezione di Milano-Bicocca, Milano, Italy

The research of valid alternatives to ³He detectors is fundamental for the detector affordability of new neutron spallation sources like the European Spallation Source (ESS). In the case of ESS it is also essential to develop high-rate detectors that can fully exploit the increase of neutron flux relatively to present neutron sources. One of the technologies fulfilling these requirements is the Gas Electron Multiplier (GEM) coupled to boron converter layers. Some developments and improvements are needed in order to make this detector technology mature to be really competitive. The detector has to be able to sustain a high rate thermal neutron flux, must have a high efficiency (similar to ³He) and the resolution of FWHM of diffraction peaks must be comparable to those of ³He systems. This presentation shows recent improvements obtained in the last two years in these directions. The neutron rate capability was tested under a very high flux thermal neutron beam (10^8 n/s/cm²) showing no decrease of performances up to several MHz/cm²; neutron diffraction experiments with a GEM detector took place (for the first time) on the INES instrument at ISIS, showing results directly comparable to those of ³He tube; a new prototype of higher efficiency boron GEM based detector was realized and recently tested showing an efficiency between 15% and 20% to 25 meV neutrons. This prototype represents a further step towards the realization of high efficiency thermal neutron GEM based detectors.

THE MANUFACTURING OF JAPANESE SWORDS: A NON DESTRUCTIVE QUANTITATIVE ANALYSIS OF STEEL COMPOSITION AND MICROSTRUCTURE THROUGH NEUTRON DIFFRACTION AND NEUTRON IMAGING TECHNIQUES

F. Grazzi¹, F. Grazzi¹, E. Barzagli¹, F. Salvemini², A. Scherillo³, A. Williams⁴, S. Peetermans⁵, V. Davydov⁵, A.M. Paradowska², F. Civita⁶, R. Franci⁶, E. Lehmann⁵, M. Zoppi¹

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³Science and Technology Facility Council, ISIS Neutron Source, Didcot, UK

⁴The Wallace Collection, London, UK

⁵Paul Scherrer Institut, SINQ Neutron Source, Villigen, Switzerland

⁶Museo Stibbert, Firenze, Italy.

In this work we present the characterization of the peculiar compositional and microstructural properties of the different kinds of steel used to forge ancient Japanese swords according to the five historical different forging traditions (*Gokaden*) and to the period [1-2]. In order to achieve such a goal, a large number of samples needs to be studied and, due to the unique nature of the artifacts, only a non-destructive approach is now possible. Japanese swords were analyzed in the past through traditional methods [3-6] aiming to characterize the steel composition and microstructure, always applying a destructive methods (metallography and electron microscopy) and the results were of great interest but this kind of approach is impossible to be applied at a large extent. Neutron diffraction and neutron imaging represent the ideal method to reach the proposed goal in a non destructive way since they permit to obtain quantitative information about composition, microstructure, morphology and spatial distribution of the material in the samples.

A total of seven intact Japanese swords and nine broken ones, pertaining to different periods ranging from 14th until 19th century, have been analyzed through neutron diffraction and neutron imaging techniques [7-10]. The samples have been made available by the Stibbert Museum and Wallace Collection and by private collectors.

Neutron experiments have been performed in two different facilities: ISIS (UK) and SINQ (CH). Diffraction measurements have been applied on all the selected samples by using the INES [11], ENGIN-X [12] and POLDI [13] diffractometers while neutron imaging measurements have been performed on the ICON [14] beam-line. Neutron imaging measurements covered the full body of most of the samples while neutron diffraction experiments were focused on specific parts of the swords as the tip, the core of the blade (differentiating among the cutting edge, the centre and the back) and the tang to determine the quantitative distribution of the metal and non metal phases. The comparative analysis of the phase distribution and the tomographic reconstruction of the samples permitted to identify peculiar characteristics related to the forging traditions and periods of the Japanese history and to determine the inner metal phase distribution thus confirming the differentiate specialization of the single parts of this kind of swords.

Due to the high quality level of the results in terms of spatial resolution and quantification of phases and microstructures, this multi-methodological non-destructive approach

presents an incomparable potential in the field of historical metallurgy.

- [1] K. Nagayama, *The Connoisseurs Book of Japanese Swords*, Kodansha International, 1997.
- [2] L. Kapp, H. Kapp and Y. Yoshihara, *The Craft of the Japanese Sword*, Kodansha International, 1987.
- [3] M. Chikashige, *Oriental Alchemy*, Samuel Weiser press, 1974.
- [4] J. Piaskowski, *Hist. Metall.* **27**, 110 (1993).
- [5] H. Hoshi and M. Sasaki, *Tetsu to Hagane* **91**, 103 (2005).
- [6] M.R. Notis, *Mater. Character.* **45**, 253 (2000), and references within.
- [7] F. Grazi et al., *J. Anal. At. Spectrom.* **26**, 1030 (2011).
- [8] F. Grazi et al., *Mater. Sci. Forum* **652**, 157 (2010).
- [9] F. Grazi et al., *Anal. Bioanal. Chem.* **400**, 1493 (2011).
- [10] F. Salvemini et al., *J. Anal. At. Spectrom.* **27**, 1494 (2012).
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EFFICIENT SHIELDING FOR THE EUROPEAN SPALLATION SOURCE: BORATED CONCRETE AND CERAMIC B₄C TILES

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This project aims to the development of new recipes for the production of low cost and high efficiency neutron shielding materials.

The concrete under study is intended to be used for neutron shielding as well as for structural components of the beam-lines. The material will be obtained by changing silica with boron rich inert sands. Three minerals have been identified and used to produce test reference samples. Mechanical properties proved to be good for two over the three sands. The results related to mechanical tests and neutron shielding tests measure using imaging with fast neutrons (at NECTAR, FRM-2) and time of flight thermal neutrons (at INES, ISIS) will be shown.

NEUTRON CROSS SECTIONS OF THE HYDROGEN LIQUIDS FROM FIRST PRINCIPLE QUANTUM CALCULATIONS

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We show that calculations of the neutron double differential cross section of liquid H₂ and D₂ can be performed accounting for the quantum nature of these fluids and ensuring the physical consistency of their computed spectral properties. The method, based on the use of quantum simulation results in place of classical models for the translational dynamics, immediately avoids the uncomfortable but typical introduction of adjustable parameters, and directly provides cross section values in excellent agreement with experiment. This tool is expected to meet the increasing need of accuracy and flexibility of cross section calculations for moderating liquids, so central nowadays for both the maintenance and new design of neutron sources.

FUNCTIONALIZED IRON OXIDE NANOPARTICLES: DEVELOPING A BIOCOMPATIBLE SYSTEM

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Fe₃O₄ iron oxide magnetic nanoparticles (MNPs) are Magnetic Resonance Imaging (MRI) contrast agents suitable for the diagnosis of several pathologies such as cancer. Our recent contribution was to develop a functionalization protocol for the introduction on MNPs surface of biocompatible molecules, such as phospholipids. Even if the functionalized MNPs were tested both in vitro and in vivo showing promising results, it is of great interest to collect information to further improve MNPs biocompatibility. The cellular membrane, being the most external cellular component, is certainly one of the main targets for functionalized MNPs. For this reason we recently started the characterization of the interaction between functionalized MNPs and lipid bilayers, systems that can be considered mimicking the lipid portion of a cellular membrane. Small Angle Neutron Scattering (SANS) and Dynamic Light Scattering (DLS) were used to characterize the nanoparticles suspension and they confirmed that by our functionalization approach monodisperse nanoparticle suspensions can be obtained. Furthermore, Neutron Reflectivity (NR) and Quartz Crystal Microbalance (QCM-D) data shed light on the behavior of lipid bilayers in presence of functionalized MNPs. The results obtained with these techniques were compared with DLS and CryoTEM measurements in which the lipid bilayer was not supported. Indeed, the functionalized MNPs resulted to be non-disruptive for the lipid scaffold of the cellular membrane.

ANIMA: IL PROGETTO DI UNO STRUMENTO MULTI-PURPOSE PER L'ANALISI DI PROPRIETÀ STRUTTURALI DALL'Å AL μM

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Il progetto ANIMA è stato presentato nel 2013: uno strumento per studiare le caratteristiche strutturali microscopiche con l'uso simultaneo della Diffrazione a grandi angoli, della Diffusione a piccoli angoli e dell'Imaging neutronici, in modo da coprire un ventaglio di distanze spaziali dall'Å al μm .

In questa comunicazione viene presentato lo stato attuale e le prospettive future di tale progetto, con una discussione delle caratteristiche tecniche e delle possibili collaborazioni nel contesto dei 16 strumenti approvati ad ESS. Saranno anche brevemente descritti alcuni degli ambiti scientifici che possono trarre beneficio dalla combinazione delle tecniche proposte.

THE ROLE OF HYDRATION IN CARBOHYDRATES PROPERTIES

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This study has revealed how the hydration of carbohydrates can be the key for explaining their different behavior in the sweetness taste perception and in bioprotection mechanism. The difference in sweetness between glucose and trehalose [1] (made up by two glucose rings), triggered our curiosity, and recently we have performed Neutron Diffraction experiments with H/D substitution (NDIS) [2] on both carbohydrates in solution to look at the solvent structure. The data analyzed via EPSR simulations, have revealed a different hydration pattern between the two. These results were also compared with those obtained with cellobiose, made up by two glucose rings but with no reported taste [3]. Moreover, these three sets of NDIS data augmented by EPSR simulations, have been analyzed with a novel tool called ANGULA. This analysis has allowed to characterize the position and orientation of water molecules around a central reference carbohydrate molecule, resulting in spatial density maps showing the probability density of water around a solute in three dimensions. The striking observation is that water molecules are located close to hydroxyl and hydroxymethyl sites of cellobiose and glucose, while, in the case of trehalose, these are located between the two rings. Based on these findings, the different hydration patterns of the three solutes might suggest a possible link between the hydration of specific solute sites with the solute specific activity as a sweet substance, as building block of cellulose fiber, and as a bioprotective agent, respectively.

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USANS FOR SANS INSTRUMENTS: THE PROJECT OPUS FOR LOKI@ESS

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Chemistry and physics have made major progresses, yielding much more complex systems with high hierarchical order on a manifold length scale. Characterization tools need to elucidate such new materials on all length scales. SANS and moreover USANS become the ideal tool to study that complexity and they could be applied to very different fields of science.

OPUS (OPtion USans) is a project dedicated to study an USANS option for the ESS SANS instrumentation suite in particular for the time-of-flight SANS instrument, LoKI, which will be constructed at the European Spallation Source. The project will consist of a basic design and simulation by ray tracing techniques of the USANS option using as starting point and bench test the prototype designed for the upgrade of D11@ILL.

The basis of our approach is a principle proposed by Roland Gähler in 2002. The technique is ideally suited as a SANS upgrade, as it uses the components of a classical SANS instrument. The only USANS-specific requirement is the addition of a high resolution detector. The principle may be used on continuous beam as well as time-of-flight instruments. The fundamental idea is to multiplex the scattering experiment in order to achieve a gain in intensity over an equivalent single pinhole geometry. The accessible Q -range can be extended to at least 10^{-5} \AA^{-1} without a loss in intensity.

This contribution will present first simulation results on a possible implementation of such an USANS option on LoKI in the frame of the project OPUS, which is financed as in-kind contribution to the ESS by the Italian government.

COUNTER-ION EXCHANGE IN GUANOSINE QUADRUPLEXES: CONTRAST-VARIATION NEUTRON SCATTERING EXPERIMENTS IN SOLUTION AND IN CONDENSED PHASE

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G-quadruplexes are helical structures formed by self-assembling of guanosine derivatives in water and in the presence of monovalent cations. G-quadruplexes are comprised of tetrads stacked one on the top of the other at a distance of 3.4 Å, each of the tetrads consisting of four planar guanine molecules, arranged in a cyclic pattern following the Hoogsteen scheme. Depending on concentration and temperature, G-quadruplexes exhibit an additional long-range organization, characterized by the formation of hexagonal and cholesteric lyotropic phases [1].

SAXS experiments demonstrated that G-quadruplexes are relatively short (typically, from 30 to 150 Å), but their length is strongly dependent on counter-ion concentration and on temperature. It has been suggested that counter-ions compete for quadruplex major and minor binding sites, stabilizing the final structure in different ways [2].

In this work, neutron scattering, in combination with contrast variation technique, has been used to study the quadruplex structural properties in the presence of different counter-ions, which competes for the different binding sites [3]. Neutron scattering experiments were performed at D16 and D11 instruments at the Institut Laue-Langevin (Grenoble, France), at room temperature. The guanosine 5'-monophosphate, K salt, was considered and G-quadruplexes in solution and in hexagonal phase were prepared in different experimental conditions (contrast and KCl/LiCl solutions). In the latter case, the osmotic stress technique was used to fix the ion activities [4]. From diffraction intensities at D16, scattering length density distribution maps were calculated, while simple cylindrical models were used to fit SANS data obtained at D11. Results show that Li⁺ preferentially fills the quadruplex inner cavity, while K⁺ condenses in the ionic atmosphere, close to the external charged surface, demonstrating that counter-ions are structurally involved in the formation and in the stabilization of the quadruplexes.

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LOCAL STRUCTURE OF TEMPERATURE AND pH-SENSITIVE COLLOIDAL MICROGELS

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Among soft colloidal systems microgels, aqueous dispersions of nanometre or micrometre-seized hydrogel particles, have been the subject of intense research in the last years because of their versatility and high sensitivity to external stimuli. Furthermore microgels allow to modulate the interaction potential through temperature and/or pH, unlike in ordinary colloids, showing unusual transitions between different arrested states [1]. In particular the responsive microgel we have studied is composed of Interpenetrated Polymer Network (IPN) of poly(*N*-isopropylacrylamide) (PNIPAM), a thermo-sensitive polymer, and polyacrylic acid (AAc), a pH-sensitive polymer, dispersed in water. Although the macroscopic swelling behavior of both the pure PNIPAM microgel [2] and the PNIPAM/PAAc IPN microgel [3] particles has been largely clarified, the response of their inner local structure to changes of the external parameters is still an open issue. Small-Angle Neutron Scattering (SANS) is a relevant technique for investigations of the spatial inhomogeneities in the length scale from a few tens of angstroms to thousands of angstroms, thanks to the accessibility of low values of the wavevectors, Q . Indeed previous SANS studies on PNIPAM microgels have shown the existence of intermediate states between the fully swollen and the completely shrunken phase [4]. The temperature dependence of the local intra-particle structure of the IPN microgels has been investigated at different pH and concentrations, in the range of temperature where a volume phase transition from a swollen to a shrunken state takes place. Data are well described by taking into account the presence of both interpenetrated polymer networks and cross-linkers, highlighting the existence of two different behaviors across the volume phase transition. Indeed at neutral pH a sharp change of the local structure from a water rich open inhomogeneous interpenetrated polymer network to a homogeneous porous solid-like structure after expelling water is observed, whilst at acidic pH the local structure changes almost continuously. These findings demonstrate that a fine control of the pH of the system allows to tune the sharpness of the volume-phase transition.

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HYBRID SUPERCONDUCTING NEUTRON DETECTORS

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A new neutron detection concept is presented that is based on superconductive niobium (Nb) strips coated by a boron (B) layer. The working principle of the detector relies on the nuclear reaction $^{10}\text{B} + n \rightarrow \alpha + ^7\text{Li}$, with α and Li ions generating a hot spot on the current-biased Nb strip which in turn induces a superconducting–normal state transition. The latter is recognized as a voltage signal which is the evidence of the incident neutron. The above described detection principle has been experimentally assessed and verified by irradiating the samples with a pulsed neutron beam at the ISIS spallation neutron source (UK). It is found that the boron coated superconducting strips, kept at a temperature $T = 8$ K and current-biased below the critical current I_c , are driven into the normal state upon thermal neutron irradiation. As a result of the transition, voltage pulses in excess of 40 mV are measured while the bias current can be properly modulated to bring the strip back to the superconducting state, thus resetting the detector. Measurements on the counting rate of the device are presented and the future perspectives leading to neutron detectors with unprecedented spatial resolutions and efficiency are highlighted.

LOOKING FOR THE SECRET OF BIOMOLECULES' FUNCTIONALITY WITH NEUTRON SCATTERING

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The ability and effectiveness of proteins in performing a plethora of essential functions in living systems depends tightly on their structural flexibility. In fact the early view of proteins as relatively rigid structures has been gradually replaced by dynamic models which encompass internal motions as essential players in building up specific protein functions. Neutron scattering experiments have already given clear suggestions that protein dynamics is key to biological activity.

Functional hydrated proteins have been shown to exhibit a sudden increase of their mean square displacements at a certain temperature, due to the onset of large-amplitude dynamical processes that are not observed in non-active dry proteins [1]. This functionally-related onset seems to be driven by the network of water molecules, that also displays a similar dynamical transition [2] when they can perform translational diffusive motions nearby the protein surface [3].

On the other hand also long-range vibrations involving dynamical networks that extend through the protein seem to play a crucial role in controlling the functional-related structural changes. Recent OKE experiments have revealed the existence of underdamped delocalized vibrational motions in the THz domain which are related to the binding of lysozyme with the inhibitor triacetylchitotriose in solution [4]. In the same THz domain we have shown that both proteins and their hydration water exhibit peculiar vibrational features, such as the Boson peak [5] and a complex collective dynamics [6]. The relationship of these features with the biological functionality is discussed.

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FUNCTIONALIZED IRON OXIDE NANOPARTICLES: DEVELOPING A BIOCOMPATIBLE SYSTEM

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Poly(vinyl alcohol) (PVA) is a biocompatible water-soluble polymer of great interest thanks to its large-scale applications as a material for drug-delivery systems or for building sensors and membranes with selective permittivity. Above the different techniques used for the preparation of PVA physical hydrogels, the cryogenic route is one of the most studied and widely employed, even though other protocols can be followed. The advantages of such gels is the absence of toxic chemicals for their preparations and the consequent possibility to obtain a completely eco-friendly product.

In this work we propose a new route for the preparation of PVA-based microgels by using the salting-out effect. The influence of the salt concentration on the aggregation properties and the kinetics of the aggregation process were deeply studied through DLS (Dynamic Light Scattering). SANS measurements threw light on the structural and morphological properties of such gels, showing the role of the salt in the aggregation process and its effect on the supramolecular organization.

Moreover, we present other possible preparation protocols, a preliminary structural study, a thermodynamic characterization of modified PVA-based microgels in aqueous solutions and their interaction with some common surfactants, with the aim of showing the potential applicability of such systems for industrial formulations. Finally, the future perspectives of this second part of the study will be clearly explained.

EXPLORING CELL BIODIVERSITY

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Brain tissue is a really complex system composed of different cell types that change in shape and size. A single neuron itself has a cell body, dendrites and an axon. About 80% of cerebral tissue consists of water molecules that are confined (intra and extra cellular) in its disordered biologic networks. Using neutron scattering on the high energy resolution backscattering instrument IN13 at ILL we are able to explore hydrogens (H) dynamics in time scale at about 40 ps and in size scale at about 1 Å. Such characteristic make it suitable to investigate cellular dependence of brain tissue heterogeneity exploiting hydrogens as a probe since major constituent of macromolecules and water. Elastic neutron scattering (ENS) gives information about mean square displacement (MSDs) and k force constant (linked to macromolecular flexibility [1]) associable even in complex and disordered system such as cellular tissue [2,3,4,5]. Cell pastes with water extra cellular removed of *E. coli* bacteria, yeast (fungus), and cancer neuronal cell from rat were investigated by ENS. Preliminary results show that MSDs and k force constants are strongly dependent on cellular biodiversity.

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L.E.N.A. – LABORATORY OF APPLIED NUCLEAR ENERGY (UNIVERSITY OF PAVIA) – NEUTRON FACILITIES & MAIN ACTIVITIES

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The TRIGA[®] (Training Research and Isotopes-production General Atomics) Mark II nuclear research reactor installed at the Laboratory of Applied Nuclear Energy (L.E.N.A.) of the University of Pavia is licensed for operating at 250 kW power in steady state. Nowadays the Pavia TRIGA reactor is available for national and international collaboration in various research fields offering different in- and out-core neutron irradiation channels. A subcritical assembly is also available at the University of Pavia (Chemistry Department – Radiochemistry Area) for experimental activities. Current scientific and Educational & Training activities are also described.

FLUX AND NEUTRON SPECTRUM MEASUREMENTS IN FAST NEUTRON IRRADIATION EXPERIMENTS

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The fast neutron irradiation experiments planned at the ISIS neutron source require a characterization of the neutron field in terms of its flux map and energy spectrum. A few measurements methods are being explored mainly as part of the collaboration between CNR and STFC. These include i) large area GEM detectors providing a time resolved map of the high energy neutron flux for varying source and collimation conditions; ii) diamond detectors for localized flux measurements (e.g. at the position of the DUT, Device Under Test); and iii) a Proton Recoil Telescope for fast neutron spectral measurements in the energy range 10–100 MeV. Along with fission chambers and other compact dosimetry instrumentation a comprehensive detector suite will be available that can match the needs of chip irradiation and other fast neutron irradiation experiments.

T-REX: A TIME-OF-FLIGHT RECIPROCAL SPACE EXPLORER FOR THE FUTURE ESS SOURCE

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We present the proposal of a direct geometry time-of-flight (TOF) chopper spectrometer for the future European Spallation Source (ESS). The instrument is optimized for mapping excitations and fluctuations in a wide dynamic range that extends from 20 μeV to 150 meV in energy transfer and from 0.01 \AA^{-1} to 17 \AA^{-1} in wave-vector transfer. The elastic energy resolution (FWHM) can be freely adjusted in the range from 1% to 3% at 3 meV and from 4% to 8% at 100 meV. The instrument has access to the thermal moderator, thus enabling uncompromised performance for neutron energies between 20 and 150 meV. The neutron guide can be fed with a replaceable extraction system from the cold moderator, which can also serve as a polarizer for cold neutrons, featuring an efficiency of 80-90% in the cold energy range. The core of the novel design is in the chopper system [1], which is specifically designed to make an efficient use of the source long pulse by means of Repetition Rate Multiplication (RRM). Ray-tracing simulations for standard instrument configurations show gain factors around two orders of magnitude compared to simulations of world leading chopper spectrometers. The total instrument length of nearly 170 m enables different means to avoid the direct view onto the moderator to provide a very good signal-to-noise ratio.

The science areas to be covered by T-REX include: magnetism, strongly correlated electron materials, functional materials, soft-matter, biophysics and disordered systems. It will implement TOF spectroscopy with Polarization Analysis as a standard option, e.g. for studying the effect of confinement on the magnetic excitations in nano-particles or to uniquely derive the vibrational hydrogen excitations in soft matter through separation of the nuclear spin incoherent scattering. Besides the polarizing extraction system, a ³He spin filter cell will be used to polarize thermal neutrons. The XYZ polarization analysis will be possible thanks to a specifically developed guide field and the so-called MAGIC Pastis coil layout. A prototype is under construction for the TOPAS spectrometer at the FMR-II, which uses a wide-angle banana-shaped ³He Neutron Spin Filter cell to cover a large range of scattering angles, both in the horizontal and vertical direction.

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Un ricordo di Marco Zoppi

Marco se ne è andato meno di un mese fa. Quella che sembrava una patologia risolvibile con un intervento chirurgico, sul quale aveva anche lo spirito di scherzare (diceva che, apparentemente, gli era scaduta la garanzia) si è dimostrata un tumore di un tipo estremamente maligno e invasivo. La malattia non ha dato tempo a nessuno, tantomeno a lui, di prepararsi.

Difficile poter riassumere in poche righe tutto quello che era, anzi che è, Marco. In questo breve ricordo non vogliamo soffermarci sulle sue indubbie qualità scientifiche e tecniche. Chiunque le può immediatamente apprezzare sfogliando i suoi più di centocinquanta lavori su riviste scientifiche internazionali o facendo esperimenti su uno dei tre strumenti neutronici da lui progettati e costruiti, in toto o in parte, e operanti con successo ad ISIS, o pensando al suo ultimo progetto, lo strumento VESPA, per la nuova sorgente europea di neutroni in Svezia, approvato pochi giorni prima della sua morte.

Non è di questo che vogliamo parlare. È del Marco scienziato e amico, compagno di lavoro di una vita, che scoprivì giorno dopo giorno lavorandoci insieme, gomito a gomito. Marco era una grande persona: generosa, diretta, sincera. Era un coraggioso, sempre pronto a buttarsi in nuove avventure, di lavoro e non solo. Ricordiamo il suo entusiasmo, la sua competenza ma anche la disponibilità a sporcarsi le mani, per qualunque problema, anche tecnico, in laboratorio. E' stato per tutti noi una guida, ma una guida discreta, che lasciava enorme libertà ai suoi collaboratori, anche giovani. Tutti ricorderanno la sua cordialità e franchezza. Era attento al lato umano delle persone, sempre al fianco dei suoi collaboratori, pronto a combattere per loro nel modo fattivo e concreto che lo contraddistingueva.

Lascia un grande vuoto. Lascia tante, tantissime, persone che lo stimano e continueranno a lavorare nel suo ricordo, portandosi dietro i suoi insegnamenti sia professionali che umani.

Grazie Marco, è stato un grande privilegio ed un grande piacere lavorare con te!

I tuoi collaboratori più vicini



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Debora Berti, Fabio Bruni, Alessio De Francesco, Alessandra Filabozzi, Yuri Gerelli, Marco Maccarini, Paolo Mariani, Antonino Pietropaolo, Francesco Spinozzi e Marco Zanatta.

COMITATO ORGANIZZATORE

Giulia Bartolomei, Fabio Bruni, Alessandra Filabozzi, Yuri Gerelli, Antonino Pietropaolo e Marco Zanatta

CON IL PATROCINIO DI

