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Neutrons matter: VII international workshop on electron-Volt neutron spectroscopy – A preface to the workshop proceedings

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Neutrons matter: VII international workshop on electron-Volt neutron spectroscopy – A preface to the workshop proceedings

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Abstract. We present here a collection of works reporting on the recent experimental and theoretical activities taking advantage of epithermal neutron spectroscopy, and in particular focusing on recent results presented during the *VII International Workshop on Electron-Volt Neutron Spectroscopy* held in Rome on 7-8 November 2018.

1. An introduction to epithermal neutrons

Neutrons are amongst the most exquisite probes to investigate and characterise materials [1]. These particles are referred to as cold and thermal when their energies are lower than ca. 500 meV, therefore matching the typical energy scales in the dynamics of condensed-matter systems. Cold and thermal neutrons are routinely employed for scientific investigations based on Quasi Elastic (QENS) and Inelastic Neutron Scattering (INS) [2], to probe diffusion and tunnelling, or lattice and internal molecular excitations, respectively. Similarly, as the wavelengths of such probes are commensurate with the interatomic distances in solid and liquids, their elastic scattering on a sample is employed for diffraction experiments characterising the structure of materials.

Traditionally, neutron sources have focused on the application of cold and thermal neutrons, by slowing down neutrons with energies in the MeV region via the interaction with moderating materials. As an example, Figure 1 shows the flux of moderated neutrons on the VESUVIO spectrometer [3] at the ISIS pulsed neutron and muon source [4], where neutrons with initial energies up to 800 MeV are slowed down in a room-temperature water moderator, so as to



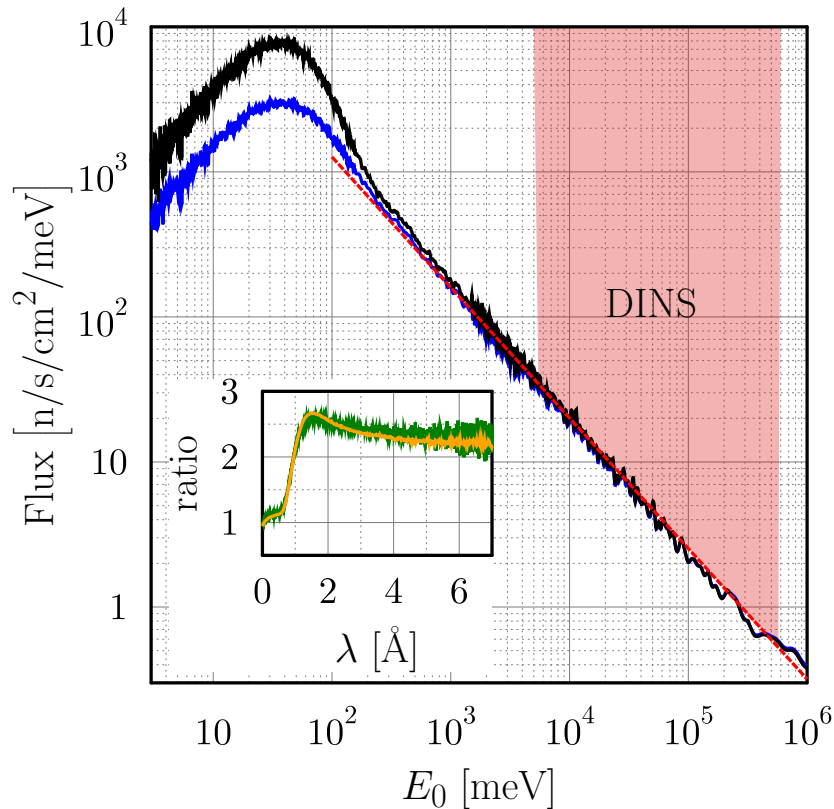


Figure 1. The incident-neutron flux on the VESUVIO spectrometer at ISIS. The red dashed line shows the epithermal tail of partially moderated neutrons, as discussed in the text. The figure is reproduced from Ref. [5].

have maximum flux in the thermal region, at about $3/2k_B T \sim 38$ meV, with k_B denoting the Boltzmann's constant, and T the temperature of the water moderator. In addition to thermal neutrons, one can notice a substantial contribution, in the shape of a long tail, of neutrons only partially moderated in the region of 1 eV – 1 keV. These neutrons are referred to as epithermal, or eV neutrons, and constitute the main subject of the articles in this collection. In particular, the flux distribution in the epithermal region is inversely proportional to the neutron energy (red dashed line in Figure 1), and is almost independent on the moderator material and geometry, as exemplified by the two overlapping spectra (blue and black lines) in the figure (see Ref. [5] for details).

Since the advent of proton-driven spallation sources in the 1970s, eV neutron spectroscopy has witnessed an ongoing development of the technique, as well as of its scientific and technological applications. The main technique based on epithermal neutrons is Deep Inelastic Neutron Scattering (DINS), also referred to as Neutron Compton Scattering (NCS) [6, 7]. The flagship instrument is the VESUVIO spectrometer [8, 9]. DINS allows for a direct measurement of nuclear kinetic energies and momentum distributions in condensed-matter systems, observables readily connected to nuclear quantum effects (NQEs), or anharmonicity in the local potential affecting a given atom. DINS is an example of MASS-selective Neutron SpEctroscopy (MANSE), where the signals from different elements are spectroscopically separated depending on their mass. Moreover, epithermal neutrons can be absorbed by some elements, usually isotopes of heavy elements such as Au, Ag, In, I, Ta, and others, in a nuclear resonant process. The study of these



Figure 2. Group picture at Centro Fermi.

resonances, namely Neutron Resonance Capture Analysis (NRCA) [10], can provide valuable information about the elemental composition of a sample, such as in archaeological or cultural-heritage investigations [11], as well as it serves as a quantum thermometer for local effective temperatures affecting atoms [12]. The cross section for such resonances can be several orders of magnitude higher than the neutron scattering cross section, and the value of the resonant energy is isotope-specific.

2. Broadening horizons

Over the past decades, a number of thematic workshops on the use of epithermal neutrons have helped defining the way forward. After a first scientific meeting in Los Alamos (USA) in 1984 [13], workshops on eV spectroscopy were held in Abingdon (UK) in 1995 and 1998, in Santa Fe (USA) in 2005, Oak Ridge National Laboratory (USA) in 2006, Rome (Italy) in 2010, and Abingdon in 2014 [14]. In the last episode of this story, an always larger and more diverse community met in Rome on 7–8 November 2017 for the VII International Workshop on electron-Volt Neutron Spectroscopy [15].

In recent years, DINS has provided, *inter alia*, a unique benchmark for the development of state-of-the-art computer simulations to describe NQEs in the hydrogen dynamics [16], such as path-integral molecular dynamics calculations [17, 18]. Yet, the 2014 edition of the workshop underlined how the realms of applicability of DINS go well beyond hydrogen [19], with an increasing number of studies focusing on moderate-weight masses such as oxygen [20], or lithium and fluorine [21]. This change in strategy of data analysis promoted MANSE as a unique technique where the momentum distribution of several atoms in a system can be analysed concurrently and independently.

In 2017, the horizon was moved well beyond MANSE. The new trend appears to be the

Table 1: Programme of the first day of the workshop.

Tuesday 7 November 2017 – Villa Wolkonsky	
11:30	Registration & lunch
	Opening
13:00	Welcome address: Ken O’Flaherty (British Embassy) and Andrew D. Taylor (STFC)
13:10	Carla Andreani – Occhialini prize lecture (“Tor Vergata”) <i>Hydrogen dynamics in stable and metastable water by deep inelastic neutron scattering</i>
	Session – Fundamental systems ; chair: Felix Fernandez-Alonso (STFC)
13:30	Alexander I. Kolesnikov (Oak Ridge National Laboratory) <i>Inelastic and deep inelastic neutron scattering study of water under ultra-confinement</i>
14:00	Francesco Mallamace (Università di Messina) <i>Nuclear Compton scattering and NMR, a common way to understand the local order</i>
14:30	Daniele Colognesi (CNR) <i>Self dynamics in simple liquids: connections between the Gaussian approximation and the asymptotic impulsive regime</i>
15:00	Coffee break
	Session – Simulation and modelling ; Chair: Roberto Senesi (“Tor Vergata”)
15:30	Roberto Car (Princeton University) <i>The momentum distribution of the nuclei as an environmental probe</i>
16:00	Angelos Michaelides (University College London) <i>Quantum effects in adsorption and diffusion at solid surfaces</i>
16:30	Michele Ceriotti (École Polytechnique Fédérale de Lausanne) <i>Theoretical benchmarks of deep inelastic neutron scattering. From the kinetic energy to the full particle momentum distribution</i>
17:00	Poster session
20:00	Conference dinner

combination of several concurrent measurements available, for example, on the VESUVIO spectrometer using NRCA, neutron diffraction, and neutron transmission. Moreover, a more systematic comparison with parent techniques, such as INS, or first-principles simulations, such as DFT-based phonon calculations, are now the new standard of eVS scientific output, as for example in Ref. [22].

To demonstrate the broad range of topics discussed, as well as the increasing interest from an always larger community in the use of eV spectroscopy, we report below the list of the registered participants in the workshop, and the list of presented posters, while Tables 1 and 2 show the programme of the two days of the workshop.

2.1. List of registered attendees

- Prof Carla Andreani – Università degli Studi di Roma “Tor Vergata”, Italy
- Ms Laura Arcidiacono – University College London, United Kingdom
- Dr Jeff Armstrong – Science & Technology Facilities Council, United Kingdom
- Prof Fabio Bruni – Università di Roma 3, Italy
- Ms Elena Budennaia – Nottingham Trent University, United Kingdom
- Prof Roberto Caciuffo – European Commission, Joint Research Centre, Germany
- Prof Roberto Car – Princeton University, United States
- Prof Michele Ceriotti – École Polytechnique Fédérale de Lausanne, Switzerland

Table 2: Programme of the second day of the workshop.

Wednesday 8 November 2017 – Villa Wolkonsky	
Session – Beyond fundamental systems; Chair: Roberto Car (Princeton University)	
8:00	Gregory Chasse (Queen Mary University of London) <i>Atomistic and vibrational source of mechanical toughness in glass bio-cements and portland cement during setting</i>
8:30	Fengge Gao (Nottingham Trent University) <i>Better understanding of self-cross linking behaviour of smectite nanoclays through VESUVIO</i>
9:00	Christoph Salzmann (University College London) <i>Ice - a miraculous material</i>
09:30 Coffee break & group photo	
Session – Methods and instrumentation; Chair: Giuseppe Gorini (University Milano Bicocca)	
10:00	Anton Tremsin (University of California at Berkeley) <i>High resolution neutron transmission imaging with single pixel spectroscopic resolution</i>
10:30	Erik Schooneveld (STFC) <i>Detection of epithermal neutrons on Vesuvio</i>
11:00	Rolando Granada (Comisión Nacional de Energía Atómica) <i>Neutron moderation: Some recent problems and results</i>
11:30 Transfer to Centro Fermi	
12:00	Welcome address: Luisa Cifarelli (President of Centro Fermi) <i>The lost notebook of Enrico Fermi and the discovery of neutron induced radioactivity</i>
12:30	Rosario Nania (Centro Fermi) <i>The Centro Fermi in Rome: the projects, the future</i>
12:45 Lunch & group picture	
14:00	Ceremony – “Neutrons Matter” prize
16:00	Closing remarks

- Dr Gregory Chasse – Queen Mary University of London, United Kingdom
- Prof Luisa Cifarelli – Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi”, Italy
- Dr Daniele Colognesi – Consiglio Nazionale delle Ricerche, Italy
- Dr Carmelo Corssaro – Consiglio Nazionale delle Ricerche, Italy
- Mr Alex Di Giulio – Università degli Studi di Roma “Tor Vergata”, Italy
- Dr Kacper Druzinski – University Adam Mickiewicz, Poland
- Prof Felix Fernandez-Alonso – Science & Technology Facilities Council, United Kingdom
- Dr Giulia Festa – Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi”, Italy
- Prof Fengge Gao – Nottingham Trent University, United Kingdom
- Prof Giuseppe Gorini – Università di Milano Bicocca, Italy
- Ms Ekaterina Gousseva – Queen Mary University of London, United Kingdom
- Dr Rolando Granada – Comisión Nacional de Energía Atómica CNEA, Argentina
- Mr Brandon Hewer – Science & Technology Facilities Council, United Kingdom
- Dr Maria Grazia Izzo – Università di Roma, La Sapienza, Italy
- Mr Alexander Jurgens – Università degli Studi di Roma “Tor Vergata”, Italy
- Mr Venkat Kapil – École Polytechnique Fédérale de Lausanne, Switzerland
- Prof Maths Karlsson – Chalmers University of Technology, Sweden
- Dr Somayeh Khazaei – Martin-Luther University, Germany
- Dr Alexander Kolesnikov – Oak Ridge National Laboratory, United States

- Dr Maciej Krzystyniak – Science & Technology Facilities Council, United Kingdom
- Ms Sveva Lungo – University of Messina, Italy
- Mr Mustafa Mahmoud – Queen Mary University of London, United Kingdom
- Dr Domenico Mallamace – CSGI, Center for Colloid and Surface Science, Italy
- Prof Francesco Mallamace – University of Messina, Italy
- Dr Adriana Mamede – University of Coimbra, Portugal
- Prof Rossana Marra – Università degli Studi di Roma “Tor Vergata”, Italy
- Prof Maria Paula Marques – University of Coimbra, Portugal
- Ms Louise McCann – Science & Technology Facilities Council, United Kingdom
- Ms Sara Miceli – Università degli Studi di Roma “Tor Vergata”, Italy
- Prof Angelos Michaelides – University College London UCL, United Kingdom
- Dr Rosario Nania – Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi”, Italy
- Mr Matteo Nardini – Università degli Studi di Roma “Tor Vergata”, Italy
- Ms Dalila Onorati – Università degli Studi di Roma “Tor Vergata”, Italy
- Dr Stewart Parker – Science & Technology Facilities Council, United Kingdom
- Dr Roberto Pinna – Università di Milano Bicocca, Italy
- Dr Rosina Ponterio – Consiglio Nazionale delle Ricerche, Italy
- Ms Sara Postorino – Università degli Studi di Roma “Tor Vergata”, Italy
- Prof Paolo Radaelli – University of Oxford, United Kingdom
- Mr James Rawlings – Nottingham Trent University, United Kingdom
- Dr Giovanni Romanelli – Science & Technology Facilities Council, United Kingdom
- Dr Alexander Rosu-Finsen – University College London, United Kingdom
- Mr Mohammed Salha – Queen Mary University of London, United Kingdom
- Dr Christoph Salzmann – University College London, United Kingdom
- Mr Valerio Scacco – Università degli Studi di Roma “Tor Vergata”, Italy
- Dr Claudia Scatigno – Università degli Studi di Roma “Tor Vergata”, Italy
- Mr Giuseppe Scionti – Università della Calabria, Italy
- Dr Erik Schooneveld – Science & Technology Facilities Council, United Kingdom
- Prof Roberto Senesi – Università degli Studi di Roma “Tor Vergata”, Italy
- Ms Zainab Sharif – University College London, United Kingdom
- Dr Goran Škoro – Science & Technology Facilities Council, United Kingdom
- Mr Fu Song – Queen Mary University of London, United Kingdom
- Dr Corrado Spinella – Consiglio Nazionale delle Ricerche, Italy
- Dr Andrew Taylor – Science & Technology Facilities Council, United Kingdom
- Dr Kun Tian – Università degli Studi di Roma “Tor Vergata”, Italy
- Dr Anton Tremsin – University of California, Berkeley, United States
- Mr Pierfrancesco Ulpiani – Università degli Studi di Roma “Tor Vergata”, Italy
- Mr Muhammed Umarji – Queen Mary University of London, United Kingdom
- Dr Cirino Vasi – Consiglio Nazionale delle Ricerche, Italy
- Ms Aurora Zaganelli – Università degli Studi di Roma “Tor Vergata”, Italy

2.2. List of presented posters

- L. Arcidiacono *et al.* – University College London; *Byzantine gold coins analysed using time resolved prompt gamma activation analysis*
- L. Arcidiacono *et al.* – University College London; *Time-resolved prompt gamma activation analysis at ISIS Spallation Neutron Source*
- J. Armstrong *et al.* – Science & Technology Facilities Council; *How do rotations alter the local potential of nanoscopic molecules? A C₆₀ case study*
- E. Budennaia *et al.* – Nottingham Trent University; *Using Vesuvio to gain better understanding of self cross-linking behaviour of smectite clays*
- C. Corsaro *et al.* – Consiglio Nazionale delle Ricerche; *The similarities between Neutron Compton Scattering and NMR spectroscopy applied to investigate the degradation of cellulosic materials*
- A. Di Giulio *et al.* – Università degli Studi di Roma “Tor Vergata”; *A McStas simulation of the incident beam in the VESUVIO spectrometer*

- K. Drubicki *et al.* – University Adam Mickiewicz; *Hydrogen dynamics in molecular solids: Insight from simulations with quantum colored-noise thermostat*
- E. Gousseva *et al.* – Queen Mary University of London; *Resolving interfacial structures and dynamics in hybrid organic - inorganic cements*
- B. Hewer *et al.* – Science & Technology Facilities Council; *Advances in the reduction and analysis of data from epithermal neutron experiments using MANTID*
- V. Kapil *et al.* – École Polytechnique Fédérale de Lausanne; *Probing the momentum distribution of protons in ab initio water*
- S. Khazaei *et al.* – Martin-Luther university; *Rotation tunnelling of coupled methyl quantum rotors in 4methylpyridine: single rotor potential versus coupling interaction*
- M. Mahmoud *et al.* – Queen Mary University of London; *Graphene nanoflake reinforced cements*
- D. Mallamace *et al.* – Center for Colloids and Surface Science; *The local structure of hydrogen bond in water studied in a wide temperature range by Neutron Compton scattering and NMR spectroscopy*
- A. Mamede *et al.* – University of Coimbra; *Shining the beam on bones Human Burned Skeletal Remains Probed by Neutron Spectroscopy*
- M. P. Marques *et al.* – University of Coimbra; *International water – a secondary target in chemotherapy? Impact of Pt/Pd anticancer drugs in breast cancer cell probed by neutron techniques*
- M. Nardini *et al.* – Università degli Studi di Roma “Tor Vergata”; *Neutron diffraction and resonance capture analysis from Sumerian pottery from the citystate of Abu Tbeirah*
- D. Onorati *et al.* – Università degli Studi di Roma “Tor Vergata”; *Optimization of gamma detection methods for neutron energy analysis on eV neutron spectrometers*
- S. Parker *et al.* – Science & Technology Facilities Council; *Observation of the stretch mode in H₂ and D₂ by INS spectroscopy*
- A. Parmentier *et al.* – Università degli Studi di Roma “Tor Vergata”; *Hydrogen mean force and anharmonicity in polycrystalline and amorphous ice*
- J. Rawlings *et al.* – Nottingham Trent University; *Towards a better understanding of the self-cross-linking behaviour of smectite clays*
- G. Romanelli and M. Krzystyniak – Science & Technology Facilities Council; *Recent upgrades on the VESUVIO spectrometer*
- A. Rosu-Finsen *et al.* – University College London; *Benchmarking acidic and basic dopants with respect to facilitating the ice V to XIII and ice VI to XV hydrogen-ordering phase transitions*
- M. Salha *et al.* – Queen Mary University of London; *Supreme toughness in Aluminium enriched cements*
- V. Scacco *et al.* – Università degli Studi di Roma “Tor Vergata”; *Analysis of neutron activation decay on the VESUVIO beam line at ISIS*
- Z. Sharif *et al.* – University College London; *Exploring new areas of the ice phase diagram for metastable ice V with varying degrees of hydrogen-order*
- F. Song *et al.* – Queen Mary University of London; *Neutron scattering on atomic structure, stabilities and dynamics of cement*
- M.B. Umarji *et al.* – Queen Mary University of London; *Water gelation as a structural scaffold in cementitious materials*
- P. Ulpiani *et al.* – Università degli Studi di Roma “Tor Vergata”; *Enhancing the YAP detectors discrimination threshold installed in the VESUVIO spectrometer at the ISIS spallation neutron source*

3. An auspice

A detailed programme and outcome of the “Neutrons Matter: VII International Workshop on electron-Volt Neutron Spectroscopy” was recently presented in Ref. [15]. Also, a copy of the flyer is shown in Figure 3 for future reference. The development of the eV spectroscopy with neutrons on the VESUVIO spectrometer has been a clear example of a successful international collaboration in science. Over the past decades, a solid agreement between the British Science and Technology Facilities Council and the Italian Consiglio Nazionale delle Ricerche has provided a fertile ground for the development of the technique, that has facilitated the growth of a world-wide scientific community. This workshop, as well as other past editions, was partially co-funded by the two councils, and for the second time it took place in Rome, the eternal city.

So as to underline this long-standing agreement, the scientific sessions of the workshop were hosted in the British Embassy in Rome, a very suggestive venue. Moreover, the time of the workshop coincided with the anniversaries of the discovery of the neutron by the British scientist

J. Chadwick, and the patent for neutron moderation by the Italian physicist E. Fermi. The group picture in Figure 2 was taken during a visit to the Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi” in the city centre, on the very stairs where a number of Nobel laureates were photographed in 1931 during the first international conference in nuclear physics. May this precedent be an auspice for the future of spectroscopy with epithermal neutrons, and for the underpinning international communities.

Acknowledgements

We would like to thank the British Embassy in Rome for their hospitality in hosting a substantial part of the workshop, as well as for supporting travel expenses for early-career researchers. A special thanks to Prof Cifarelli and Dr Nania for the visit to the Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi”. We acknowledge the financial support of the Science & Technology Facilities Council, of the School of Neutron Scattering “F. P. Ricci”, of the Museo Storico della Fisica e Centro Studi e Ricerche “Enrico Fermi”, and of the Consiglio Nazionale delle Ricerche.

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NEUTRONS MATTER


VII International Workshop on Electron-volt Neutron Spectroscopy

85th anniversary - J. Chadwick (1932)

80th anniversary - Enrico Fermi (1937)

7th – 8th November 2017

Villa Wolkonsky and Centro Studi e Ricerche Enrico Fermi
Rome, Italy

Neutrons Matter, the seventh edition of the *International Workshop on Electron-volt Neutron Spectroscopy*, celebrates the 85th anniversary of the discovery of the neutron by Chadwick, and the 80th anniversary of the Patent issued by the Ministero delle Corporazioni on 27th October 1937 to Enrico Fermi for the use of neutrons to enhance artificial radioactivity. The latest discovery took place at the Istituto di Fisica di Via Panisperna at the very heart of Rome. Following a successful sixth edition of this workshop series in the United Kingdom in 2014, the workshop aim to bring to the fore and highlight the most recent (and quite exciting) advances in the field, with an emphasis on the use of the technique across condensed matter research, as well as the concurrent use of contemporary computational materials modelling. The workshop will be held in Rome, in the beautiful setting of Villa Wolkonsky and at the Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi.

PROGRAMME
Programme includes invited oral presentations and posters

Dates & Venue

7th Nov 2017 All day: Villa Wolkonsky.
Evening: conference dinner

8th Nov 2017 Morning: Villa Wolkonsky
Lunch and Afternoon: Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi

International Advisory Committee

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- ❖ British Embassy, Rome, Italy
- ❖ Consiglio Nazionale delle Ricerche (CNR), Italy
- ❖ Centro Studi e Ricerche Enrico Fermi, Italy
- ❖ School on Neutron Scattering "Francesco Paolo Ricci" (SoNS), Italy
- ❖ Science & Technology Facilities Council (STFC)
- ❖ UK Government Science and Innovation Network, UK
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Dr Dalila Onorati, Università di Roma Tor Vergata, Italy
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APPLICATION ABSTRACT HOTEL REGISTRATION

Attendance 60-70 participants, early-career researchers welcome

Topics

- ❖ New Materials for Energy and Functional Materials
- ❖ Fundamental Systems
- ❖ Information & Communication Technologies
- ❖ Simulation and Modelling
- ❖ Applications to cultural heritage
- ❖ Recent instrumentation and methodological developments resulting from joint collaborative efforts across the Consiglio Nazionale delle Ricerche and the UK Science & Technology Facilities Council.

"NEUTRONS MATTER" Prize

A prize will be awarded to the best poster presented by an early-career researcher. Poster session is scheduled on the 7th November at Villa Wolkonsky. The Prize ceremony will take place on the 8th November at Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi. [Poster Abstract](#).

Proceedings

Workshop Proceedings will be published in the *Journal of Physics*, UK Institute of Physics. Contributions will be reviewed by the International Advisory Committee. [Proceedings Abstract](#).

Scientific Secretariat

Sara Miceli, Università di Roma Tor Vergata, Italy

Important dates

Request of hotel reservation extended deadline	25th September 2017
Proceedings abstract extended deadline:	27th September 2017
Notification of abstract acceptance	15th October 2017
Deadline for Poster Abstract:	25th September 2017

For questions related to the science programme:
Carla Andreani and Felix Fernandez Alonso

For questions related to the conference proceedings:
Giulia Festa and Giovanni Romanelli

For any other question:
Sara Miceli









Figure 3. The flyer of the workshop.