

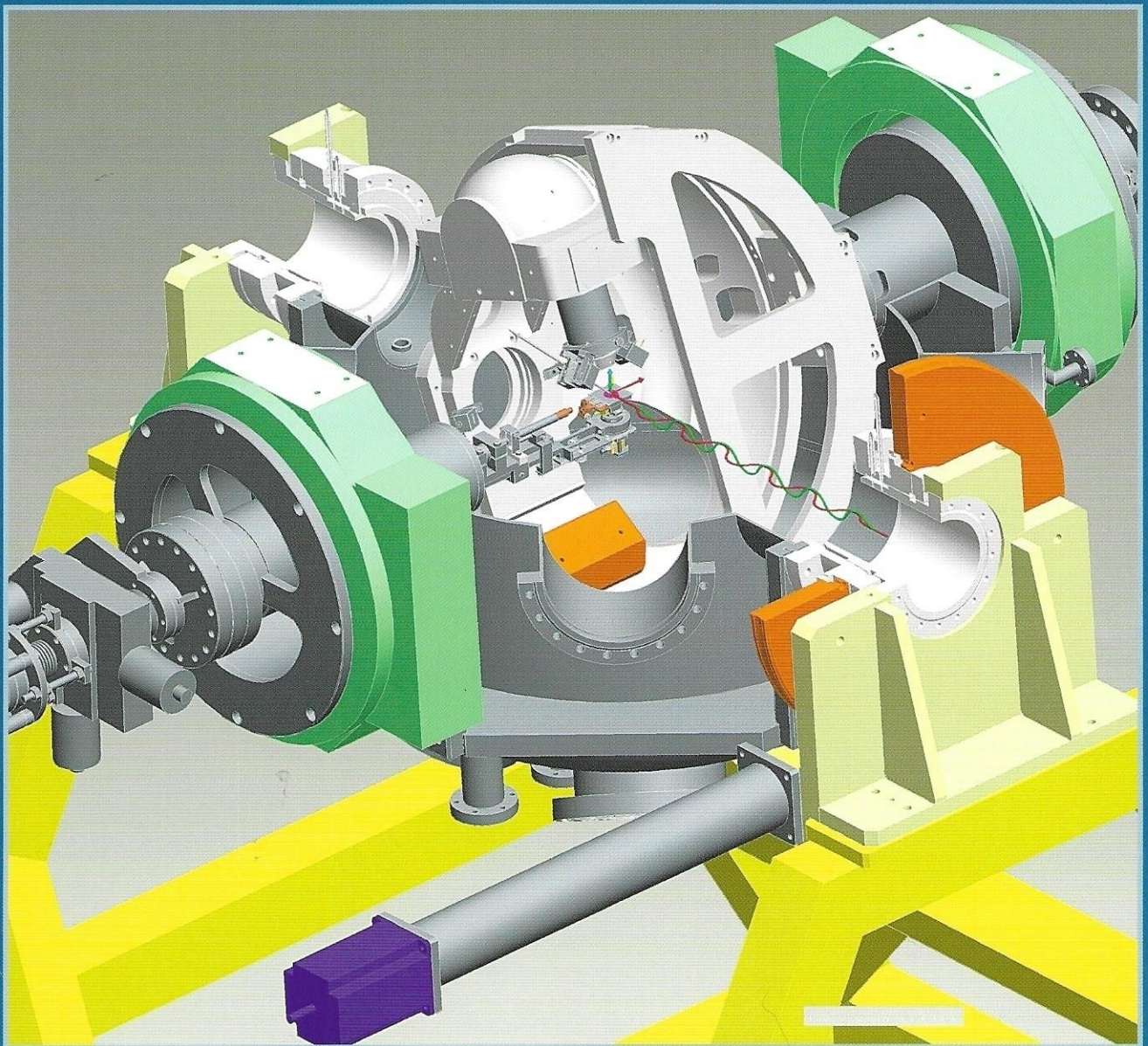


Rivista del  
Consiglio Nazionale  
delle Ricerche

# NOTIZIARIO

## Neutroni e Luce di Sincrotrone

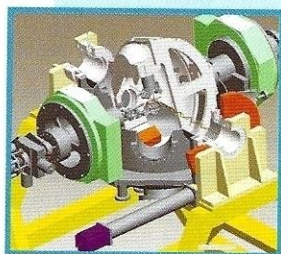
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Cover photo:  
CAD drawing of BEAR  
experimental room



**NOTIZIARIO**  
Neutroni e Luce di Sincrotrone

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# SUMMARY

## EDITORIAL NEWS

Well Deserved Prize for Jack Carpenter..... 2  
I. Anderson

## SCIENTIFIC REVIEWS

Using Neutrons to Track Ancient Pottery  
Firing Technology..... 3  
A. Botti, A. Sodo, M.A. Ricci

BEAR: a Bending Magnet for Emission Absorption  
and Reflectivity ..... 8  
S. Nannarone, A. Giglia, N. Mahne, A. De Luisa, B. Doyle,  
F. Borgatti, M. Pedio, L. Pasquali, G. Naletto, M.G. Pelizzo,  
G. Tondello

## MUON & NEUTRON & SYNCHROTRON RADIATION NEWS

News from ESRF ..... 20  
News from ILL ..... 20  
News from LCLS..... 24  
News from NCXT ..... 25  
News from NMI3 ..... 25  
News from SNS..... 32

SCHOOL AND MEETING REPORTS ..... 34

CALENDAR ..... 40

CALL FOR PROPOSAL ..... 42

FACILITIES ..... 43

## Sea Waves and Spin Waves Meet in Santa Margherita di Pula

The biennial School of Neutron Scattering, named after the late Francesco Paolo Ricci, prominent neutron scatterer and one of the founding fathers of the Italian neutron scattering community, has become a fixture of the scientific calendar, and has steadily grown in prestige and international standing over the years.

The eighth edition, which I had the privilege to direct together with Dante Gatteschi (University of Florence – INSTM), co-funded by the Association “School of Neutron Scattering Francesco Paolo Ricci”, NMI3 and a number of institutional sponsors\*, was held at the beautiful Hotel Flamingo in Santa Margherita di Pula (Sardinia) on Sept. 25-Oct. 6 2006.

This year’s theme, for the first time in the history of the School, addressed the structure and dynamics of magnetic systems, as investigated with a variety of neutron scattering tools.

Equal emphasis was placed on theory and practice, with a mix of introductory lectures, specialised lectures providing the theoretical basis of each discipline, scientific seminars on topical subjects and a series of hands-on tutorials.

The latter proved extremely popular with the students, who enjoyed the sophisticated, computer-based data analysis sessions, such as “Slicing and dicing of  $Q$ - $\Omega$  space” by Toby Perring (ISIS-RAL) as well as the pen-and-paper exercises, such as “Guess the final polarisation” by Jane Brown (ILL) of “Find the spiral phase” by Mechthild Enderle (ILL). Helped in no small part by the unquestionable charm of the School venue, we had managed to lure the very best Lecturers and Tutors on each topic from around the world, and this, in turn, attracted a group of highly competent and motivated Italian, European and International students from as far away as Australia and India.

The downside was that the scenic setting could have been an almost irresistible distraction for the students. Nevertheless, the quality of the teaching was so high that the Directors had no difficulty in recalling the afternoon sessions after the lunchtime break on the beach or at the pool or the after-dinner sessions after a good dose of “Mirto Rosso” (well, *almost* no difficulty...).

The School started on Monday afternoon with introductory lectures on Small Angle Neutron Scattering by

Fabrizio Lo Celso (University of Palermo) and on Inelastic Neutron Scattering by Marco Zoppi (CNRS – Florence), who also gave an interesting after-dinner seminar on the Italian Neutron Experimental Station (INES) at ISIS.

The next two and a half days were largely devoted to the theory and practice of magnetic powder diffraction, taught by Juan Rodriguez-Carvajal (ILL), Laurent Chapon (ISIS) and myself.

At the end of this section, most of the students were competently refining neutron powder diffraction data, performing simulated annealing to solve magnetic structures and visualising the results in 3D.

But, alas, just when they thought that they were mastering the subject, Jane Brown provided a much-needed “reality check”, shown that there is far more depth to the subject, and initiating the students on the intricacies of neutron polarimetry.

Polarised neutron diffraction, with particular reference to measurements of spin density on single crystals, was the subject of the lectures presented by Arsen Gukasov (LLB).

A full day was devoted to magnetic neutron reflectometry, with theory lectures by Giampiero Felcher (Argonne National Laboratory), hands-on tutorials by Tim Charlton (ISIS) and a final topical seminar, given again by Giampiero, on the exciting opportunities provided by the new SERGIS technique.

After a much-needed free morning on Sunday, the lectures restarted in the afternoon with Albrecht Wiedemann (HMI), who provided an extremely clear introduction to magnetic SANS, later followed by a seminar on the investigation of magnetic nanostructures.

Having thoroughly explored  $Q$



Participants to the eight edition of the biennial School of Neutron Scattering (Sept. 25 - Oct. 6, 2006)



space in all its facets, the students found themselves on Monday faced with a new dimension (energy transfer), and the relevant techniques of Triple Axis Spectroscopy (Mechthild Enderle – ILL) and time-of-flight chopper spectroscopy (Toby Perring – ISIS). Roberto Caciuffo introduced the formalism of Crystal Field levels and excitations, and its applications to molecular magnetism.

This was followed by a Lecture/Tutorial by Roberto Senesi on the unusual but extremely interesting topic of Intermultiplets Transition in Pr probed by high-energy INS.

The highly topical subject of molecular magnetism was further pursued by Hans Güdel (University of Bern), with a series of lectures on "Inelastic Neutron Scattering of Spin Clusters and Single Molecule Magnets" and Dante Gatteschi, who lectured on "Molecular Magnets".

The last few days of the School were very busy for the students, who were asked to work in groups to prepare a series of reports, which were presented during the final day. The subjects chosen ranged from an in-depth treatment of some of the problems presented in the Tutorials to the application of the methods learned during the School to the Students' own research topics.

All reports demonstrated the effort and dedication perfused by the Students during what amounted to two very intense weeks of work.

The reports were also humorous and at times truly hilarious, clearly indicated that, in addition to hard work, the School was also good fun.

One particularly valuable contribution from the Lecturers and Tutors was a full set of lecture notes (available on the School web site [http://www.fis.uniroma3.it/sns\\_fpr/index.html](http://www.fis.uniroma3.it/sns_fpr/index.html)), which represents a useful summary of the state of the art in the field of magnetic neutron scattering.

Many have expressed the wish to put this to a good use, either in the

form of a new edition of the School, perhaps under different auspices, or of a published collection – a suggestion that we are now considering very seriously.

Paolo G. Radaelli  
ISIS-Spallation Neutron Source

\* Sponsors

The Association "School of Neutron Scattering Francesco Paolo Ricci" acknowledges the support of Consiglio Nazionale delle Ricerche, NMI3, Università di Milano Bicocca Università di Milano, Università di Palermo (and Dip. di Chimica Fisica), Università di Roma Tor Vergata, Università di Roma Tre (and Dip. di Fisica).

## ETSF European Theoretical Spectroscopy Facility Opening New Eyes to the Nanoworld

**What can the ETSF do?  
Some examples:**

- Surface reconstruction puzzle:**  
solution from theory + simulation  
The structure of the surfaces of Si, Ge or Ga with varying composition and reconstruction can be established thanks to the comparison of measured spectra to high level calculations.
- A biological marker: the Green Fluorescent Protein**  
Recently developed theories accurately describe the properties of the GFP leading to a better understanding of its fluorescent behaviour.
- Optical data storage and rewritable DVDs**  
Computer simulation gives new insights into the design of more efficient data storage devices.

For more information about these examples, and others such as photovoltaics, quantum transport, supra-molecular chemistry, etc., see [www.etsf.eu](http://www.etsf.eu)

For more information about theory, code development, training events, please see: [www.etsf.eu](http://www.etsf.eu)

The ETSF is an initiative of the Nanoquanta Network of Excellence

Nanoquanta's constituent nodes have developed, in close collaboration since the 90's, many of the theoretical approaches and computational solutions which are commonly used in the framework of electronic excitations.

**Nanoquanta's ten nodes:**

- University of York
- Ulm Universität
- Freie Universität Berlin
- Università degli Studi di Milano
- Friedrich-Schiller-Universität, Jena
- Laboratoire des Solides Irradiés, Palaiseau
- Università degli Studi di Roma "Tor Vergata"
- Universidad del País Vasco URV/EHU, San Sebastian
- Université Catholique de Louvain, Louvain-la-Neuve
- Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

**Nanoquanta's associate members:**

- Institut d'Electronique, de Microelectronique et de Nanotechnologies, Lille; Institut Hétéo, CNRS Grenoble, St. Martin; Universidad Nacional de Educación a Distancia, Madrid; University of Coimbra; Slovak University of Technology, Bratislava

**Nanoquanta Network of Excellence**

Additional support is provided by national engineers.

For more information about Nanoquanta, see: [www.nanoquanta.eu](http://www.nanoquanta.eu)

**Opening new eyes to the nanoworld**

### Why theoretical Spectroscopy?

Interaction between matter and radiation (electrons, light, X-rays, lasers) is the key to the study of materials, ranging from solids to atoms, from surface to nanoscale systems.

Through the powerful combination of quantum-based theory such as the Bethe-Salpeter equation or Time-Dependent Density functional Theory with computer simulation applied to electronic excitations (theoretical spectroscopy), researchers are now able to:

- analyse and explain experimental data (ellipsometry, EELS, Raman, IR, NMR, X-Ray, ARPES, STS, IV transport, etc.)
- achieve remarkable technological and fundamental breakthroughs, such as new functionality (e.g. spinoelectronics) or biological applications ("bottom-up" assembly of molecular machines)

To design and optimise:

- biological devices
- nanosstructures
- new materials

### European Theoretical Spectroscopy Facility

**1-The core of the ETSF**

A network of preeminent European Condensed Matter Theory groups

- They develop theory and code, and provide services to users.
- They take responsibility for the management of the ETSF and the development of its user community.

**2-Associate theory groups**

A broad community of theoretical research groups working in related topics

- They develop theory and code, and provide services to users just like members of the Core.

**3-Users**

A large and varied group of researchers from the public and private sectors

- Demand for collaboration using software developed by the ETSF and support for calculations is growing rapidly amongst theoreticians and experimentalists working at large institutions such as synchrotrons, in individual laboratories, and in private companies.
- They benefit from the ETSF in different ways, depending on their proximity to the field through:
  - collaboration by proposing relevant projects that require full-time work by ETSF members;
  - commissioning customer-driven software development and applications;
  - promotion of new ideas for theory and software development;
  - ongoing project consultancy;
  - participation in training events;
  - software downloads with added personalised support (complete tutorials, e-learning and e-doc modules)

The ETSF will bridge the gap between fundamental research and technological applications

An innovative Infrastructure... to contribute significantly to nanoscience and nanotechnology through the development and application of theoretical spectroscopy. It involves close collaboration between theorists (from core and associate groups) and a new community of experimental and industrial researchers who wish to apply modern first principles theories of spectroscopy.

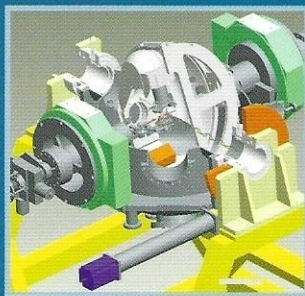
First call for user projects, early 2007.  
Check our web site:  
<http://www.etsf.eu>



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