

The Newsletter of the ISIS Molecular Spectroscopy User Group

Welcome!

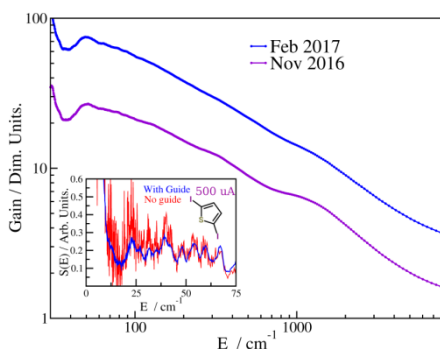
In the second issue of our Newsletter in 2017, we welcome Brandon Hewer, our new sandwich student working on the Mantid development. We bid farewell to Louise McCann, who completed her placement at the end of August, and we welcome back to RAL two of the past sandwich students, Daniel Nixon and Elliot Oram.

abINS and Mantid

The new version of Mantid will be available on the first week of October, with the latest additions available in this technical report. The abINS algorithm in Mantid to calculate INS spectra from ab-initio lattice dynamics simulations is fully functional. If you use abINS, please cite this link. The FABADA minimiser for fitting using the Bayesian methodology is available with the option of simulated annealing. Here more details to global-fit QENS data.

Tosca upgrade

After the guide upgrade, experiments can be performed on much smaller samples, and spectra can be collected in minutes (note the log scale in the figure). What used to be challenging experiments are now at reach!



In situ calorimetry

Good progress is being made on equipment to measure thermodynamic transitions in parallel to QENS. Expressions of interest for use are welcome by contacting Vicky.

The future of epithermal neutrons

MSc and PhD students (below) from the University of Roma "Tor Vergata" have participated in experiments to improve the detection procedure on VESUVIO, obtaining interesting preliminary results.



Renewing detection electronics on Vesuvio

The next-generation data acquisition electronics, DAE3, has been installed on Vesuvio and will be tested during the next cycles. During the summer, detection electronics has been updated as well, with the installation of new cables, high-voltage supplies, and racks.

**Next Proposal Round
Deadline: October 16th
Submit your proposals here**

Science Highlights

- [Atomic Quantum Dynamics in Materials Research](#)
- [Neutron Scattering - Applications in Biology, Chemistry, and Materials Science](#)
- [Detecting Molecular Rotational Dynamics Complementing the Low-Frequency Terahertz Vibrations in a Zirconium-Based Metal-Organic Framework](#)
- [Understanding the Role of Molecular Diffusion and Catalytic Selectivity in Liquid-Phase Beckmann Rearrangement](#)
- [Unravelling exceptional acetylene and carbon dioxide adsorption within a tetra-amide functionalized metal-organic framework](#)
- [Inelastic Neutron Scattering study of Reline: shedding light on the hydrogen bonding network of deep eutectic solvents](#)
- [Ionic Liquids: evidence of the viscosity scale-dependence](#)
- [Resilience of Malic Acid Natural Deep Eutectic Solvent Nanostructure to Solidification and Hydration](#)
- [Effect of Phosphorylation on a Human-like Osteopontin Peptide](#)



Forthcoming Events

➤ [Neutrons Matter – VII International Workshop in Electron-Volt Neutron Spectroscopy, Roma, 7-8 November 2017](#)

A splendid occasion to celebrate the long-standing collaboration between Italy and UK in neutron science. The workshop will be held at the Villa Wolkonsky, the British Embassy in Roma, and at the Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi. In the seventh edition in this series of thematic meetings about Electron-Volt Neutron Spectroscopy, many contributions linked to VESUVIO science are expected. The "Neutrons Matter" Prize will be awarded to the best poster presented by an early-career researcher.

➤ [ISIS Student Meeting, Abingdon, 30-31 October 2017](#)

Please be reminded that the representatives of our group, C.G. Salzmann and R. Senesi, are always open for feedback.

Please inform us of your publications arising from ISIS-related work. Remember to include ISIS staff as co-authors on publications when deemed appropriate.