

The Newsletter of the ISIS Molecular Spectroscopy User Group

News

Welcome!

It is time for the second issue of our Newsletter in 2016! Farewell to Elliot Oram who greatly helped us with Mantid. His work can be found [here](#). We welcome Louise McCann, a *sandwich student* to develop Mantid further. We also welcome Mattia Gaboardi who joined the MSG on May with Rutherford International Fellowship.

Mantid

Mantid 3.7 can now be [downloaded](#). During last summer, Bartomeu Llopis Vidal upgraded the Bayesian minimiser and the results will be available in version 3.8 on 10 October. [The recruitment campaign](#) for the next year *sandwich student* is now started.

If you experience any issue with Mantid while analysing your data, please have a chat with your local contact. In case the issue is due to a software bug, we will share it with the MANTID team.

Tosca: The next chapter!

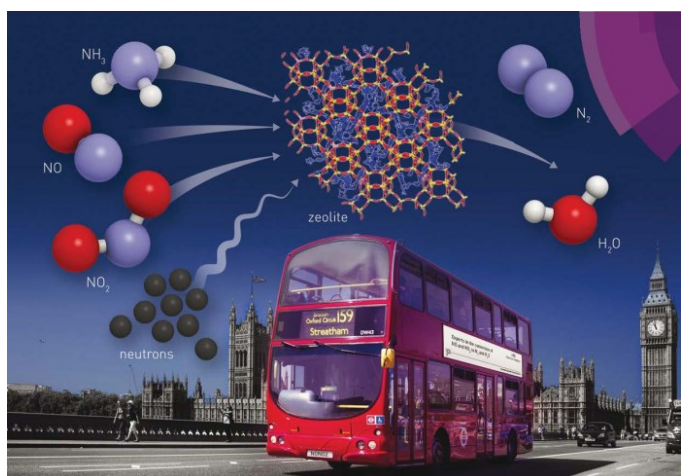
The Tosca neutron guide project is progressing well, thus if you have a proposal, please apply for beam-time during this proposal round (October 2016).

Extending the energy range on Vesuvio

Cold neutrons reaching samples in TS1 while the proton beam is directed to TS2 are now measured on VESUVIO, allowing diffraction and transmission measurements on an extended neutron energy range.

Special Issue: Catalysis and Energy Materials

[By clicking here](#), you can access the full PCCP special issue focusing on the use of neutron scattering to interrogate catalysts and other materials for energy applications. The issue was guest-edited by Richard Catlow (University College London), Stewart Parker and Ian Silverwood (ISIS Neutron and Muon Facility, STFC).



Ibex arrives to Iris

Iris will be the first instrument at ISIS to switch from SECI to **IBEX**, a new and modern interface for data collection already used on some new instruments such as Larmor.



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

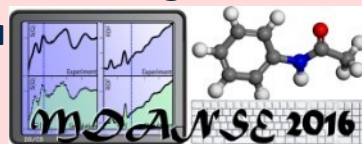
**Next Proposal Round
Deadline: October 16th
Submit your proposals here**

Science Highlights

- [Reactivity of Hydrogen on and in Nanostructured Molybdenum Nitride: Crotonaldehyde Hydrogenation](#)
- [A comprehensive approach to investigate the structural and surface properties of activated carbons and related Pd-based catalysts](#)
- [Selective adsorption of Sulfur Dioxide in a robust metal-organic framework material](#)
- [Neutron scattering study of the terminating protons in the basic structural units of non-graphitising and graphitising carbons](#)
- [Osteometrics in burned human skeletal remains by neutron and optical vibrational spectroscopy](#)
- [Quantum Tunneling of Water in Beryl: A New State of the Water Molecule](#)
- [Soft confinement of water in graphene-oxide membranes](#)
- [Picosecond to nanosecond dynamics provide a source of conformational entropy for protein folding](#)
- [Heads or tails: How do chemically substituted fullerenes melt?](#)



**In November, join the MSG at the
Cosener's House in Abingdon for
two events you
cannot miss!**



The **Molecular Spectroscopy Science Meeting** will be held on 9 – 10 November. You can find the program [here](#). **Registration closes on 14 of October** and you are more than welcome to present a poster and win a prize!

One after the other, the workshop **Molecular and Lattice Dynamics to Analyse Neutron Scattering Experiments**, organised in collaboration with ILL Computing for Science Group, will be held on 10 – 12 November. The school will show how widely-available simulation tools can be applied to the analysis and interpretation of neutron scattering data. Please, register [here!](#) **Registration closes on 30 of September!**

Forthcoming Events

- [Faraday Joint Interest Group Conference, 11-13 April 2017, Warwick](#)
- [ICANS XXII, 27-31 March 2017, Oxford](#)