

The Newsletter of the ISIS Molecular Spectroscopy User Group

Welcome!

In the first issue of our Newsletter in 2018, we welcome Hamish Cavaye, the new PDRA working with Stewart on catalysis projects.

Mantid

The new release of Mantid (Mantid 3.12) is now available. In this release, the QENS data analysis interface has been redesigned to provide more control on fitting parameters, and more options are added in the QENS data-correction interface. The abINS algorithm in Mantid has been improved to run one order of magnitude faster. The working principles of abINS have been published [in this paper](#). If you use abINS for your research, please cite this paper.

Automation on Iris

Changing samples on Iris is becoming less labour intensive! An automated script-driven system is in place to enable measurements over a wide temperature range (4 – 600 K), and the 3-position sample changer with independent sample-temperature control is now routinely used for measurements up to a maximum of 350 K. An updated version of the Iris user guide is now available [here](#).

Vesuvio Workshop

A great success at the [VII International Workshop on Electron-Volt Neutron Spectroscopy](#), held in Rome on last November with about 70 participants (picture below). The proceedings will be coming soon!

**Next Proposal Round
Deadline: April 18th
Submit your proposals here**

We wish you a
happy Easter break!

Science Highlights

- [Measurement of the para-hydrogen concentration in the ISIS moderators using neutron transmission and thermal conductivity](#)
- [Mechanism of enhancement of ferroelectricity of croconic acid with temperature](#)
- [Molecular orientational melting within a lead-halide octahedron framework: The order-disorder transition in \$\text{CH}_3\text{NH}_3\text{PbBr}_3\$](#)
- [Modelling of structure and dynamics of molten NaF using first principles molecular dynamics](#)
- [On the microscopic mechanism behind the disorder-disorder transition in the plastic phase of 1-Chloroadamantane](#)
- [New Insights into Hydride Bonding, Dynamics, and Migration in \$\text{La}_2\text{LiHO}_3\$ Oxyhydride](#)
- [Measurement of Magnetic Exchange in Asymmetric Lanthanide Dimetallics: Toward a Transferable Theoretical Framework](#)
- [Dynamical Transitions and Diffusion Mechanism in DODAB Bilayer](#)



Changes to the Proposal Deadlines

Following the discussion within the ISIS User Committee, the proposal deadline has been changed to the 3rd Wednesday in April & October.

Our next Science Meeting

More information about MSSM2018 will be available soon!

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.

Forthcoming Events

- [Neutron & Muon Science and User Meeting, Warwick, 25 – 27 April 2018](#) – with the student meeting on the first day!
- [19th International Seminar on “Neutron Scattering Investigation in condensed matter”, Poznan, 23 – 25 May 2018](#)
- [International Meeting of the Spanish Neutron Society, Santander, 17 – 20 June 2018](#)
- [Membranes Beyond, Hamilton \(Canada\), 2 – 4 July 2018](#)
- [Erice School on Neutron Science and Instrumentation, Erice \(Italy\), 4 – 13 July 2018](#)
- [QENS/WINS, Hong Kong, 15 – 20 July 2018](#)
- [MDANSE2018, Spain on 23 – 29 September 2018](#)