

The Newsletter of the

ISIS Molecular Spectroscopy User Group

People

We're very happy to welcome Alex Hawkins as a member of the Molecular Spectroscopy Group at ISIS. Alex will be working with us for 6 months from the start of February, providing local contacting support for group members on parental leave.

COVID-19

While vaccinations continue to roll out and case numbers fall, ISIS remains vigilant in its commitment to remain a COVID-secure facility. In the forthcoming cycle (27th April – 17th June) we will again be running primarily without user presence on site. Please ensure that you stay in contact with your local contacts if you have an experiment coming up and get in touch ASAP if you are hoping to attend in person so that the appropriate paperwork can be completed.

The long shutdown

The long shutdown is still scheduled to begin immediately after the next cycle, from the end of June. With the majority of the group instruments on TS1, we expect no beam for approximately 14 months from this date. The next proposal round will take place for TS2 only towards the end of this year, with a full proposal round for all instruments expected in early 2022. Further information can be found on the [ISIS website here](#).

New *in-situ* mass spec capabilities



The group have acquired a Hiden HPR-30 mass spectrometer with automatic leak valve. This will allow measurement to be made on the beamline at pressures from vacuum to ambient without user intervention. It can therefore be used to perform temperature-programmed or post neutron-measurement gas desorption characterisation in addition to flow monitoring in continuous reactions.

If you'd like any more information about the new equipment, please get in touch with Ian Silverwood (ISIS).

Molecular Spectroscopy Science Meeting 2020

In October (28th and 29th) last year, despite the difficulties of the pandemic we held a very successful virtual user group meeting. The meeting was well attended with between 40-60 delegates across both days logging in to see talks from nine invited speakers as well as four update talks from members of ISIS staff. We very much look forward to the next MSSM and hope it can return to taking place in person.

Data analysis and Mantid

[Mantid](#) 6.0 is now available to download from [mantidproject.org](#). This is the Workbench only release using Python version 3. Documentation regarding the preparation of publication quality plots can be found [here](#). Please post to the [Mantid Forum](#) to report any bug or to ask for help.

Please use your ISIS user office login to access IDAaaS. A general FAQ is available on IDAaaS facility [here](#). DLPOLY and CASTEP software for atomistic simulations are now available on IDAaaS.

The [LAGRANGE](#) instrument option has also now been implemented in the [abINS code](#) for analysing INS spectroscopic data. If you use abINS for your INS data analysis please cite [this article](#).

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

Spectroscopy Science Highlights

- Cation Dynamics and Structural Stabilization in Formamidinium Lead Iodide Perovskites - [J. Phys. Chem. Lett.](#)
- New Spectroscopic Insight into the Deactivation of a ZSM-5 Methanol-to-Hydrocarbons Catalyst - [ChemCatChem](#)
- Control of zeolite microenvironment for propene synthesis from methanol - [Nat. Commun.](#)
- Profiling of human burned bones: oxidising versus reducing conditions - [Sci. Rep.](#)
- Structure and spectroscopy of methionyl-methionine for aquaculture - [Sci. Rep.](#)
- Vibrational Motions Make Significant Contributions to Sequential Methyl C–H Activations in an Organometallic Complex - [J. Phys. Chem. Lett.](#)
- The neutron cross section of barite-enriched concrete for radioprotection shielding in the range 1 meV–1 keV - [Eur. Phys. J. Plus](#)
- A Python Algorithm to Analyze Inelastic Neutron Scattering Spectra Based on the γ -Scale Formalism - [J. Chem. Theory Comput.](#)
- Thermal neutron cross sections of amino acids from average contributions of functional groups - [arXiv](#)
- Cation Dynamics and Structural Stabilization in Formamidinium Lead Iodide Perovskites - [J. Phys. Chem. Lett.](#)
- Effect of pore geometry on ultra-densified hydrogen in microporous carbons - [Carbon](#)
- Diffusional Dynamics of Hydride Ions in the Layered Oxyhydride SrVO₂H - [Chem. Mater.](#)
- The low energy phonon modes of the hydrogenated and deuterated π -conjugated system 7,7,8,8-tetracyanoquinodimethane: an inelastic neutron scattering study - [Phys. Chem. Chem. Phys.](#)
- The Effect of an Intramembrane Light-Actuator on the Dynamics of Phospholipids in Model Membranes and Intact Cells - [Langmuir](#)
- Human hair: subtle change in the thioester groups dynamics observed by combining neutron scattering, X-ray diffraction and thermal analysis - [Eur. Phys. J. Spec. Top.](#)
- Short-Time Dynamics of PDMS-g-PDMS Bottlebrush Polymer Melts Investigated by Quasi-Elastic Neutron Scattering - [Macromolecules](#)
- Ammonia Storage in Hydrogen Bond-Rich Microporous Polymers - [ACS Appl. Mater. Interfaces](#)

Forthcoming Events

*Note all events and dates could be subject to change

- [UK Neutron & Muon Science and User Online Meeting and Student Meeting 2021 \(NMUM\)](#) – 30th April 2021
- [QENS/WINS 2021 \(Online\)](#) – 17th-21st May 2021

Job & PhD Listings

- [Experimental and computational studies of the methanol synthesis catalyst – where is the hydrogen? – University of Lincoln](#)
- [PhD student position in energy related materials physics – Chalmers University](#)

Please be reminded that the representatives of our group, [R. Senesi](#) and [A. O'Malley](#), are always open for feedback.