

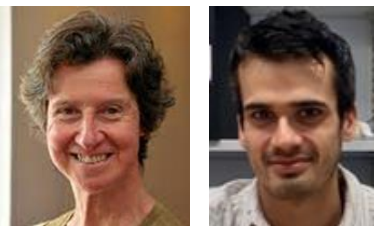
## The newsletter of the ISIS Molecular Spectroscopy User Group

### Staff news

We are very happy to welcome two new placement students. Matei Pascariu will work on the Raman set-up and Rachel Rushworth will work with the *in-situ* calorimeter for IRIS. We say thank you and goodbye to Gui Pereira and Ratislav Turanyi. Welcome also to Maciej Bartowiak who will work on MDANSE.

### User Group Representatives

Maria Paula Marques from the Univ. Coimbra, Portugal, is your new user group representative and joins Alexander O'Malley (Bath University, UK).



Alex is also this year's recipient of the BTM Willis Prize 2022. Congratulations!!

### Data Analysis & Software

Mantid 6.5 will be available soon to download. New scripts are available for diffraction data on OSIRIS, multiple scattering corrections, and additional functions for convolution fitting of S(Q,E) in the Data Analysis interface. Questions or suggestions welcome at the Mantid Forum. A new algorithm, abINS2D, is now available from Mantid 6.4 for calculating INS spectrum for direct geometry instruments at ISIS (MAPS, MARI) and ILL (PANTHER). The up to date version of the MDANSE code is available for download here. A Users guide to use the code is also available now. A new release based on python 3.0 will be available soon. The course materials of the MDANSE course are available here.

### Forthcoming Events

- 10<sup>th</sup>-11<sup>th</sup> November NSG-ECM 2022, Cosener's House Abingdon
- ECNS 20<sup>th</sup>-23<sup>rd</sup> March 2023, Garching, Germany
- RSC Faraday Joint Interest Group Conference 3<sup>rd</sup>-5<sup>th</sup> April 2023, Sheffield
- 2023 UK Neutron & Muon Science and User Meeting, 19<sup>th</sup>-21<sup>st</sup> April, 2023, University of Warwick
- Neutron Scattering Gordon Research Seminar, 24<sup>th</sup>-25<sup>th</sup> June, 2023, California, USA
- Neutron Scattering Gordon Research Conference, 25<sup>th</sup>-30<sup>th</sup> June, 2023, California, USA

Please send any feedback for our group, to our User Group representatives, A O'Malley and M. P. Marques.

### ISIS Call for Proposals for TS1 and TS2

**Deadline: 17:00 GMT, 19<sup>th</sup> October**

Submit your proposals using the new system here. Remember it is a good idea to discuss with the instrument scientist first!

### TS1 Neutrons

The third cycle with the new LINAC tank 4 is currently underway on TS2. Progress of work on TS1 is on track and the new target is now in place (see ISIS website). We are looking forward to commissioning and welcoming our first users later in the year.

### Instrument Updates

TOSCA's secondary upgrade project is progressing well. An international review has held in May and the design was approved. As part of the Endeavour instrument programme portfolio, it is en route to receiving funding approval.

Work on building the case for SHERPA, a dedicated polarised backscattering spectrometer, is ongoing. We are looking for scientific case studies, so let Ian know!

### Science Highlights

- Structure and Spectroscopy of Iron Pentacarbonyl, Fe(CO)<sub>5</sub>
- Light it up – Disentangling the structure of next-generation photovoltaic materials with TOSCA
- Controlling Amyloid Fibril Properties using Ionic Liquids. The representative case of EAN and TMGA on the Amyloidogenesis of Lysozyme
- Combined spectroscopic and computational study for optimising catalyst design in hydrocarbon transformations
- Water dynamics in human healthy and cancerous tissues
- Microscopic diffusion in cationic vesicles across different phases
- Neutron spectroscopy as a method for classical force-field parameterization: Past methods, present successes and future challenges
- Sodium diffusion and dynamics in Na<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub> as probed by neutron scattering and ab-initio simulations
- Pressure dependence of rotational dynamics in barocaloric ammonium sulfate
- Short-range magnetic order within the multiferroic erythrosiderite mineral (NH<sub>4</sub>)<sub>2</sub>FeCl<sub>5</sub>·H<sub>2</sub>O
- Conduction Mechanism in Graphene Oxide Membranes with Varied Water Content: From Proton Hopping Dominant to Ion Diffusion Dominant
- The Impact of Surface Charges of Carboxylated Cellulose Nanofibrils on the Water Motions in Hydrated Films
- Anisotropy of the proton kinetic energy captures structural transition in water confined in a graphene nanoslit pore
- Changes in the hydrogen nuclear kinetic energy across the several phases of methylammonium lead tribromide
- Force constant disorder in the Ni<sub>44</sub>Nb<sub>56</sub> bulk metallic glass as observed on Vesuvio

### Instrumentation Highlights

- Upgrade of the OSIRIS primary spectrometer
- On the spectral resolution of the broad-band indirect-geometry time-of-flight neutron spectrometer TOSCA
- Unlocking high-pressure science with broadband neutron spectroscopy at ISIS

Please inform us of your publications arising from ISIS related work. Remember to include ISIS staff as co-authors, when deemed appropriate, to cite instruments and software, and include a DOI for your experiment RB.