

Good Vibrations

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The newsletter of the ISIS Molecular Spectroscopy User Group

Staff news

We welcome Chi Cheng who has joined the MDANSE team.

IRIS and OSIRIS are BACK!!

The new hydrogen moderator has successfully been installed and commissioned, meaning that all Molecular Spectroscopy instruments were operational in the 2023/5 cycle. The upgrade has delivered a flux increase of a factor of 2 for both IRIS and OSIRIS. We are very happy to welcome back our QENS users!

<u>Next ISIS Call for Proposals*</u> TS1&TS2 Deadline: 17:00 17th April 2024

*due to backlog, all our TS1 instruments will be offering reduced time



QENS/WINS 2024 Call for abstracts

We await you at QENS/WINS on the 10th – 14th June in Manchester. We are accepting abstracts until 12th April, <u>here</u>.

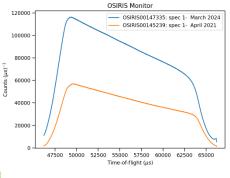
SiMol: Last year 30^{th} Oct – 1^{st} Nov we merged our user meeting with a simulation meeting and held the SiMol meeting at Milton House. The book of abstracts for the talks and posters can be found <u>here</u>. An article abou the meeting can be found here.

Data Analysis & Software

Data Analysis & Software <u>Mantid 6.9</u> has been released. Notable changes include the move of some of the QENS data analysis under the name <u>Inelastic</u>, as these interfaces are applicable for both indirect geometry (IRIS/OSIRIS) and direct geometry (LET) instruments, and an upgraded online <u>QENS model repository</u> where users can deposit their QENS models. Also, an automated Data Reduction facility is now available provided for TOSCA on IDAaaS. We ask users to test these new features and provide us with feedback, and report any Mantid related bug reports to Mantid Forum. Finally, we are now testing a new release MDANSE2. We encourage users to take part in testing the alpha version, which can be downloaded from <u>here</u>. The online Users guide for <u>MDANSE</u> is available <u>here</u>. Users are requested to post any Mantid related bug reports to <u>Mantid Forum</u>.

Forthcoming Events

- <u>NMSUM</u> 10th-12th April, 2024, Warwick
- QENS/WINS 10th -14th June, 2024, in Manchester
- MDANSE school 5th-7th November, 2024, at the ILL



Successful Placement Students

Three new publications have resulted from our latest cohorts of placement students, Matei Pascariu, Rastislav Turanyi and Rachel Rushworth.

Matei <u>published</u> his work on methyl- β -D-riboforanoside probed by the INS, Raman and IR spectroscopies. The experimental techniques were complemented by DFT computational methods using both gas-phase (Gaussian) and solid-state (CRYSTAL, CASTEP) approaches. Rastislav published his work on computational methods and neutron spectroscopy in the design and development of sodium-ion batteries. Rachel's paper on thianthrene was recently accepted for publication as well. She was able to characterise bending modes at 200-300 cm⁻¹ for the first time using the INS, Raman spectroscopy and periodic DFT.

Science Highlights

- <u>Cellular dynamics as a marker of</u> <u>normal-to-cancer transition in human</u> <u>cells</u>
- Investigation of the Dynamic Behaviour of H2 and D2 in a Kinetic Quantum Sieving System
- Neutron thermal cross sections of 3Dprinting organic polymers using the Average Functional Group Approximation
- Cation Dynamics as Structure Explorer in Hybrid Perovskites – The Case of MAPb13
- The Advantages of Flexibility: The Role of Entropy in Crystal Structures Containing C-H…F Interactions
- Silver Jubilee for the OSIRIS spectrometer: Achievements and Outlook
- New insights into the protein stabilizing effects of trehalose by comparing with sucrose
- Nanocomposite materials as observed by mass-selective neutron spectroscopy
- Exploring asymmetry induced entropy in tetraalkylammonium–urea DES systems: what can be learned from inelastic neutron scattering?
- Tuning of structure and host dynamics via yttrium doping in Bi2O3 to enhance oxygen ion diffusion
- Quasi Elastic Neutron Scattering model library
- <u>A Multimodal Study on the Unique</u> <u>Sensing Behavior of a</u> <u>Guest@Metal-Organic Framework</u> <u>Material for the Detection of Volatile</u> <u>Acetone</u>

Please send any feedback for our group, to our User Group representatives, <u>Maria-</u> <u>Paula Marques and Matthew Potter</u>.

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 <u>DOI for your experiment RB</u>.