

The newsletter of the ISIS Molecular Spectroscopy User Group

Staff news

We are happy to announce that Victoria Garcia Sakai is now Head of the newly created Neutron Spectroscopy Division which oversees the Molecular Spectroscopy and Excitations Groups.

TS1 Neutrons

Commissioning of the TS1 systems continues following completion of the upgrade. A number of issues still need resolution, in particular around the CH₄ and H₂ moderator systems. We hope to provide some user beam on Tosca and Vesuvio in late May, however, Iris and Osiris will be unavailable until the summer at the earliest. We apologise for the impact this will cause and will keep you updated.

Data Analysis & Software

Mantid 6.6 has a new interface, Inelastic Data Manipulation, for all QENS instrument data. Analysis of diffraction on OSIRIS can now be done in scripting mode. The new Autoconvolution option in abINS and abINS2D can calculate up to 10 quantum events. abINS2D can now be used to plan INS experiments on direct geometry instruments. A Users guide for MDANSE is available here and the up to date version of the software is available to download from here.

Characterising Ancient Egyptian Leathers with neutron spectroscopy

A series of leather objects from a collection of Museo Egizio (Italy) recovered throughout Egypt and dated to different historical periods (ranging from ca. 2700 BC-AD 600), used VESUVIO and TOSCA amongst a suite of techniques to inform on the chemical and elemental composition and link to morphology. The study documented extensive denaturation, co-called gelatinisation due to leather deterioration over time.



(a)

(b)

Forthcoming Events

- RSC Faraday Joint Interest Group Conference 3rd-5th April 2023, Sheffield
- 2023 UK Neutron & Muon Science and User Meeting, 19th-21st April, 2023, University of Warwick
- Neutron Scattering Gordon Research Seminar, 24th-25th June, 2023, California, USA
- Neutron Scattering Gordon Research Conference, 25th-30th June, 2023, California, USA
- SiMolSpec, 30th Oct-1st Nov, 2023, Milton House, Didcot

Further Information: Molecular Spectroscopy Homepage [IRIS-LET-MAPS-OSIRIS-TOSCA-VESUVIO](#)

Science Highlights

- [Vibrational spectra of neutral and doped oligothiophenes and polythiophene](#)
- [Experimental and computational studies of sulfided NiMo/Al-PILC: Catalyst activation and guaiacol adsorption sites on Mo- and Ni-edges](#)
- [Nuclear quantum dynamics in Hexamethylenetetramine and its deuterated counterpart: a DFT-augmented neutron study](#)
- [Neutron-Enhanced Information on the Laboratory Characterization of Ancient Egyptian Leathers: Hydration and Preservation Status](#)
- [Quantum Effects of Neutron Scattering on Indistinguishable Particles](#)
- [Soft anharmonic coupled vibrations of Li and SiO₄ enable Li-ion diffusion in amorphous Li₂Si₂O₅](#)
- [Geometric Frustration and Concerted Migration in the Superionic Conductor Barium Hydride](#)
- [Origin of the Large Entropy Change in the Molecular Caloric and Ferroelectric Ammonium Sulfate](#)
- [Collective dynamics of liquid sulfur scrutinized over three decades in frequency](#)
- [Exceptional Hydrogen Diffusion Rate over Ru Nanoparticle-Doped Polar MgO\(111\) Surface](#)
- [Characterisation of ethylene adsorption on model skeletal cobalt catalysts by inelastic and quasi-elastic neutron scattering](#)

ISIS Call for Proposals for TS2 only

Deadline: 17:00 19th April 2023

Job & PhD Listings

- There is one PhD position available, please find details here.

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

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.