

The newsletter of the ISIS Molecular Spectroscopy User Group

People

We are very happy to welcome Gui Maciel Pereira and Ratislav Turanyi who have joined us as sandwich students. Gui is working on introducing the parametric bootstrap technique for Neutron Compton Scattering on Vesuvio. Ratislav is working on the integration of molecular dynamics simulations for QENS spectroscopy, in particular for the [MDANSE project](#).

The long shutdown

The ISIS shutdown is well underway and progress can be followed on the [ISIS website](#). Next beamtime will be available to TS2 only, likely to be scheduled March to July 2022. The next call for both TS1 and TS2 instruments will close on 20th April 2022, with beamtime planned for autumn 2022.

We are recruiting!

- We are looking for an **instrument scientist** on [Vesuvio](#) (deadline 7th November)
- We have several **sandwich student** positions available [here](#) (deadline 31st October)
- A number of **open ended positions** in scientific software development, are available including one on the [MDANSE](#) cde. Apply [here](#) by the 31st October 2021.

New Instrument Concept – SHERPA – Polarisation Analysis on IRIS

We are working on a new concept to upgrade the IRIS spectrometer that would provide the community with the first ever backscattering spectrometer with polarisation analysis. This will allow separation of coherent and incoherent scattering from a sample and will open up an exciting range of possibilities. If you are interested, please get in touch with Ian.

In-situ illumination cell for TOSCA

A new prototype in-situ illumination cell has been developed by Hamish in collaboration with the ISIS electronics department. It was successfully used on TOSCA to perform photoisomerisation on a photochromic material. Hamish hopes to continue development of the hardware for general use in the user programme. For more information please see ([Physical Chemistry Chemical Physics](#)), or [contact Hamish](#).



In-situ calorimeter for QENS

Thanks to the work of sandwich student Cameron Twigg over the last year, there has been good progress on the design of powder cells for measurements of thermodynamic changes and QENS in parallel. This aims to complement the existing liquid cells. Further work is ongoing. Expressions of interest are welcome by [contacting Mona](#).

Data Analysis & Software

[Mantid 6.2](#) is now available to [download](#). The Data Analysis GUI for QENS has been upgraded. A reminder to please cite [this](#) if you use QENS tools from Mantid. A users guide can be found [here](#).

[abINS](#) can now simulate INS up to the 10th order. A reminder to please cite [this](#) if you use abINS for your INS data analysis.

The remote data analysis service [IDAaaS](#) has a new web-front. Please use your user office login to access IDAaaS to open a workspace in the browser. A general FAQ is available on IDAaaS facility [here](#).

Spectroscopy Science Highlights

- [Glass Transition in Rice Pasta as Observed by Combined Neutron Scattering and Time-Domain NMR](#)
- [Time-resolved Prompt-Gamma Activation Analysis at Spallation Neutron Sources and Applications to Cultural Heritage, Security, and Radiation Protection](#)
- [MWCNT/rGO/natural rubber latex dispersions for innovative, piezo-resistive and cement-based composite sensors](#)
- [Probing the dynamics and structure of confined benzene in MCM-14 based catalysts](#)
- [Origin of natural and magnetic field induced polar order in orthorhombic PrFe_{1/2}Cr_{1/2}O₃](#)
- [Thermal neutron cross sections of amino acids from average contributions of functional groups](#)
- [Purification of propylene and ethylene by a robust metal-organic framework mediated by host-guest interactions](#)
- [Atomically Dispersed Copper Sites in Metal-Organic Framework for Reduction of Nitrogen Dioxide](#)
- [Metalloprotein Interaction Probed by Synchrotron Terahertz and Neutron Scattering Spectroscopy](#)
- [Spectroscopic Identification of Disordered Molecular Cations in Defect Perovskite-like Aln\(HCO2\)\(C2O4\)1.5 \(Ln=Tb-Er\) Phases](#)
- [Predicting the impact sensitivity of a polymorphic high explosive: the curious case of FOX-7](#)
- [Topics in Catalysis](#)
- [Net Zero and Catalysis: How Neutrons Can Help](#)
- 3 STFC Air Quality Network (SAQN) scoping studies awards have been granted to MSG scientists. More information will be found [here](#), [here](#) and [here](#).

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

Please send any feedback for our group, to our User Group representatives, [R. Senesi](#) and [A. O'Malley](#). If you are interested in becoming a user rep for the group please contact [Victoria Garcia Sakai](#), group leader.

Forthcoming Events

- ISIS Student meeting 28th and 29th October at RAL
- QENS/WINS 23rd to 27th May 2022, San Sebastian, Spain
- International Conference on Neutron Scattering 2022 21st to 25th August 2022 Buenos Aires Argentina
- 15th International Conference on Nuclear Data for Science and Technology 24th to 29th July 2022 Sacramento, California USA

(*Note all 2021/2022 events and dates could be subject to change)