

## The Newsletter of the ISIS Molecular Spectroscopy User Group

### People

We are very happy to announce that Victoria García Sakai has become the new head of the Molecular Spectroscopy Group at ISIS. We'd like to thank Stewart Parker for his work as acting group leader. We say welcome to Mona Sarter, who joins the QENS team and IRIS bringing expertise in biophysics. Sadly, we also say goodbye to José Martínez González who is moving to take a postdoc in MD simulations in Spain.

### COVID-19 and ISIS

A lot has changed in a short period of time as a result of the recent outbreak of coronavirus. To comply with government advice and to keep people as safe as possible the decision was made to finish the user cycle 2019/04 on 18 March, 9 days early. Further to this and in light of the predicted nature of the pandemic, the user cycle 2020/01 (28 April-5 June) has also been cancelled along with the next proposal round, previously scheduled to close on 15 April. As the situation is still changing rapidly, please keep checking for notifications from the user office regarding experiments that have been cancelled and experiments that are already scheduled later in the year.

### ISIS Long Shutdown

After a comprehensive readiness meeting in January it was decided that the forthcoming ISIS long shutdown would be delayed by 4 months. The new start date has been set as 4 January 2021. This means that the previously planned dates for the 2020/02 cycle have been moved to start on 8 September and an additional 2020/03 cycle has been added to the schedule, running from 10 November. [Up-to-date information is online.](#) These new dates currently remain unchanged, however please be aware that the progress of the COVID-19 pandemic may lead to further adjustments being made in the future.

### Mantid – [send us your feedback!](#)

The Mantid project is preparing for an [international review](#). Your feedback and participation in very important in this review process. If you use Mantid in any capacity, please [fill out the online survey](#) and give your feedback, it only takes a couple of minutes and is very helpful.

[Mantid 5.0](#) is also now available to download from [mantidproject.org](#). This is the first version run only on Python 3. Tips or help migrating your scripts to Python 3 can be found on the [Mantid forum](#). In this new release, data reduction and analysis for all MSG instruments are available on Mantid Workbench. This workbench is flexible to use and equipped with enhanced plot settings and performance improvements. For MSG, we have a brand new GUI for simultaneous multidataset fitting for QENS data analysis.

### ISIS Impact Awards

The ISIS Impact Awards nominations deadline has been extended to 24 April! The awards celebrate socio-economic impact generated by the user community. For more information please visit the [ISIS website](#).



### Instrument Updates - OSIRIS

Adrien Perrichon and Franz Demmel have recently published a report demonstrating the potential benefits of a neutron guide upgrade on the performance of QENS instrument OSIRIS. The report can be [found on ePubs](#). Additionally, a new Si(111) crystal analyser is scheduled for installation during the long shutdown, improving the spectral resolution and dynamic range of the instrument when ISIS comes back online.

Don't miss our  
supplementary  
special page below!

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

Mantid International Review  
Feedback Survey  
Your feedback is important!

## Spectroscopy Science Highlights

- High-resolution neutron spectroscopy using backscattering and neutron spin-echo spectrometers in soft and hard condensed matter - [Nature Reviews](#)
- An effective hydrogen scattering cross section for time-of-flight neutron experiments with simple organic molecules – [J. Appl. Cryst.](#)
- Affecting an Ultra-High Work Function of Silver - [Angew. Chem. Int. Ed.](#)
- Quantitative production of butenes from biomass-derived  $\gamma$ -valerolactone catalysed by hetero-atomic MFI zeolite - [Nature Materials](#)
- Diffusion of sodium ions in amorphous Na<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>: Quasielastic neutron scattering and ab initio molecular dynamics simulations - [Phys. Rev. Materials](#)
- Identification of normal modes responsible for ferroelectric properties in organic ferroelectric CBDC - [J. Phys. Commun.](#)
- Accelerated Local Dynamics in Matrix-Free Polymer Grafted Nanoparticles - [Phys. Rev. Lett.](#)
- Intracellular water as a mediator of anticancer drug action - [Int. Rev. Phys. Chem.](#)
- Imidazolium-based ionic liquids cause mammalian cell death due to modulated structures and dynamics of cellular membrane - [Biochim. Biophys. Acta Biomembr.](#)
- Dynamic Landscape in Self-Assembled Surfactant Aggregates - [Langmuir](#)
- Asymmetric Monomer, Amorphous Polymer? Structure–Property Relationships in 2,4-FDCA and 2,4-PEF – [Macromolecules](#)
- Secondary relaxation in the terahertz range in 2-adamantanone from theory and experiments – [Phys. Rev. B](#)

## Forthcoming Events

\*Note all 2020 events and dates could be subject to change

- **CANCELLED** - UK Neutron and Muon Science & User Meeting (NMSUM). Dates for rescheduling to follow.
- [QENS/WINS 2020 – 8-12 June - San Sebastian, Spain](#)
- [Joint ESS ILL User Meeting “Neutrons 4 Europe” – 23-25 September – Lund, Sweden](#)
- [MDANSE2020 – 26-29 September \(tentative\) – Lund, Sweden](#)
- [Molecular Spectroscopy User Group Science Meeting \(MSSM2020\) – 28-29 October – Cosener’s House, Abingdon](#)
- [Faraday joint interest group conference 2020](#) - postponed to 29-31 March 2021 - Sheffield
- [Gordon Research Conference and Seminar on Neutron Scattering – 5-11 Jun 2021 - Hong Kong](#)

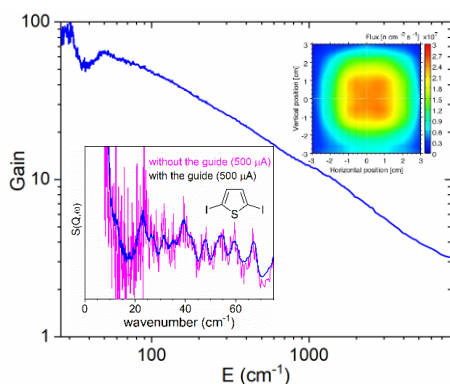
## Job & PhD Listings

- [Postdoc position on low-dimensional metal halides for lighting](#)
- [PhD student position in time-resolved spectroscopy on proton- and hydride-ion conducting perovskites for energy applications](#)
- [PhD Studentships with ILL and UK Universities](#)

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

TOSCA is an indirect-geometry inelastic neutron spectrometer optimised for high resolution vibrational spectroscopy in the energy transfer region between  $-24 \text{ cm}^{-1}$  and  $4000 \text{ cm}^{-1}$ . The instrument has been operational over the last two decades and during that time has set the standard for broadband chemical spectroscopy with neutrons. Since February 2017 the instrument has been upgraded with high- $m$  neutron guide composed of ten sections in order to boost the neutron flux at the sample position. In the low energy region a gain in neutron flux of as much as 82 times has been observed. The much improved count rate allows faster measurements where useful data of hydrogen-rich samples can be recorded within minutes, as well as opening the ability to perform experiments involving smaller samples.

Such a development has allowed detailed studies of industrially relevant systems containing weak neutron scatterers, as well as parametric studies, particularly for hydrogen containing molecules. Additionally, as neutron scattering is an inherently flux-limited technique, studies of smaller samples, which are too expensive to produce in large quantities, has become possible. A report of the upgrade as well as examples of the abovementioned studies are given below:

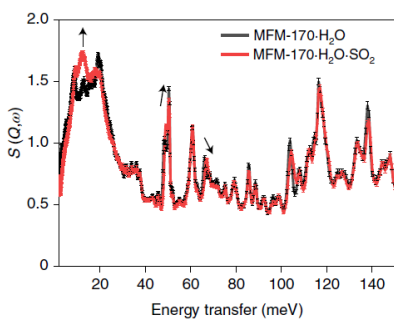
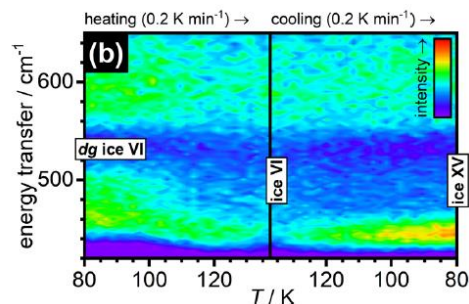


**NEUTRON GUIDE UPGRADE:** [The neutron guide upgrade of the TOSCA spectrometer, R.S. Pinna \*et al.\*, Nuclear Instruments and Methods in Physics Research A 896, 68 \(2018\)](#)

Gain in the neutron flux at the TOSCA sample position as a function of neutron energy.

**PARAMETRIC STUDIES:** [Deep-glassy ice VI revealed with a combination of neutron spectroscopy and diffraction, A. Rosu-Finsen \*et al.\*, J. Phys. Chem. Lett. 11, 1106 \(2020\)](#)

Contour plot of the librational region upon heating deep-glassy ice VI from 80 to 138 K, followed by cooling back to 80 K.



**WEAK NEUTRON SCATTERERS:** [Reversible coordinative binding and separation of sulfur dioxide in a robust metal–organic framework with open copper sites, G.L. Smith \*et al.\*, Nature Materials 18, 1358 \(2019\)](#)

Shifts in water modes are observed, indicating  $\text{H}_2\text{O} \cdots \text{SO}_2$  interaction.

**STUDIES OF SMALLER SPECIMENS:** [A new look into the mode of action of metal-based anticancer drugs, M.P.M. Marques \*et al.\*, Molecules 25, 246 \(2020\)](#)

The mode of action of Pt- and Pd-based anticancer agents (cisplatin and Pd2Spm) was studied by characterising their impact on DNA.

