Science and Technology Facilities Council
ISIS

Good Vibrations

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The Newsletter of the ISIS Molecular Spectroscopy User Group

The virtual User Group Science Meeting MSSM2020 registration is open now! CLICK HERE!

People

We're very happy to welcome Adrien Perrichon as a full member of the Molecular Spectroscopy Group at ISIS. Adrien has been working as a visiting researcher for the past two years and in his new role becomes an instrument scientist to support energy materials research and instrument upgrade projects. We also welcome sandwich student Cameron Twigg, who is going to be working on in-situ calorimetry capabilities for QENS instrument IRIS. Hamish Cavaye, who was previously on a fixed-term contract has become a permanent member of ISIS staff. Hamish spends half his time as industrial liaison for Johnson Matthey and the other half of his time as local contact, primarily doing INS on the instrument MAPS. Lastly, we are sorry to say farewell to Matthew Andrew, who helped us in development of QENS data analysis in Mantid Workbench. We wish him a bright future ahead.

Covid-19 and ISIS

The pandemic continues to pose challenges to people all around the world. At ISIS we are now approaching the end of our first user cycle and we are all adapting to the Covid-secure work practices. This cycle has remained a primarily user-free cycle, with samples mailed in and handled by the instrument scientists. Overall this has worked very successfully and we are still awaiting management decisions regarding visiting users in upcoming cycles.

Unfortunately, Covid-19 restrictions have caused another delay to the start of the long shutdown. The shutdown is now set to begin on 29th March 2021, with an additional cycle to be run in Feb/Mar next year. At present there are no additional FAP proposal rounds scheduled. Up-to-date information can be found on the ISIS website here.

Placement Student Success

Local school student Emilie Revill-Hivet joined the Molecular Spectroscopy Group for a two-week placement in the summer of 2019 working with Stewart Parker (ISIS) to study the INS of lithium and potassium methanesulfonate salts. The work has subsequently been published in Royal Society Open Science, a great feat for someone who hasn't even left school yet! More can be read in the full story, featured on the Royal Society Blog. To find out more about applying for work experience places, please see the UKRI web page here.

Data Analysis & Mantid

ISIS Data Analysis as a Service (IDAaaS) server is now available for MSG environment. We request users to login here with your User Office login ID and go to the MSG environment to access data and to analyse it using our central data analysis facilities. We would like to hear your feedback and suggestions.

Mantid 5.1 is also now available to download from mantidproject.org. This is the final release available with Mantidplot as the GUI. Users are requested to familiarise themselves with the Mantid Workbench facility for their data analysis. There will be only Workbench from the next release. Please cite Mantid when you use it for your data reduction.

In addition to the online Users's Guide available for QENS data analysis using Mantid, there is an online tutorial available in STFC training portal for those who are new users in QENS spectroscopy. If you use Mantid for your QENS data analysis please cite this.

The abINS code for analysing INS spectroscopic data has now load data from VASP and DMol output. If you use abINS for your INS data analysis please cite this paper.

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

Spectroscopy Science Highlights

- Unraveling the Ground-State Structure of $BaZrO_3$ by Neutron Scattering Experiments and First-Principles Calculations – Chem. Mater.
- Measurement of neutron total cross sections at the VESUVIO spectrometer – Nucl. Instrum. Meth. A
- Volatile hydrogen intermediates of CO_2 methanation by inelastic neutron scattering – Catalysts
- A HF loaded Lewis-acidic aluminium chlorofluoride for hydrofluorination reactions – Chem. Eur. J
- Green reconstruction of MIL-100 (Fe) in water for high crystallinity and enhanced guest encapsulation - ACS Sustainable Chem. Eng.
- Spontaneous formation of an ordered interstratification upon Ni-exchange – Appl. Clay Sci.
- Discovery of neutron-moderating materials at ISIS Neutron and Muon Source – EPJ Web of Conferences
- Phonons and oxygen diffusion in Bi_2O_3 and $(Bi_{0.7}Y_{0.3})_2O_3$ – J. Phys.: Condens. Matter

Queen's Birthday Honours

We'd like to offer up our warmest congratulations to Prof Sir Richard Catlow (UCL) as a long-standing ISIS molecular spectroscopy user, who has been awarded a knighthood for Leadership in Science and Research.

A short article with more information can be found on the ISIS website.

Forthcoming Events

*Note all 2020/2021 events and dates could be subject to change

- Molecular Spectroscopy User Group Science Meeting (MSSM2020) – 28-29 October – Cosener's House, Abingdon
- Virtual MRS Fall Meeting – 27 November – 4 December 2020
- Faraday joint interest group conference 2021 – 29-31 March 2021 – Sheffield, UK
- MDANSE (2020) – Postponed until April, 2021

Job & PhD Listings

- The advertisement for Industrial placement students on data analysis and simulations of energy materials and development of online training is now out. Please apply!

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