

The Newsletter of the ISIS Molecular Spectroscopy User Group

**Next Proposal Round
Deadline: October 16th
Submit your proposals here**

News

In this second issue of Good Vibrations for 2019 we regret to announce that Felix Fernandez-Alonso (ISIS & UCL) has stepped down as head of the Molecular Spectroscopy Group at ISIS. Felix has been instrumental in sculpting the group over the past decade, during which time it has grown dramatically both in size and in expertise. We all owe Felix many thanks and wish him all the best for the future.

We also say goodbye to Joel Ponsonby, a sandwich student who worked on the QENS capability for in-situ calorimetry and is now back studying at the University of Bath. A report of this work will be published soon.

We welcome Ciara Nightingale, Matthew Andrew, and Adam Jackson to the group. Ciara and Matthew will work on development of data analysis facilities in Mantid, and Adam will work on the abINS algorithm. We have said farewell to Robert Applin, the sandwich student, who worked on Mantid 2018-19.



Newton Fund

Indri Badria Adilina (Indonesian Institute of Sciences, 2nd from right) and her team were successfully awarded funding from the UK government Newton Fund in 2018. Their research concerns the conversion of biomass waste

from the palm oil industry into fuel. During their time at ISIS, Indri and her team made great use of the inelastic and quasielastic scattering instruments to investigate the complex reactions occurring within the catalysts they were studying. Indri was also awarded the Economic Impact ISIS Award at the NMSUM meeting (29th April – 1st May 2019, Warwick University). You can read more about Indri and her research on the [ISIS website](#).

Long Shutdown

Please remember that the long shutdown for ISIS is scheduled to begin on 1st September 2020. Due to this fact the forthcoming October 2019 FAP proposal round (round 20/1) is the last proposal round for experiments that will be scheduled before the long shutdown. There will be no proposal round in April 2020 (round 20/2).

More information regarding the schedule for proposal rounds and the long shutdown can be found on the [ISIS website](#).

Mantid

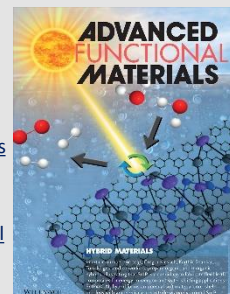
[Mantid 4.1](#) was released at the end of July. More data treatment facilities are now available in the new Mantid [Workbench](#). The latest development of Mantid is documented in a [RAL Technical Report](#). New updates also have been posted in the on-line [QENS data analysis Users Guide](#). There is also a [citable publication](#) of these SINE2020 funded developments. An improved version of the [abINS algorithm](#), suitable for INS interpretations, also can be found in Mantid 4.1.

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

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

Science Highlights

- [Chasing the “Killer” Phonon Mode for the Rational Design of Low-Disorder, High Mobility Molecular Semiconductors](#)
- [Flexible and Ultrasoft Inorganic 1D Semiconductor and Heterostructure Systems Based on SnIP](#) (Adv. Funct. Mater. front cover)
- [Hydrodeoxygenation of Guaiacol as a Bio-Oil Model Compound over Pillared Clay-Supported Nickel–Molybdenum Catalysts](#)
- [Perovskite solar cell resilience to fast neutrons](#)
- [Water dynamics in MCF-7 breast cancer cells: a neutron scattering descriptive study](#)
- [Fibre formation in calcium caseinate influenced by solvent isotope effect and drying method – A neutron spectroscopy study](#)
- [Structural dynamics of a metal–organic framework induced by CO₂ migration in its non-uniform porous structure](#)
- [In Vivo Water Dynamics in Shewanella oneidensis Bacteria at High Pressure](#)
- [Modulating proton diffusion and conductivity in metal–organic frameworks by incorporation of accessible free carboxylic acid groups](#)
- [Predicting the reactivity of energetic materials: an ab-initio multi-phonon approach](#)
- [First analysis of ancient burned human skeletal remains probed by neutron and optical vibrational spectroscopy](#)
- [Experimental Evidence for Vibrational Entropy as Driving Parameter of Flexibility in the Metal-Organic Framework ZIF-4\(Zn\)](#)
- [Visualisation of the catalysed nuclear-spin conversion of molecular hydrogen using energy-selective neutron imaging](#)
- [A modern approach to QENS data analysis in Mantid](#)
- [Adsorbed States of Hydrogen on Platinum: A New Perspective](#)



Forthcoming Events

- [ISIS Student Conference, 28th-29th October 2019, Abingdon](#)
- [Artificial Intelligence Applied to Photon and Neutron Science, 12th-14th November 2019, ESRF-ILL, Grenoble, France](#)
- [Neutrons @ Materials Research Society, 1st-6th December, Boston, USA](#)
- [Faraday joint interest group conference 2020, 6th-8th April 2020, Sheffield](#)
- [UK Neutron & Muon Science and User Meeting 2020 \(NMSUM\), 8th-10th June 2020, Warwick](#)
- [QENS/WINS 2020, 8th-12th June 2020, Spain](#)

ISIS Job Listings

- [ISIS Molecular Spectroscopy Group Leader](#)
- [ISIS Instrument Scientist – MAPS](#)
- [ISIS Instrument Scientist – LET](#)