

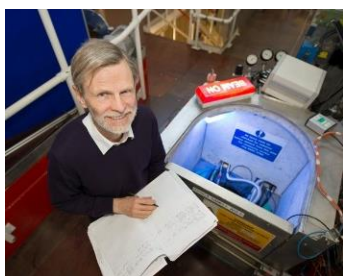
The newsletter of the ISIS Molecular Spectroscopy User Group

People

We are very happy to welcome Andrew Seel to the VESUVIO team. We say goodbye to Giovanni Romanelli who takes up the post of assistant professor at the University of Rome “Tor Vergata”.

Norman Sheppard award

We are very happy to announce that our Stewart Parker, ISIS Catalysis Scientist, has been awarded the Norman Sheppard award by the Infrared and Raman discussion group. Congratulations Stewart.



VESUVIO+ update

We have a programme of work to improve the current performance of VESUVIO and prepare the ground for an entirely new epithermal neutron spectrometer, ETNA, in the future. We are currently repositioning the backscattering detectors closer to the sample position, which will increase the count rate without compromising the resolution. In addition, an optimisation and re-design of the beam stop is planned with work beginning at the end of the long shutdown, to minimise the parasitic gamma background to optimise the working conditions of the forward scattering detector banks.

Data Analysis & Software

Mantid 6.3 is now available to [download](#). The Data Analysis for QENS GUI and calculations of DensitiesofStates have been upgraded, a [users guide](#) is available. [abINS code](#) can now load force constant data from castep_bin file, if you use abINS please [cite this](#). The newest version of the MDANSE code is available [here](#).

Forthcoming Events

- NMSUM 2022 25th to 27th April 2022 at Warwick University
- QENS/WINS 23rd to 27th May, San Sebastian, Spain
- [MSSM](#) 27th to 28th June, Cosener’s House Abingdon
- [MDANSE](#) 29th June to 1st July, Cosener’s House Abingdon
- 15th International Conference on Nuclear Data for Science and Technology 24th to 29th July 2022 Sacramento, California, USA
- International Conference on Neutron Scattering 2022, 21st to 25th August, Buenos Aires, Argentina

ISIS neutrons are back

The first cycle with the new LINAC tank 4 is currently underway on TS2. Progress of work on TS1 is on track (see [ISIS website](#)). Neutrons are expected in the autumn.

SHERPA: QENS + polarisation

On March 8th we held a very successful online workshop to discuss the idea of a new polarised QENS instrument (SHERPA). Thank you to everyone who attended for the interest and positive feedback. The introductory talks are [available online](#). We would like to hear your thoughts and requirements. If you are interested please fill out the following [questionnaire](#).

Endeavour Instruments

Design work is progressing well for the OSIRIS guide and TOSCA secondary upgrade projects, alongside effort by ISIS to secure funding from government for the full Endeavour program.

OSIRIS updates

New low-noise detector electronics for the spectroscopy detector unit on OSIRIS are almost finished and will be ready for users after the long shutdown. In addition, the new Silicon analyser is under construction and will provide higher energy resolution from summer 2023 onwards.

Pressure cell for TOSCA

A new high-pressure cell for TOSCA, that makes the most of the recent guide upgrade, is ready for use. The cell allows measurements up to 1.7 GPa within a matter of hours with excellent signal to background. If you are interested in using this for the upcoming proposal round, please contact [Jeff Armstrong](#).

ISIS Call for Proposals for TS1 and TS2 Deadline: 20th April

Science Highlights

- [Hydrogen Detection Limits and Instrument Sensitivity of High-Resolution Broadband Neutron Spectrometers](#)
- [Understanding the ZIF-L to ZIF-8 transformation from fundamentals to fully costed kilogram-scale production](#)
- [Water in Deep Eutectic Solvents: New Insights From INS](#)
- [Dynamics & Spectroscopy with Neutrons—Recent Developments & Emerging Opportunities](#)
- [Density of Phonon States in Cubic Ice Ic](#)
- [Sodium diffusion and dynamics in Na₂Ti₃O₇: neutron scattering and ab-initio simulations](#)
- [Lattice Dynamics in Organic Ferroelectrics Using Neutron Spectroscopy and Ab-Initio Modeling](#)
- [A Ferrotoroidic Candidate with Well-Separated Spin Chains](#)
- [Diffusional Dynamics of Hydride Ions in the Layered Oxyhydride SrVO₂H](#)
- [Contrasting Effects of FA Substitution on MA/FA Rotational Dynamics in FA_xMA_{1-x}PbI₃](#)
- [Disentangling water, ion and polymer dynamics in an anion exchange membrane](#)
- [The intimate relationship between structural relaxation and the energy landscape of monatomic liquid metals](#)
- [Universality of Time–Temperature Scaling Observed by Neutron Spectroscopy on Bottlebrush Polymers](#)
- [Activated Transport in Polymer Grafted Nanoparticle Melts](#)
- [Characterisation of ethylene adsorption on model skeletal cobalt catalysts by INS and QENS](#)
- [Exploring ultra-fast proton dynamics in water under a static electric field](#)

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](#).