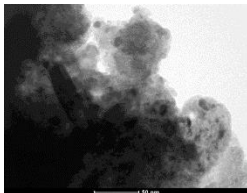


The newsletter of the ISIS Molecular Spectroscopy User Group

Staff news

We are pleased to announce that Stewart Parker has been appointed as our new group leader with Sanghamitra Mukhopadhyay as his deputy.

VESUVIO helps reveal the dynamics of the elusive hydrogen spillover



Hydrogen spillover is an elusive process, and its experimental and ab initio characterisation poses a serious challenge. In this work, the nuclear quantum dynamics of hydrogen in a palladium-decorated cubic polymorph of tungsten oxide, Pd/cWO₃, is described in terms of the hydrogen momentum distribution. Ab initio modelling of lattice dynamics yields theoretical predictions for the widths of proton momentum distributions in hydrogen-terminated beta-palladium hydride and hydrogen in acid centres (OH⁺ groups) on the surface of the cubic phase of tungsten oxide. This provides the contribution and the width of the momentum distribution of the quasi-free atomic hydrogen inside the saturated hydrogen bronze resulting from the spillover process.

QENS/WINS: Save the date!

We are delighted to announce that next years QENS/WINS will be jointly organised by ISIS and the IoP. It will take place in Manchester 10th – 14th June 2024. Please save the date and watch out for the official announcement that will be circulated shortly.

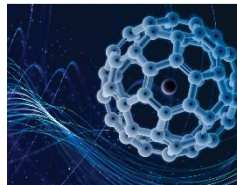
Data Analysis & Software

Mantid 6.8 will be released in early October. For details on what has changed please look [here](#). An online Users guide for MDANSE is available [here](#) describing how to use MDANSE in scripting mode and the up to date version of the software is available to download from [here](#). Users are requested to post any Mantid related bug reports to [Mantid Forum](#).

Forthcoming Events

- SiMolSpec, 30th Oct-1st Nov, 2023, Milton House, Didcot
- QENS/WINS 10th -14th June, 2024
- HiRes 2023 Synergies in High Resolution Spectroscopy (12-15 December 2023), ILL

Molecular Surgery on TOSCA features on the cover of PCCP



Recent work on TOSCA has been featured on the cover of PCCP. In this study, a complex set of reactions, known as "molecular surgery" allowed the inclusion of He within a C60 cage. This system represents a near perfect textbook example of the "particle in a box" scenario from quantum mechanics. The unique resolution and wide energy range on TOSCA allowed a direct comparison to theoretical models. These measurements were performed on milligram quantities of He, and could not have been performed on TOSCA before the massive flux gain granted by the TOSCA guide.

TS1 Neutrons

The last run cycle (26 June – 4 Aug) saw good running at both ISIS target stations. The methane moderator performed well, but the hydrogen moderator is still not operational. This means that IRIS, OSIRS, SURF, and LoQ are currently unavailable.

The investigations into the issues with the hydrogen system were successful and they were diagnosed. It is anticipated that the moderator will be replaced during the 2023 Christmas shutdown.

We would like to remind you that LET on TS2 also accepts QENS proposals and has polarisation analysis (PA) capabilities for QENS. For more information on PA here is a link to [two papers](#).

Endeavour Programme and MSG

ISIS has secured £90M for its Endeavour Programme and two MSG instruments will be benefitted from that. More information about the [Endeavour programme](#) and upgrade for Tosca+ and OSIRS+ will be found here.

Science Highlights

- [Untangling the Fundamental Electronic Origins of Non-Local Electron-Phonon Coupling in Organic Semiconductors](#)
- [Experimental and Modelling Studies of Local and Nanoscale *para*-Cresol Behaviour: A Comparison of Classical Force Fields](#)
- [Control of H-Related Defects in \$\gamma\$ -MnO₂ in a Hydrothermal Synthesis](#)
- [Quantum tunnelling rotor as a sensitive atomistic probe of guests in a metal-organic framework](#)
- [Cooperative Change in the Internal Dynamics of Streptavidin Caused by Biotin Binding](#)
- [Neutron Scattering Studies of Heterogeneous Catalysis](#)
- [Nuclear quantum dynamics in Hexamethylenetetramine and its deuterated counterpart: a DFT-augmented neutron study](#)
- [Hydrogen Spillover in Tungsten Oxide Bronzes as Observed by Broadband Neutron Spectroscopy](#)
- [A combined inelastic neutron scattering and simulation study of the ³He@C₆₀ endofullerene](#)
- [Online learning to train users of muons and neutrons at ISIS](#)

**[ISIS Call for Proposals for TS1&TS2](#)
Deadline: 17:00 18th October 2023**

Job & PhD Listings

- [VESUVIO Instrument Scientist](#)
- [VESPA Instrument Scientist](#)
- [Industrial placement student Raman Spectroscopy on TOSCA](#)
- [Industrial placement student Developing a DSC on IRIS](#)
- [Neutron and Muon Online Scientific Training Development Industrial Placement](#)

Please send any feedback for our group, to our User Group representatives, [A O'Malley](#) and [M. P. Marques](#).

Please inform us of your publications arising from ISIS related work. Remember to include ISIS staff as co-authors, when deemed appropriate, to cite instruments and software, and include a [DOI](#) for your experiment RB.