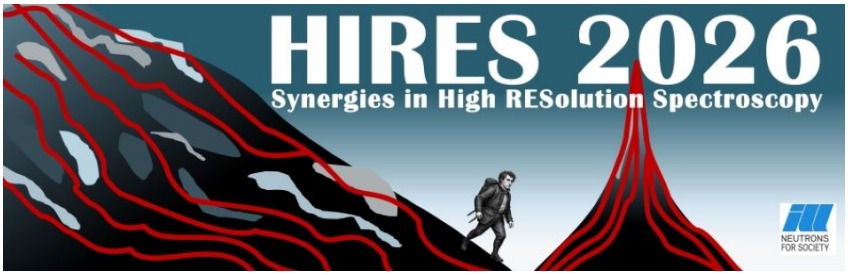

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Combining Inelastic Neutron Scattering with Nuclear Magnetic Resonance Spectroscopy for Molecular Hydrogen Endofullerenes

Endofullerenes consist of supramolecular complexes in which fullerene cages, consisting only of carbon atoms, completely confining single atoms or molecules, or in rare cases, multiple atoms or molecules. Endofullerenes are practical realisations of the classic "particle in a box" problem of quantum mechanics, in which confinement leads to energy quantization. We have studied the quantised translational-rotational dynamics of the confined H_2 molecules in the endofullerenes $H_2@C_{70}$ and $2(H_2)@C_{70}$. The allowed dynamical states of the endohedral hydrogens are heavily restricted due to the Pauli Principle. The effect of this is the existence of spin isomers and a metastable rotational state of H_2 at cryogenic temperatures. The translational and rotational excitations of these systems have been measured using IN5 and IN1-Lagrange spectrometers at the ILL-Grenoble.

In the INS spectrum we are able to directly observe transitions between corresponding translational and rotational states.

This measurement allows us to observe interactions between the protons which would be invisible to conventional solution state NMR. The complementary of the NMR experiments means we can deduce information about the positioning and orientation of the confined molecules within the fullerene cage. The combination of INS and NMR measurements allows the study of molecular confinement, spanning both the quantum and classical regimes.

Session

Hard Condensed Matter

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