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Molecular Spectroscopy, Computer Modelling and the State of the Art in INS spectroscopy for Energy Materials

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Molecular spectroscopy is a very powerful tool to study the dynamical properties of solid, liquid and gases. Inelastic Neutron scattering (INS) is a very powerful tool to study hydrogen-containing materials. With the development of neutron spallation sources, and the use of epithermal neutrons, inelastic neutron scattering can measure the vibrational spectra of materials on the whole range of vibrational motions (0-4400 cm−1) and effectively opening up the field of neutron spectroscopy [1]. The recently commissioned Lagrange instrument at the ILL, although based at a reactor source can also access up to similar energy transfers. With the new generation of neutron instruments, like the ones at the ESS it will be possible to expand the realm of INS spectroscopy to time resolved experiments and beyond hydrogen.

These sources have increased neutron fluxes and are making possible to increase the number of spectroscopic neutron studies of gas adsorption, catalysis, energy materials etc. Computer modeling is crucial in understanding and interpreting vibrational spectroscopy, in particular the correlation between model and experiment is bridged by the aClimax program [2].
In this paper I will present the state of the art in neutron scattering spectroscopy showing applications to study in-situ ammoniation reactions, metal hydrides for hydrogen storage applications [3] as well as CO2 and SO2 gas sequestration at source using MOFs [4]. I will also discuss the use of computer modeling to aid the interpretation of results and future science that will be possible when the ESS comes on-line.

References:
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