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Inelastic Neutron Scattering applied to porous materials

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Neutron scattering is a rare experimental technique because there are only a few places worldwide where it is
possible to perform the required experiments. The Spallation Neutron Source at ORNL in East Tennessee is the most advanced pulsed neutron source. The interaction of neutrons with the nuclei provides unique information on light elements (like hydrogen). It can distinguish between neighboring elements and isotopes, complementing X-ray capabilities and other photon-based techniques. In the case of Inelastic Neutron Scattering (INS), the technique is the neutron analog of Raman and infrared spectroscopies. Instead of using photons as the probing beam, a neutron beam illuminates the sample. The penetrating power of neutrons means that with the adequate selection of materials, it is possible to build sample environments that can manage extreme conditions in pressure and temperature without the need for optically transparent windows—giving the technique much versatility. Gas handling experiments are trivial. The main disadvantages of INS are that measurements usually require cryogenic temperatures, the neutron fluxes are low when compared with photons, and accessing neutron scattering facilities is challenging.
Atomistic computer modeling, particularly DFT, molecular dynamics, etc., is routinely used to interpret and analyze experimental results. The interplay of atomistic modeling and experimental data is unique and allows access to a precious insight into the mechanistic interpretation of the data.
Porous materials have space voids where it is possible to adsorb molecules. Trapping these molecules to "store" them or sometimes react chemically is used in many applications. This talk will present examples of INS spectroscopy applied to small molecule adsorption on porous
materials, with particular emphasis on hydrogen molecules. Materials from zeolites and carbons to metal-organic frameworks highlight the unique information the technique provides and how computer models are essential to interpreting the data.

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