INTERACTION OF MOLECULAR HYDROGEN WITH POROUS FRAMEWORKS STUDIED BY INS

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Understanding the properties of molecular hydrogen within restricted geometries is a requisite to improve the current hydrogen storage technologies. In particular, the understanding of the microscopic dynamics of molecular hydrogen within confinement, which is directly correlated to the interaction with the host. Inelastic neutron scattering (INS) has been a leading experimental technique to study physisorbed H_2 because it is a direct spectroscopic probe of the dynamics and local environment of H_2 molecule, providing valuable microscopic information on the effects of both surface interactions and confinement. In solid state, the molecular hydrogen shows rotational transitions. The lowest possible rotational transition (J=1 to J=0) has a characteristic energy of 14.6meV, known as the free rotor transition. Such transition is directly visible by an INS experiment and is affected by the local environment of the H_2 molecule (hindered rotor). Hence, following the rotational transition of H_2 can directly provide information about the confinement, local adsorption potential, and the dynamics of the H_2 molecule.

This talk will focus on the characterization of porous frameworks, i.e., metal-organic frameworks, as H2 adsorbents combining INS and adsorption isotherms. Two examples will be visited to demonstrate the potential of neutron vibrational spectroscopy to study such complex interactions. First, the effects on the thermodynamical stability of the adsorbed phase produced by the confinement in narrow pores. Second, the response of a flexible framework upon H2 adsorption.

Rafael Balderas-Xiconhténcatl recently started a postdoc at the Max Planck Institute for Intelligent Systems after finishing his first postdoc at the Chemical Spectroscopy group of Oak Ridge National Laboratory, paid directly by the Fuel Cell Technologies Office of the Department of Energy US DoE. He received his doctoral degree working in hydrogen adsorption in porous materials and isotope separation by Max Planck Institute for Intelligent Systems/Uni Stuttgart, Germany. He was born in Puebla, Mexico, received a Bachelor´s degree in Physics from the National Autonomous University of Mexico (UNAM) and a Master´s degree in Physics by Centre for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV), Mexico. His current research interests are focus on the study of the fundamental principles to develop energy sustainability such as hydrogen physisorption, as well as the development of efficient isotope separation technologies using porous materials.