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VABILO NA INŠTITUTSKO PREDAVANJE / INVITATION TO THE INSTITUTE LECTURE

Prof. Juergen Eckert

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petek / Friday, 29. 05. 2015, ob / at 11:00

v Preglovi seminarski sobi / Pregl Lecture room at the Pregl Research Centre, National Institute of Chemistry, Hajdrihova 19, Ljubljana

Potential Energy Surfaces for Hydrogen in Porous Materials Probed by Rotational Tunneling Spectroscopy

A detailed knowledge of the interactions responsible for binding hydrogen molecules in porous materials is essential for any further improvements of their hydrogen storage properties. Characterization of H_2 adsorption is almost exclusively carried by thermodynamic measurements, which only give average properties for all the sites occupied by H_2 molecules at a particular loading. One of the few molecular level experimental probes available is that of the observation of transitions between the hindered rotor energy levels of the adsorbed H_2 by inelastic neutron scattering spectroscopy. The lowest of these transitions may be described as rotational tunneling, and its observation provides extraordinarily fine detail on the interaction of molecular hydrogen with porous host materials, particularly when analyzed in conjunction with computational analysis on the potential energy surfaces, which govern the H_2 quantum rotations.

We have carried out an extensive series of computational studies on H_2 in several MOF's employing a general purpose materials sorption potential along with explicit many-body polarization interactions. The latter assisted in the determination of the binding sites through the distribution of the induced dipoles that led to strong adsorbate interactions, and was crucial in obtaining an accurate representation of the observed rotational transition frequencies. The results of our systematic spectroscopic and computational studies on a large number of porous materials provide detailed information on the effectiveness of hydrogen binding at different types of sites, and thereby could give direction for efforts in the synthesis of new materials with improved hydrogen interactions with hybrid porous materials.

This talk is based on a collaboration with Tony Pham of USF.

Vljudno vabljeni! / Kindly invited!

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