Neutron and Thermodynamic Studies of Hydrogen on Pd Decorated Metal Oxides

PAIGE LANDRY, University of Tennessee, A. RAMIREZ-CUESTA, ISIS, E. CRUZ SILVIA, B. SUMPTER, Oak Ridge National Lab, J.Z. LARESE, University of Tennessee — We report our investigations of thermodynamic, inelastic and quasielastic neutron scattering (INS and QENS) studies of H2 adsorbed on bare and Pd decorated metal oxide (MO) surfaces, specifically ZnO, SBA-15 silica, and alumina. Guided by our volumetric adsorption measurements, we used INS and QENS to probe the dynamics of the adsorbed hydrogen molecules. These measurements provide insight into how the microscopic behavior of hydrogen is changed when it is confined at interfaces or interacts with a Pd catalyst. Using INS, the motion of the adsorbed hydrogen are examined as a function of surface adsorbate composition. For rotational motion we use the ortho-to-para transition as a guide and find that the rotational barrier for H2 adsorbed on some of these MO surfaces shift to lower energy (relative to bulk H2). For comparison, the hydrogen adsorption and microscopic behavior when the MO are decorated with 1% Pd metal will be discussed. Evidence for the presence of adsorbed H2, Zn hydroxide and the potential role of spillover will be discussed. This work was partially supported by the U.S. DOE, BES under contract No. DE-AC05-00OR22725 with ORNL managed and operated by UT-Battelle, LLC, the NSF under grant DMR-0412231 and a grant from the University of Tennessee, JINS.