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Neutron, Thermodynamic, and Modeling Studies of Hydrogen Interaction with MgO(100) JOHN LARESE, University of Tennessee, L.L. DAEMEN, Los Alamos National Lab, J. OLLIVIER, T. SEYDEL, Institut Laue-Langevin, E. CRUZ SILVIA, B. SUMPTER, Oak Ridge National Lab — We report our investigations of thermodynamic, neutron diffraction, inelastic and quasielastic neutron scattering (INS and QENS) studies of hydrogen adsorbed onto MgO(100). Guided by our volumetric adsorption measurements, we used INS and QENS to probe the dynamics of the adsorbed H2 molecules. Our structural studies indicate that near monolayer completion the intermolecular distance of the H2 molecules on MgO are ∼20% more compressed than the closest packed bulk solid plane. The melting of this compressed solid takes place at temperatures above the bulk triple point, whereas most other 2D films melt at about 70% of the triple point. Using INS, the motion of the adsorbed hydrogen is examined as a function of film thickness. For rotational motions, we use the ortho-to-para transition as a guide and find that the rotational barrier for H2 adsorbed on MgO is shifted to lower energy at low surface coverage. These results are compared with modeling for additional insight into the microscopic processes that underpin the observed behavior. This work partially supported by the U.S. DOE, BES under contract 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 TN, JINS.

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