

Abstract Submitted
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Evidence of Near Surface Layer Stabilization by Liquid Multi-layer Adsorbed Films NICHOLAS STRANGE, J.Z. LARESE, Univ of Tennessee, Knoxville — Molecular adsorption on surfaces is fundamentally important in a variety of scientific and technological processes. Surface adsorption plays a key role in catalysis/catalytic supports, optoelectronic devices, lubrication and adhesion, wetting phenomena, and separations. We present the results of a comprehensive investigation of the first ten members of the homologous series of n-alkanes (methane-decane) adsorbed on the basal plane of hexagonal boron nitride using high-resolution, volumetric adsorption isotherm measurements (more than 30 separate temperatures per molecule). The experimentally determined heats of adsorption vs. carbon chain length follow the well-known “odd-even” behavior of the n-alkanes. While this may not be surprising we will illustrate additional potential surface configurations that can lead to an increase in entropy. Potential phase transitions are identified using changes in the 2D-compressibility. In addition, we describe the results of companion molecular dynamics modeling to provide microscopic insight to the wetting behavior as a function of alkane chain length and film thickness. A comparison with the behavior of the same n-alkane set on MgO and graphite will also be included. These studies can serve as the basis for developing accurate, robust models of the potential energy surfaces and can be used for future investigations of the microscopic structure and dynamics of these adsorbed films using neutron/xray diffraction and neutron spectroscopy.

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