

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Thermodynamic Studies of Decane on Boron Nitride and Graphite Substrates Using Synchrotron Radiation and Molecular Dynamics Simulations NICHOLAS STRANGE, University of Tennessee, THOMAS ARNOLD, MATTHEW FORSTER, JULIA PARKER, Diamond Light Source, J.Z. LARESE, University of Tennessee, UNIVERSITY OF TENNESSEE TEAM, DIAMOND LIGHT SOURCE COLLABORATION — Hexagonal boron nitride (hBN) has a lattice structure similar to that of graphite with a slightly larger lattice parameter in the basal plane. This, among other properties, makes it an excellent substrate in place of graphite, eliciting some important differences. This work is part of a larger effort to examine the interaction of alkanes with magnesium oxide, graphite, and boron nitride surfaces. In our current presentation, we will discuss the interaction of decane with these surfaces. Decane exhibits a fully commensurate structure on graphite and hBN at monolayer coverages. In this particular experiment, we have examined the monolayer structure of decane adsorbed on the basal plane of hBN using synchrotron x-ray radiation at Diamond Light Source. Additionally, we have examined the system experimentally with volumetric isotherms as well as computationally using molecular dynamics simulations. The volumetric isotherms allow us to calculate properties which provide important information about the adsorbate's interaction with not only neighboring molecules, but also the interaction with the adsorbent boron nitride.

Nicholas Strange
University of Tennessee

Date submitted: 15 Nov 2013

Electronic form version 1.4