Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Thermodynamic Studies of n-Octane Thin Films Adsorbed on Magnesium Oxide(100) DAVID FERNANDEZ-CANOTO, J.Z. LARESE, Oak Ridge National Laboratory — Thermodynamic properties of $n-$octane adsorbed on the MgO(100) surface were investigated using high-resolution adsorption isotherms in the temperature range of 225 K to 295 K. Two distinct adsorption steps were observed in all isotherms. The average area occupied by an n-octane molecule was estimated to be 139.1 $Å^2$. The temperature variation of the two dimensional compressibility was used to identify phase transitions near 265.9 K and 271.4 K for the first and second layers, respectively. COMPASS force field has been used to calculate the minimum energy configuration of a single n-octane molecule sited on the MgO (100) facet. Calculations suggest that the most likely configuration for the adsorbed molecule is with the carbon backbone parallel to the (100) plane, and with the center of mass atop the Mg^{2+} site. U.S. DOE, Materials Science Division under contract No. DE-AC05-00OR22725 with ORNL operated by UT-Battelle, LLC, and the NSF under grant DMR-0412231.

David Fernandez
Oak Ridge National Laboratory

Date submitted: 05 Dec 2007 Electronic form version 1.4