

Abstract Submitted  
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**Adsorption of Methane and Propane on a LJ Wall and on Molybdenum Surface: A Simulation Study** ALI ABU NADA, Southern Illinois University at Carbondale, GARY LEUTY, MESFIN TSIGE, University of Akron — Atomic-scale MD simulations were used to study multilayer adsorption as a function of temperature for two different alkanes ( $\text{CH}_4$  and  $\text{C}_3\text{H}_8$ ) on a fixed Lennard-Jones wall and on the (001) surface of molybdenum. In sets of simulations on the molybdenum surface, the substrate atoms were made to interact via a Lennard-Jones potential in one study and via an embedded-atom model (EAM) potential in the next. The results show that  $\text{CH}_4$  and  $\text{C}_3\text{H}_8$  on the flat wall possess a highly ordered packing arrangement exhibiting a higher degree of order than films adsorbed on the molybdenum substrate. Additionally, the number of ordered layers seen in the case of adsorption of  $\text{CH}_4$  was noted to be greater than the number of ordered layers in the case of adsorption of  $\text{C}_3\text{H}_8$ . In each case, the first layer appears frozen, implying there is no translational motion for the molecules in this layer, and we can confidently surmise that the first adsorbed layer exists in the solid phase far above the bulk melting temperature.

Ali Abu Nada  
Southern Illinois University

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