EXPLICIT – HYDROGEN MOLECULAR DYNAMICS SIMULATIONS OF VARIOUS ALKANES ON GRAPHITE AT SUBMONOLAYER COVERAGES: TOWARDS PERCOLATION

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Abstract

Alkanes are a family of carbon chain molecules with many industrial uses, such as lubrication, adhesion, detergent manufacture and crude oil refining, to name a few. When placed on surfaces, such molecules can exhibit novel and interesting behavior. Much insight can be gained from computer simulation of real systems, but alkanes on surfaces have been studied by modeling efforts mainly when the layer is complete. When the layer is not complete, it can have vacancies and may even form connecting (percolating) networks over the surface which can affect the thermodynamics of the system greatly and in novel ways. In this study we present initial results for pentane and hexane, and discuss the significance of studying alkanes with varying chain length.

Acknowledgment is made to the Donors of The American Chemical Society Petroleum Research Fund (PRF43277-B5), and the University of Missouri Research Board, for the support of this research. This material is based upon work supported in part by the Department of Energy under Award Number DE-FG02-07ER46411. The authors acknowledge useful discussions with Haskell Taub and Flemming Hansen.

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