

# Molecular Dynamics Simulations of Hexane Deposited onto Graphite: An Explicit-Hydrogen Model at $\rho = 1$

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*Received: January 15, 2007*

*Accepted: March 19, 2007*

## ABSTRACT

We present the results of parallel Molecular Dynamics computer simulations of hexane ( $C_6H_{14}$ ) adlayers physisorbed onto a graphite substrate in the density range  $0.5 \leq \rho \leq 1$  in units of monolayers, with emphasis on monolayer completion ( $\rho = 1$ ). The hexane molecules are modeled to explicitly include hydrogens and the graphite is modeled as a six – layer all atom structure. In the explicit hydrogen simulations, the herringbone solid loses its orientational order at  $T_1 = 140$  °K, fairly consistent with results of UA simulations. However there is almost no nematic meso-phase or negative energy change at the loss of herringbone order. The explicit hydrogen melting temperature is  $T_2 = 160$  °K—somewhat lower than seen in experiment and in UA simulations. Generally, results for the all-atom model agree well with experiment, as the molecules remain overall flat on the substrate in the solid phase. At densities below about  $\rho = 0.875$  the system supports a connected network which stabilizes it against thermal fluctuations and yields much more reasonable sub-monolayer- melting behavior. The united atom picture, on the other hand, departs significantly from experiment at most sub-monolayer- densities and gives melting temperatures several decades below what is experimentally observed. The purpose of this work is to compare the results of UA and explicit hydrogen MD simulations of hexane on graphite mainly at  $\rho = 1$ , to discuss cursory explorations at sub-monolayer- densities and mention open questions related to the system that are worth pursuing. Various structural and thermodynamic order parameters and distributions are presented in order to outline such differences.

## I. INTRODUCTION

Extensive Molecular Dynamics (MD) studies of hexane on graphite using the United Atom (UA) approximation have provided a framework for advancing our understanding of physisorbed alkanes. In

the UA approximation, methyl ( $CH_3$ ) and methylene ( $CH_2$ ) pseudo-atoms replace the actual corresponding functional groups in a molecule. The main utility of such an approximation is a considerable savings of computational effort. Because of the highly anisotropic nature of the hexane molecule