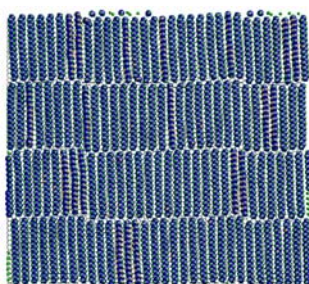


Physics Colloquium

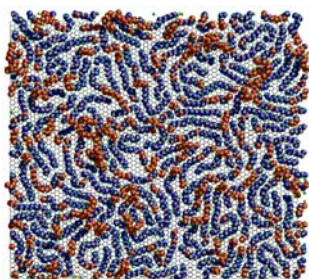
UNIVERSITY OF MISSOURI-KANSAS CITY
DEPARTMENT OF PHYSICS

Professors Lucyna Firlej & Bogdan Kuchta
Department of Physics & Astronomy
University of Missouri-Columbia

Modeling of alkanes adsorbed on graphite



We present Molecular Dynamics (MD) simulations of tetracosane ($C_{24}H_{50}$) monolayer physisorbed on graphite. $C_{24}H_{50}$ molecules are simulated with explicit hydrogens and the graphite is represented by six graphene layers. We show that the all atom representation of $C_{24}H_{50}$ is much more sensitive to the model of intramolecular interactions than united atom model. In particular two components: electrostatic forces and scaled 1-4 internal non-bonded interactions can shift melting temperature by several tenths of degree.



We focus our analysis on the microscopic mechanism of melting, experimentally observed at 340 K. We are looking for the pre-melting transformations and analyze if there is a correlation between translational disordering of molecules and their internal degrees of freedom. We analyze several order parameters and their fluctuations along the MD trajectories and show that correlation between molecular stiffness and the intermolecular forces causes molecules' footprint reduction during melting which involves a simultaneous lost of intramolecular and translational order. This cooperative mechanism is related to an abrupt increase of gauche defects within the central region of the chain.

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September 26, 2008

Coffee at 3:10, Colloquium at 3:30 in Room 310