ALL - ATOM MOLECULAR DYNAMICS SIMULATIONS OF TETRACOSANE (C24H50)
MONOLAYERS ADSORBED ON GRAPHITE

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Abstract

Results of massively parallel Molecular Dynamics (MD) computer simulations tetracosane (C24H50) monolayers physisorbed onto the basal plane of graphite are discussed. The adlayer molecules are simulated with explicit hydrogens, and the graphite substrate is represented as an all-atom structure having six graphene layers. The low-temperature ordered solid organizes in a rectangular centered structure, presenting lamellae and being incommensurate with the underlying graphite. Above T = 200 K, as the molecules start to lose their translational and orientational order via gauche defect formation, a weak smectic mesophase (observed experimentally but never reproduced in United Atom (UA) simulations) appears and the lamellae disorder. Then, at a little above T = 350K the system melts in concert with molecule deformation. The behavior of the adsorbed layer is critically sensitive to the way the electrostatic interactions are included in the model, and changes in the electrostatic scaling factor can alter the melting temperature by decades of degrees. An optimal scaling factor is discussed.

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