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 simu-lated 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, pre-senting lamellae and being incommensurate with the underlying graphite. Above T = 200 K, as the mole-cules 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 de-formation. The behavior of the adsorbed layer is critically sensitive to the way the electrostatic interac-tions are included in the model, and changes in the electrostatic scaling factor can alter the melting tem-perature by decades of degrees. An optimal scaling factor is discussed.

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