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Improved Molecular Dynamics simulations of hexane on graphite near monolayer completion[1] M.W. ROTH, M.J. CONNOLLY, University of Northern Iowa, CARLOS WEXLER, University of Missouri - Columbia, PAUL A. GRAY, University of Northern Iowa — We present the results of computer simulations of hexane on graphite near monolayer completion utilizing NAMD Scalable Molecular Dynamics in parallel computing environments. We include hydrogens explicitly on the hexane molecules, and the graphite substrate is represented as six all - atom graphene sheets. Results presented for temperatures between T = 100 K and T = 200 K have features which differ from those obtained using the united Atom (UA) model, where hydrogens are suppressed. Various structural and thermodynamic quantities show that the improvement obtained from explicitly including hydrogens come not only from their interaction with the substrate but also by their manipulation of in - plane space.

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