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Molecular dynamics simulations of hexane on graphite at various coverages: the difference explicit hydrogens make

[1] M.W. ROTH, M.J. CONNOLLY, University of Northern Iowa, Department of Physics, PAUL A. GRAY, University of Northern Iowa, Department of Computer Science, CARLOS WEXLER, University of Missouri Columbia, Department of Physics and Astronomy — Molecular Dynamics simulations of hexane (C_6H_{14}) adlayers on graphite are carried out for coverages of $0.5 \leq \rho \leq 1$ monolayers. The hexanes have explicit hydrogens and the graphite is modeled as an all – atom, six – layer structure. Above $\rho \cong 0.9$ the herringbone solid loses orientational order at $T_1 = 140$ K $\pm$ 3 K. At $\rho = 0.878$ the system presents vacancy patches and T_1 decreases to ca. 100 K. As coverage decreases further, the vacancy patches become larger and by $\rho = 0.614$ the solid is a connected network of randomly oriented domains. All cases show a weak nematic mespohase. The melting temperature is $T_2 = 160$ K $\pm$ 3 K and falls to ca. 145 K by $\rho = 0.614$. The dynamics and energetics observed demonstrate that the explicit-hydrogen model of hexane is substantially more realistic than the UA approximation.

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