Abstract Submitted
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Molecular Dynamics computer simulations of hexane on graphite at submonolayer coverages[1] M.J. CONNOLLY, University of Northern Iowa, CARLOS WEXLER, University of Missouri - Columbia, M.W. ROTH, PAUL A. GRAY, University of Northern Iowa — Results of Molecular dynamics computer simulations of hexane on graphite at submonolayer densities are presented. Two models are utilized; the first is a united atom (UA) representation which suppresses hydrogen atoms and the second is NAMD Scalable Molecular Dynamics in parallel computing environments with explicit hydrogens. Large UA systems having N = 1008 molecules and smaller (N = 112) explicit - hydrogen systems both show three distinct regimes: vacancy dominated at higher densities, a connected network at intermediate densities and individual islands at low densities. Various structural and thermodynamic quantities are utilized to understand how the systems behavior correlated to the topology it exhibits.

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