Abstract Submitted
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All-atom Molecular Dynamics simulations of partial pentane and hexane films on graphite[1] M. KASPAR, M.W. ROTH, University of Northern Iowa, CARLOS WEXLER, University of Missouri, L. FIRLEJ, Université Montpellier, B. KUCHTA, Université de Provence — We compare the self-assembly patterns of pentane (C_5H_{12}) and hexane (C_6H_{14}) adlayers physisorbed onto graphite at various coverages using the results of molecular dynamics simulations. Near monolayer coverage, the solid low temperature structure of the pentane film is nematic-like, and that of hexane-herringbone-like. At submonolayer coverages both systems exhibit three distinct topological regimes: vacancy patches at higher densities, percolating networks at intermediate densities and ultimately individual patches. The systems' orientational behavior and melting dynamics is discussed with respect to its unique density-dependent topology. The simulations explicitly include hydrogens of pentane and hexane and the graphite is modeled as a six-layer all atom structure.

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