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Phase Transitions in Hexane Physisorbed onto Graphite[1] CARLOS WEXLER, MICHAEL ROTH, University of Northern Iowa, CARY PINT, University of Northern Iowa — We report the results of molecular dynamics (MD) simulations of hexane physisorbed onto the basal plane of graphite. At low temperatures the system forms a herringbone solid. For monolayer coverages a solid to nematic liquid crystal transition takes place at $T_1 = 138 \pm 2$K followed by another transition at $T_2 = 176 \pm 3$K into an isotropic fluid. We characterize the different phases by calculating various order parameters, coordinate distributions, energetics, spreading pressure and correlation functions, most of which are in reasonable agreement with available experimental evidence. In addition, we perform simulations where the Lennard-Jones interaction strength, corrugation potential strength and dihedral rigidity are varied in order to better characterize the nature of the two transitions through. We find that both phase transitions are facilitated by a "footprint reduction" of the molecules via tilting, and to a lesser degree via creation of gauche defects in the molecules. Furthermore, submonolayer coverages see a diminished role for the nematic phase, whereas supramonolayer coverages present a more robust nematic.

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