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Simulated Effects of Odd-Alkane Impurities in a Hexane Monolayer on Graphite CARY L. PINT, M.W. ROTH, Department of Physics, University of Northern Iowa — We present the results of molecular dynamics (MD) simulations of odd alkane impurities present within the hexane (even alkane) monolayer. We simulate a series of temperatures at 3%, 5%, 10%, and 15% impurities of propane (C_3H_8), pentane (C_5H_{12}), heptane (C_7H_{16}), nonane (C_9H_{20}), and undecane ($C_{11}H_{24}$) to study both the changes in the monolayer structure and the phase transitions when odd alkanes, whose low-temperature solid structure has been experimentally observed to be much different than that of hexane, occupy space within the hexane monolayer in the low-temperature herringbone (HB) phase. We find that the most significant changes in the melting transition are imposed by impurities whose chain lengths are much different than that of hexane, and the impurities whose chain lengths most closely resemble hexane still give a melting temperature that is within 10K of the pure hexane monolayer melting temperature at high impurity composition. However, due to "lattice misfits," we find that the transition into the intermediate phase exhibits drastic changes as compared to the pure hexane monolayer with the exception of pentane impurities, whose optimal impurity chain length allows the monolayer to exhibit a commensurate phase that is similar to the hexane monolayer, even with a high impurity composition.

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