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# Simulated effects of odd-alkane impurities in a hexane monolayer on graphite

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We present the results of molecular-dynamics simulations of odd-alkane impurities present within the hexane (even alkane) monolayer. We simulate various temperatures at approximately 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 ($C_{11}H_{24}$), each having a low-temperature solid phase belonging to a different space group as compared to hexane, to study the effects of impurities on the various phases and phase transitions for hexane monolayers that are well characterized through previous experimental and theoretical work. Based upon preferential adsorption, we provide two emerging pictures of how impurities could affect the monolayer, for impurity chain lengths longer and shorter than that of the hexane molecules. We provide evidence that impurities in the monolayer, even in small proportion to the hexane, could induce significant changes in the phase behavior and phase transitions, and we propose that because of the size of pentane

with respect to hexane, and the nature of the solid herringbone (HB) phase, pentane impurities give the best representation of the phase behavior observed for the pure hexane monolayer. We find that impurities with chain lengths longer than hexane tend to distort the sublattices of the solid HB phase, and hence lead to a phase transition into an "intermediate" phase significantly prior to that observed for a pure hexane monolayer. We discuss possible application of our results toward experiment, as we find that extremely small amounts of impurities in the monolayer often induce significant changes in phase-transition behavior. 

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