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Molecular Dynamics simulations of tetracosane ($C_{24}H_{50}$) bilayers physisorbed onto the basal plane of graphite[1] MICHAEL ROTH, E. MALDONADO, University of Northern Iowa, L. FIRLEJ, LCVN, Université Montpellier 2, B. KUCHTA, Laboratoire Chimie Provence, Université de Provence, CARLOS WEXLER, University of Missouri Department of Physics and Astronomy — We present and discuss the results of explicit - hydrogen Molecular Dynamics computer simulations of tetracosane ($C_{24}H_{50}$) bilayers deposited on a graphite substrate in the temperature range 100 K $\leq \quad T \leq$ 450 K. Both layers exhibit strong coupling between the internal molecular degrees of freedom and bulk behavior but because of the different boundary conditions between layers, they exhibit distinctly different dynamics and phase transition signatures. Structural, thermodynamic and bond - orientational distributions and parameters are utilized in understanding the solid, intermediate and liquid phases presented in and phase transitions presented by the system.

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