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Molecular Dynamics simulations of perpendicular tetracosane films¹ MICHAEL ROTH, University of Northern Iowa, CARLOS WEXLER, University of Missouri - Columbia — We present the results of Molecular Dynamics computer simulations of perpendicular tetracosane ($C_{24}H_{50}$) films adsorbed onto a bilayer of tetracosane on graphite in the temperature range [100K, 500K]. Various structural and thermodynamic quantities are utilized to characterize the system's temperature evolution. The system goes from the low – temperature solid phase supporting a perpendicular third layer to the collapse of the perpendicular film near $T = 300K$ to a dense, coalesced patch at high temperature.

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