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Tetracosane ($C_{24}H_{50}$) trilayers physisorbed onto the basal plane of graphite: perpendicular patches[1] MICHAEL ROTH, 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 — Results of explicit - hydrogen Molecular Dynamics computer simulations of tetracosane ($C_{24}H_{50}$, or C24) trilayers deposited on a graphite substrate in the temperature range 100 K $\leq \quad T \quad \leq$ 550 K are presented. The third layer is perpendicular to the alkane underlayers as well as to the graphite substrate. Diffusion thakes place predominantly at the bottom of the patch through a ratcheting mechanism that is coupled to dihedral (torsional) defects. In the low - temperature solid the patch exhibits a dome - like shape and, with increasing temperature rolling of the interior molecules couple to the collapse of the patch into a droplet - like shape and, ultimately a liquid C24 patch atop the graphite layer results. Structural, thermodynamic and bond - orientational distributions and parameters are utilized in understanding the temperature evolution of the system and results are compared to those under the United Atom approximation.

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Michael Roth
University of Northern Iowa

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