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**Tetracosane ( $C_{24}H_{50}$ ) trilayers physisorbed onto the basal plane of graphite: perpendicular patches<sup>1</sup>** MICHAEL ROTH, University of Northern Iowa, L. FIRLEJ, LCVN, Universit Montpellier 2, B. KUCHTA, Laboratoire Chimie Provence, Universit 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  $100\text{ K} \leq T \leq 550\text{ K}$  are presented. The third layer is perpendicular to the alkane underlayers as well as to the graphite substrate. Diffusion takes 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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- Prefer Oral Session  
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