

Abstract Submitted
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The role of local domain formation in the melting of hexane adlayers on graphite¹ M.W. ROTH, Univ. of Northern Iowa, L. FIRLEJ, B. KUČHTA, C. WEXLER, Univ. of Missouri — Hexane is the shortest alkane [$\text{CH}_3-(\text{CH}_2)_{n-2}-\text{CH}_3$] whose flexibility has any considerable impact on its dynamics. When adsorbed on graphite, a monolayer of hexane melts at a temperature of approximately 175 K. To understand the mechanisms of this transition we have performed large scale molecular dynamics simulations (several runs over 100 ns, total computation time ~ 10 cpu-years), using the most realistic model of the system (a fully atomistic representation of hexane, explicit site-by-site interaction with graphite carbons and CHARMM force field with carefully chosen adjustable parameters of interactions). We show that the melting of the low temperature herringbone solid phase starts with the formation of gauche defects at the ends of neighboring molecules, followed by molecular reorientation within a lamellae, without perturbing the overall structure of the adsorbed film. The melted phase has a domain-type structure with domains' orientation that reflects the 6-fold symmetry of graphite. The size of domains decreases progressively when the temperature increases and the deformation of molecules to quasi globular shape is driven by progressive formation of gauche defects.

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Carlos Wexler
University of Missouri

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