Condensed Matter Physics

MOLECULAR DYNAMICS COMPUTER SIMULATIONS OF PARTIAL HEXANE AND PENTANE ADLAYERS DEPOSITED ON GRAPHITE, M.W. Roth[1*], M. Kaspar,[1] Carlos Wexler[2] , L. Firlej[3] , B. Kuchta[4] and Paul A. Gray[5], *[1]Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614, [2]Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, [3]LCVN, Université Montpellier 2, 34095 Montpellier, France, [4]Laboratoire Chimie Provence, Université de Provence, 13396 Marseille, France, [5]Department of Computer Science, University of Northern Iowa, Cedar Falls, IA 50614 Faculty sponsor email: rothm@uni.edu*

We discuss results of Molecular Dynamics computer simulations of hexane (C_6H_{14} , or C6) and pentane (C_5H_{12} , or C5) adlayers deposited onto a graphite substrate for various coverages below monolayer completion. The alkane molecules incorporate explicit hydrogens and the graphite is modeled as a six–layer all atom structure. Both systems present four distinct topological regimes involving empty space: at densities closest to full coverage there are large domains with individual vacancies, then with decreasing density, large vacancy patches appear first, followed by formation of connected networks of smaller domains with multiple orientations that ultimately separate into individual patches. The physical behavior of the systems is related to their topological behavior.

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