

Abstract Submitted
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Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces HENDRIK HEINZ, University of Akron, RICHARD A. VAIA, BARRY L. FARMER, Air Force Research Laboratory, WPAFB — Characterization through experiment and simulation shows that the orientation of the alkyl layers and reversible phase transitions on heating are a function of the cross-sectional area of the alkyl chains in relation to the available surface area per alkyl chain (packing density). On even surfaces, a packing density less than 0.2 leads to nearly parallel orientation of the alkyl chains on the surface, conformational disorder, and no reversible melting transitions. A packing density between 0.2 and 0.75 leads to intermediate inclination angles, semi-crystalline order, and reversible melting transitions on heating. A packing density above 0.75 results in nearly vertical, lattice-like alignment of the surfactants on the surface and no reversible melting transitions. The same principle applies to curved surfaces, taking into account a local radius of curvature and a distance dependent packing density on the surface. The chain length (minimum C10) and interface chemistry have little impact on this behavior but determine chemical functionality and transition temperatures.

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