

Steady Packing, Changing Friction: Simulations of Confined Semi-Ordered Monolayers under Shear

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Molecular simulations were conducted on confined films of surfactant-like molecules. Parameters were chosen such that one chain end was more strongly attracted to the surface than the remainder of the molecule, leading to adsorbed packing perpendicular to the surface. Long-range order at levels intermediate between that of a liquid and a solid was maintained over times longer than 5 ns in directions both perpendicular and parallel to the surface, and the ordering was strikingly independent of sliding velocity (0–7.5 m/s). Friction force, in contrast, increased with sliding velocity for systems in which one or two fluid layers were confined between the perpendicularly adsorbed films. A fluctuation analysis of the density profile revealed regions with differing amounts of flexibility, especially near the boundary between the adsorbed film and additional confined fluid.