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The Role of Confinement-induced Ordering on the Slow Dynamics of Confined Fluids[1] JIANPING GAO, W.D. LUEDTKE, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Grand canonical molecular dynamics simulations have been performed to study molecular diffusion in confined thin liquid films. Thin liquid films (modeled as spherical LJ particles) confined by atomically flat, or rough, gold surfaces are studied, and their properties are compared. This includes layering, in-layer ordering, solvation forces and in-plane molecular diffusion. Atomic-scale roughness, with a rms roughness of about 2 Angstroms, significantly reduces ordering in the confined fluid and quenches the oscillations in the solvation forces. Molecular diffusion remains high for films with a thickness as small as four molecular widths. For atomically flat surfaces where the thin films form well defined layers, sharp slowdown of the molecular diffusion correlates well with the occurrence of in-layer ordering.

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