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Crossover in the local diffusive dynamics of equilibrium and supercooled confined fluids JONATHAN BOLLINGER, THOMAS TRUSKETT, University of Texas at Austin — Confined fluids are ubiquitous in natural and technological contexts, and relating emergent structural motifs to dynamics is critical to facilitate the inverse design of nano- and micro-fluidic systems. Crucially, such thin film systems are frequently tuned between equilibrium and glassy states, as during, e.g., processing of polymer thin films. We use molecular dynamics simulations and a Fokker-Planck equation based method to examine the position-dependent diffusive dynamics of binary hard-sphere fluids confined to slit pores that are designed to mimic realizable thin films [Nugent et al. PRL 2007, 99]. At moderate densities, local single-particle mobilities normal to the direction of confinement are higher in regions of high local packing fraction. However, as the average packing fraction is increased into the supercooled regime, this local positive correlation between packing fraction and mobility is reversed. We discuss the outlook for a universal mechanistic framework that can unite these disparate local correlations between packing and mobility and also predict average diffusivities of the inhomogeneous fluids. Auxiliary measurements of the simulated films suggest that this behavioral dichotomy should also emerge in structurally similar experimental colloidal suspensions.

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