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Counterintuitive connection between layering and mobility in confined fluids GAURAV GOEL, WILLIAM KREKELBERG, University of Texas at Austin, JEFFREY ERRINGTON, State University of New York at Buffalo, THOMAS TRUSKETT, University of Texas at Austin — Fluids confined to narrow spaces adopt a spatially inhomogeneous distribution of density due to the interactions between the fluid particles and the boundaries. This “density profile” is the most common measure of inhomogeneous structure in confined fluids, but its connection to fluid transport coefficients is poorly understood. We explore via molecular simulations how tuning particle-wall interactions to flatten or enhance the particle layering of a model Weeks-Chandler-Andersen (WCA) confined fluid impacts its self-diffusivity, viscosity, and entropy. Counterintuitively, interactions that eliminate particle layering significantly reduce confined fluid mobility, while those that enhance layering have the opposite effect. Excess entropy helps to both understand and predict these trends.

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