A Systematic, Multiscale Approach to Simple Liquid-State Property Models

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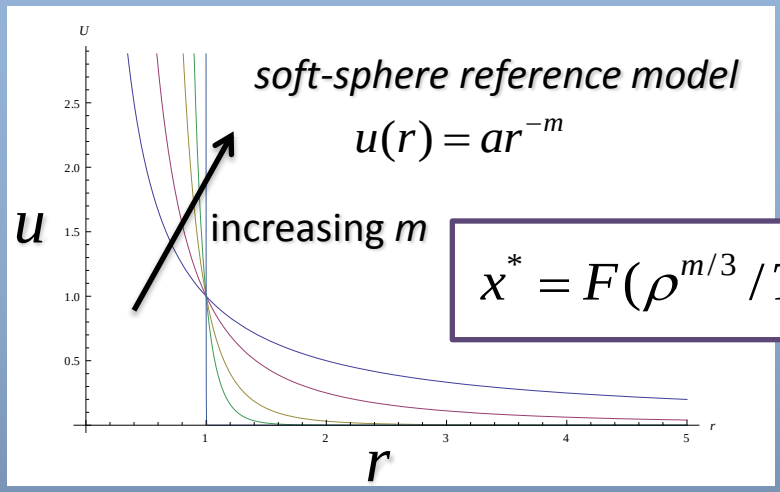
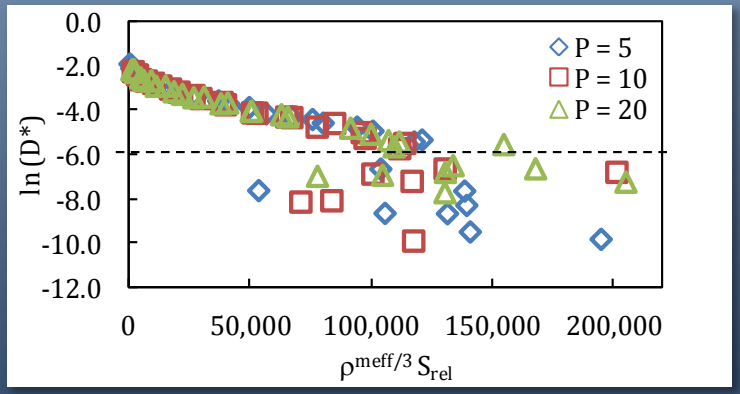
Understanding the determinants and behavior of liquid-state transport coefficients like diffusivity and viscosity is essential to quantitative modeling in the chemical process industries. Recent efforts show promise for predicting such dynamics by mapping complex molecular systems to much simpler, analytically-tractable reference "soft-sphere" systems with purely repulsive interparticle interactions. We use a novel strategy to "coarse-grain" arbitrarily complex liquids to effective soft sphere ones, which provides an exciting new way to predict their dynamic behavior.



Soft spheres interact through a pairwise inverse power law repulsion, and their appropriately-normalized transport coefficients are unique functions of the single thermodynamic variable $\rho^{m/3}/T$.



The density-scaled relative entropy predicts the diffusion constant over a wide range of state conditions above the supercooled regime.

$$\min_{\{a,m\}} S_{rel} \rightarrow \text{effective scaling exponent } m$$

Complex molecular architectures are mapped to soft spheres by minimizing the relative entropy, which quantifies the latter's relevance as a simple model.