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

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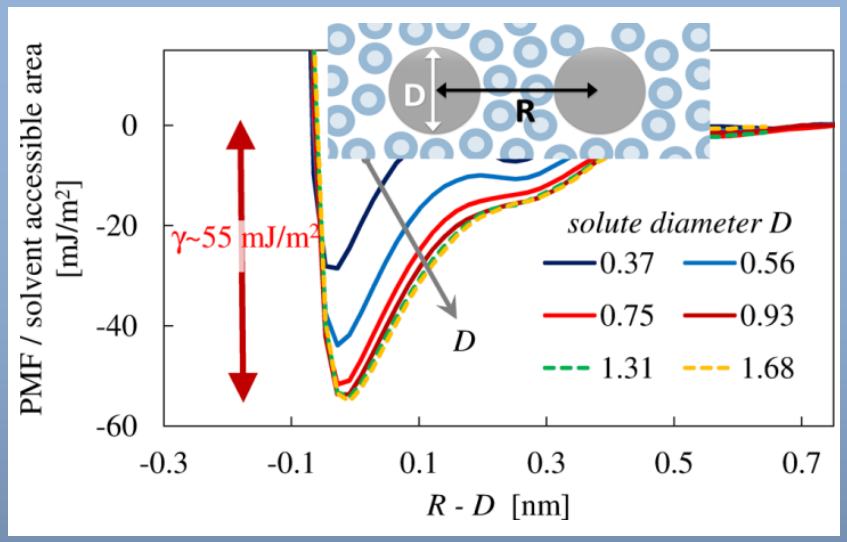
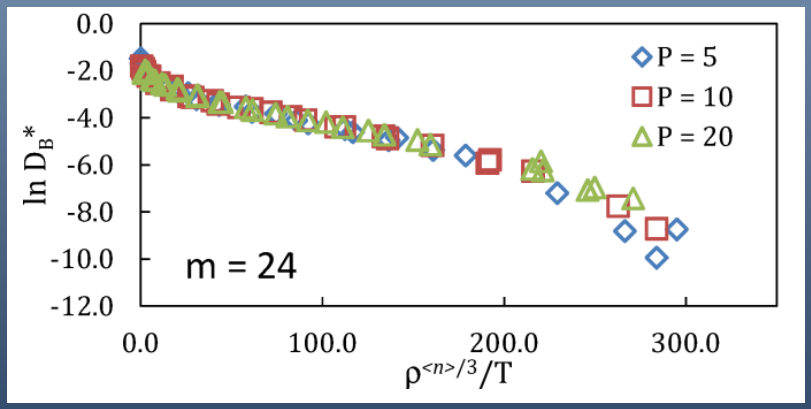
New theories of the liquid state can be achieved through systematic coarse-graining techniques. We use a novel relative entropy approach for building simple liquid models that minimizes information loss upon coarse-graining. (1) We show that the approach predicts temperature-density scaling laws for transport coefficients by coarse-graining arbitrary systems to soft-spheres. (2) We develop a simple, isotropic, core-softened model of water that successfully captures small and large scale behavior of the hydrophobic force law, offering a natural simulation-experiment link.



A coarse water model predicts the scale-dependence of the hydrophobic force law. The area-normalized potential of mean force (PMF) agrees with experimental water-hydrocarbon surface tensions for large solutes.



The relative entropy predicts soft-sphere scaling laws for Lennard-Jones mixtures that capture the diffusion constant over a wide range of conditions.

complex all-atom model

$\min S_{rel}$

simplified model

(e.g., soft spheres or isotropic water)

Complex molecular architectures are mapped to simple models by minimizing the relative entropy.