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An Improved Lattice Gas Model of the Hydrophobic Effect
PATRICK VARILLY, AMISH PATEL, DAVID CHANDLER, UC Berkeley — Biological systems are characterized by length scales where the hydrophobic effect crosses over from being dominated by volume exclusion to being dominated by interface formation. This crossover behavior, successfully described by Lum-Chandler-Weeks theory, precludes modeling the hydrophobic contribution to solvation free energies of solutes by an effective surface area term, as is done in GBSA-style implicit solvent models in common use in the biological community. Instead, what is needed is a dynamical model of the hydrophobic effect that explicitly captures this crossover behavior, yet is simple enough for use in a biological context. In this work, we extend the simple lattice gas model of ten Wolde and Chandler by correcting its salient deficiencies at small and large length scales. We demonstrate good agreement between our model and explicit-water simulations, particularly at the crossover length scale, and then proceed to apply the theory to model several instances of hydrophobic assembly in biologically-motivated systems.

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