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Modeling the hydrophobic effect by coupling solutes to a lattice gas AMISH PATEL, DAVID CHANDLER, University of California, Berkeley — In problems of biological assembly, manifestation of the hydrophobic effect is complex depending on the size as well as the conformation of the solute. The solute disrupts the inherent structure of the solvent by causing an unbalancing of attractive interactions experienced by the solvent molecules The extent of this disruption determines the relative ease with which the solute is solvated. The theory of Lum, Chandler and Weeks (LCW) successfully describes this rich interplay between the solute and solvent structures by coarse-graining the solvent density and analytically integrating out solvent fluctuations on length-scales smaller than the coarse-graining length (L_c). Since the implementation of LCW theory can be computationally very demanding the coarse-grained solvent density was mapped onto a lattice gas by ten Wolde, Sun and Chandler. In this work, we further improve upon the theory by relaxing certain assumptions about the unbalancing of attractive interactions on length scales smaller than L_c. In addition to a brief overview of the theory, results obtained by application of the theory to several pertinent problems of hydrophobic assembly will be presented.

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