Implicit Models for Short-Range Contributions to Solvation Energies from Exchange Repulsion, Dispersion Attraction, and Hydrogen Bonding

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Implicit models can provide a very efficient and reasonably accurate estimation of solvation energies for use in conjunction with electronic structure calculations on solutes. For polar solutes in polar solvents the solvation energies are dominated by long-range electrostatic effects that can now be treated by a variety of well-established implicit methods based on classical dielectric continuum theory. However, additional short-range contributions between solute and first-shell solvent molecules that are generally not well described by dielectric models can also make significant contributions, and may become dominant if either the solute or the solvent is nonpolar. We describe here recent successful efforts to obtain implicit models for short-range interactions between solute and solvent arising from exchange repulsion, dispersion attraction, and hydrogen bonding. These new models are easy to implement, and used in conjunction with dielectric continuum methods lead to good estimations over a large data set of experimental solvation energies.