Implicit Models of Short-Range Solvation Effects

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Solvation energies strongly influence the thermodynamic and reactive properties of chemicals in solution. Implicit solvation models have been found to be very useful for quick semiquantitative estimates of solvation energies. This category includes dielectric continuum theories, which account for the important long-range electrostatic interactions of polar solutes in polar solvents.

In addition to such bulk dielectric effects, various short-range interactions are usually also significant, such as dispersion attraction, exchange repulsion, cavitation, and hydrogen bonding among others. We are developing implicit models for these short-range effects to be used in conjunction with existing dielectric continuum models in order to obtain a more complete description of solvation. It has very recently been found that hydrogen bonding energies are proportional to the extrema of the electric field the solute presents to solvent on the surface of the cavity separating them. A report will also be given of progress on finding simple descriptors of dispersion and exchange interactions.