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Implicit solvent model for density functional theory calculations
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don — There has been a considerable amount of work in developing simulation
techniques for processes in solution. Implicit solvation is one such method which
成功fully addresses the difficulty of achieving a reliable statistical average over the
many solvent degrees of freedom, and this property makes it the prime candidate
for use within efficient density functional theory (DFT) calculations on biological
systems. The implicit solvation method replaces the complex arrangement of solvent
molecules with a continuous polarizable medium with the intention of replicating the
electrostatic response of the bulk solvent. The method we have implemented uses
the electron density to describe the solvation cavity and thus departs from standard
implicit solvation methods which are burdened by a large number of parameters
to define the solvent cavity. We present the validation of this model through the
calculation of energies of solvation, as well as an investigation of the solvation effect
on NMR chemical shifts of small biologically relevant molecules.

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