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Implicit solvent model for density functional theory calculations
HATEM HELAL, MIKE PAYNE, Cavendish Laboratory, University of Cambridge, ARASH A. MOSTOFI, Department of Physics and Materials, Imperial College London — There has been a considerable amount of work in developing simulation techniques for processes in solution. Implicit solvation is one such method which successfully 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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