Polarizable embedding for biological systems: Modeling photoactive proteins with the Effective Fragment Potential method

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Accurate description of solute-solvent interactions is a key for understanding photochemical processes in biological systems. The effective fragment potential (EFP) is a polarizable model providing rigorous description of non-covalent interactions from first principles. When coupled to a QM region, hybrid QM/EFP methods belong to polarizable embedding schemes. Recently, we extended the EFP method to modeling flexible macromolecules and polymers, which allowed us to analyse importance of polarization for biological processes. We apply the new flexible EFP methodology to model excitonic interactions in the Fenna-Matthews-Olson photosynthetic protein. Specifically, we decompose effects of polarization, electrostatics, and short-range terms on electronic properties of pigments and demonstrate importance of a balanced description of solute-solvent interactions for predictive modeling of absorption and circular dichroism spectra of this protein.