The *effective* modeling of photobiology with the Effective Fragment Potential method

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Accurate description of solute-solvent interactions is an essence for modeling and understanding of photochemical processes in biological systems. The Effective Fragment Potential (EFP) is a quantum mechanical-based model potential providing rigorous description of non-covalent interactions from first principles. In biological systems where intermolecular interactions span a broad range from non-polar to polar and ionic forces, EFP is superior to classical force fields. With the presence of *ab initio* region, EFP-based QM/MM schemes (so called QM/EFP) describe biological environment with explicit inclusion of polarization. In the present study, we elucidate excitonic interactions in the Fenna-Matthews-Olson (FMO) photosynthetic pigment-protein complex with the QM/EFP approach. In photosynthetic genus, the FMO complex transfers the excitation energy from light harvesting antenna chlorosome to the reaction center with high efficiency. We demonstrate that QM/EFP absorption and circular dichroism spectra of the FMO complex are in good agreement with experiment. Building upon these results, we characterize effects of local amino acids and of long-range electrostatic and polarization interactions on the electronic properties of *bacteriochlorophyll a* (*Bchl a*) pigments. We also find that internal geometries of pigments are strongly coupled with several neighboring amino acids and accurate description of pigment geometries is essential for predicting excitonic interactions in the FMO complex.