The importance of polarizable embedding in biological systems: The effects of protein on the excitation energy transfer among photosynthetic pigments

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In photosynthesis, sunlight is collected by chlorosome antenna, and then transferred to the reaction center (RC) through the excitation energy transfer (EET) process initiated by the light-harvesting pigment-protein complexes (PPC). This photosynthetic process occurs with almost perfect efficiency in many living organisms, such as plants and photosynthetic bacteria. It is of interest to study these processes because sunlight is considered a renewable and almost infinite energy resource. However, the current use of solar energy is limited due to extremely low efficiency of artificial devices such as solar cells and solar panels. Therefore, understanding the exact photosynthetic mechanism within a PPC is necessary to increase the performance of these solar energy devices. The key factor in the efficiency of the photosynthetic process is the electronic couplings among photosynthetic pigments during the course of EET within the protein. We work on computational investigation of the EET processes using Fenna-Matthew-Olson complex from *prosthecochloris aestuarii* as our model PPC (PDB ID: 3EOJ). Specifically, we explore the effect of protein environment on the excitation energies of individual pigments and the electronic couplings that exist between them. In order to obtain relevant structures of the FMO complex, classical molecular dynamic simulations are performed. Then, excited state calculations using QM/EFP method are conducted. QM/EFP is a polarizable QM/MM model developed in our group and recently extended to biological systems. We aim at comparing results from QM/MM, QM/EFP and FMO (Fragment Molecular Orbital) methods and elucidating the importance of polarizable embedding to EET in biological systems.