

The Summer Undergraduate Research Fellowship (SURF) Symposium

2 August 2018

Purdue University, West Lafayette, Indiana, USA

The Exciton Spectra Simulator of Photosynthetic Protein-pigment Complex

Qifeng Chen, Yongbin Kim, Danil Kaliakin, and Lyudmila Slipchenko

Department of Computer Science, Purdue University

Department of Chemistry, Purdue University

ABSTRACT

The solar energy is one of the most successful alternative energy sources because of its unlimited availability and environmental friendliness. However, the energy transfer rate in artificial solar devices is significantly lower than the energy transfer rate in plants and bacteria. The key factor that governs efficient energy transfer is the electronic couplings between photosynthetic pigments within living organisms. We are applying quantum mechanical / molecular mechanical (QM/MM), quantum mechanical / effective fragment potential (QM/EFP) and fragment molecular orbital (*fmo*) methods to elucidate the energy transfer pathway in Fenna-Matthews-Olson (FMO) complex through computing the site energies of bacteriochlorophylls and the electronic couplings between them. Based on the values of site energies and couplings computed with QM/MM, QM/EFP and *fmo methods* we generate the multiple electronic Hamiltonians describing the energy transfer within the FMO complex. In this research, I am focusing on the improving the algorithm and developing the GUI for computing emission and absorption spectra for molecular systems with multiple chromophores. After taking the Hamiltonians matrixes as inputs, the researchers were able to predict the theoretical absorption and circular dichroism spectra. By comparing these spectra to experimental data, we managed to compare the efficiency and accuracy of the chosen methods and demonstrate the importance of accurate description of protein environment when studying the energy transfer within the pigment-protein complexes.

KEYWORDS

Exciton Spectra, Photosynthetic protein-pigment complex, Exciton Spectra Simulator, Energy transfer pathway, Bacteriochlorophylls, couplings, absorption spectra