

Examination of Chlorophyll-Chlorophyll Excitation Energy Transfer based on Local Induced Dipoles Analysis

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More than 50% of the light captured by green plants for use in photosynthesis is absorbed by the light harvesting complex (LHCII). This complex contains a variety of chromophores that allow the system to absorb in a broad range of the solar spectrum. A common chromophore present in most of the complexes involved on the photosynthesis is the chlorophyll molecule.

After absorption of a photon by one chlorophyll molecule, the exciton energy is transferred to a set of chlorophylls until reaching the active center, where this energy will be transformed into chemical energy.

One standard method to interpret the excitation energy transfer between a donor and an acceptor molecule is the so-called Förster's resonance energy transfer theory (FRET). FRET theory describes the non-radiative energy transfer mediated by a quantum-mechanical coupling between the transition dipole moment of the donor and acceptor molecules. One of the central assumptions of FRET is that the coupling can be described by a dipole-dipole interaction.

OCTOPUS code enable us to perform real-time and real-space TDDFT calculations for a systems containing hundred of atoms. By fragmenting the global computed density, we are able to compute local properties of the components of the system under study.

We present here the study of the dipole-dipole coupling between different pairs of chlorophyll molecules. The analysis is based on the variation of the local dipole moment and the induced electron density after excitation of one chromophore. The analysis techniques presented on this work enable to graphically understand the dipole-dipole coupling that governs the energy transfer on light harvesting systems.