TDDFT Study on Light Harvesting Systems: LHC-II case

Joaquim Jornet Somoza, Nano-Bio Spectroscopy Group, Departamento de Física de Materiales, Universidad del País Vasco

The current increase in energy demands across the world makes fossil-fuel based energy resources unsustainable. Solar energy conversion is one alternative to produce green renewable energy. However, the efficiency of current organic photovoltaic cells is still low (<10%) compared with natural biological systems (~100%). A deeper understanding of the mechanism that governs the energy transfer inside natural light-harvesting systems will be essential to design highly efficient and bio-inspired devices. In this work we present a full first–principles calculations within the framework of real–space time–dependent density functional theory (TD-DFT) for the complete chlorophyll (Chl) network (~7000 atoms)of the light–harvesting complex from green plants, LHC–II.

A local analysis method of the time dependent densities (ρ(t)) developed for this work has made possible quantum–mechanical studies of the optical response of individual chlorophyll molecules subject to the influence of the remainder of the chromophore network. The site-specific alterations in chlorophyllexcitation energies support the existence of distinct energy transfer pathways within the LHC-II complex.

We propose here a new *t*reatment of the ρ(t) that enables the calculation of exciton energy transfer inside chlorophyll network going beyond Förster's model.