

Abstract:

Photosynthesis is the essential process for the conversion of solar light into energy forms usable by living organisms on earth. The first two tasks performed by photosynthetic systems are the absorption of light and the transport of excitation energy to a reaction center. A key step towards the understanding of these processes on a molecular level lies in the characterization of the antenna systems responsible for light-harvesting.

Subsystem density-functional theory (DFT) offers a unique way for the investigation of quantum mechanical processes in such biological units. This talk introduces basic concepts of subsystem DFT and highlights recent developments that allow for a theoretical investigation of cooperative phenomena in the response of complex systems to external electromagnetic fields. The capabilities of this method are demonstrated in a study on the light-harvesting complex LH2 of purple bacteria and other biological pigment aggregates.