UNIVERSITY of L'AQUILA
Department of Engineering

Master Thesis
in
Mathematical Modelling in Engineering

Effect of The Protein Electric Field on The Spectral Tuning Of A Photosynthetic System

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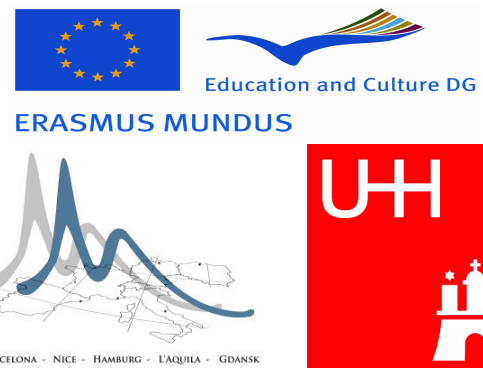

Abstract

Peridinin-chlorophyll-a proteins (PCP) are a class of light-harvesting antenna systems proteins only found in photosynthetic dinoflagellates. Due to their exceptional stability they are an excellent model system to study carotenoid to chlorophyll energy transfer. PCP contains both chlorophylls and carotenoids molecules, the latter being responsible to extend the spectral range of captured light to regions where chlorophylls are transparent.

The high resolution X-ray structures of Main-form-PCP (MFPCP has a peridinin:chlorophyll ratio of 4:1) and the less common high-salt-PCP (HSPCP which has a peridinin:chlorophyll ratio of 3:1) have been solved [1] . The absorption and fluorescence spectra from both complexes exhibit several distinguishing features that become evident only at cryogenic temperatures. In particular, at low temperatures the Q_y transitions of the Chlorophyll-a pigment's bound in the HSPCP complex are split into two well-resolved bands. [2]

In this thesis classical molecular dynamics simulations of the HSPCP complex in explicit water solution are carried out at different temperatures in order to investigate the protein flexibility and the impact of this on the different spectral properties of the HSPCP. The influence of the protein environment on the spectral properties of the chlorophyll-a pigment's in HSPCP proteins is further characterised by analysing the site energies shifts of the pigments, by using the Charge Density Coupling (CDC) method [3] .

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