Center for Green Energy Technology
PONDICHERRY UNIVERSITY

Lecture

On

"Exciton Energy Transfer Dynamics in Light Harvesting Complexes "

By

Dr. Suryanarayanan Chandrasekaran,

PhD Jacobs University, Bremen, Germany.

DST - Inspire faculty 2017

Date : 29th August 2017
Venue: CGET Seminar Hall, PU
Time : 10:45 AM

All are invited

Seminar Coordinator

Centre Head
Dr.B.M.JAFFAR ALI
CENTRE HEAD
CENTRE FOR GREEN ENERGY TECHNOLOGY
PONDICHERRY UNIVERSITY
PUDUCHERRY 605014

Exciton Energy Transfer Dynamics in Light Harvesting Complexes

Dr. Suryanarayanan Chandrasekaran,
PhD Jacobs University, Bremen, Germany.
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sonofsunsurya@gmail.com

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The process of harvesting sun light in an efficient way have become the quest to solve our daily energy demands. The straightforward way to construct an artificial photosynthetic device for practical use of solar energy is to understand the structural and functional organization of the natural photosynthetic machinery. For that atomistic theoretical modeling of natural Light Harvesting complexes (LHC) containing chromophoric pigment-protein complexes are needed to understand the exciton transfer mechanism occurring in them. The multi-scale modeling using classical molecular dynamics simulation with subsequent electronic structure calculations and quantum dynamics are done for natural LHC to understand the underlying quantum coherence phenomena observed through 2D photon-echo experiment. The complete theoretical study for classification of system(pigment) and it's environment along with analysis of excitation energy of individual pigments by density of states and spectral density will be presented in detail. The excited state coupling calculations are done with respect to distance between the pigment molecules inside the LHC through point dipole approximation (PDA) and transition state electrostatic potential method (TrESP).

How natural LHC defy the concept of self assembly and use efficient exciton transfer mechanism in it ? To explain this phenomena the two studied natural light harvesting complex known as Fenna-Matthews-Olson (FMO) complex of green sulfur bacteria and the Phycoerythrin 545 (PE545) antenna of marine algae results will be presented in detail. Finally my Inspire proposal objective of modeling of chlorosome exciton transfer mapping to match with pi-conjugated systems to predict the exciton recombination problem occurring in artificial solar cell will be presented.

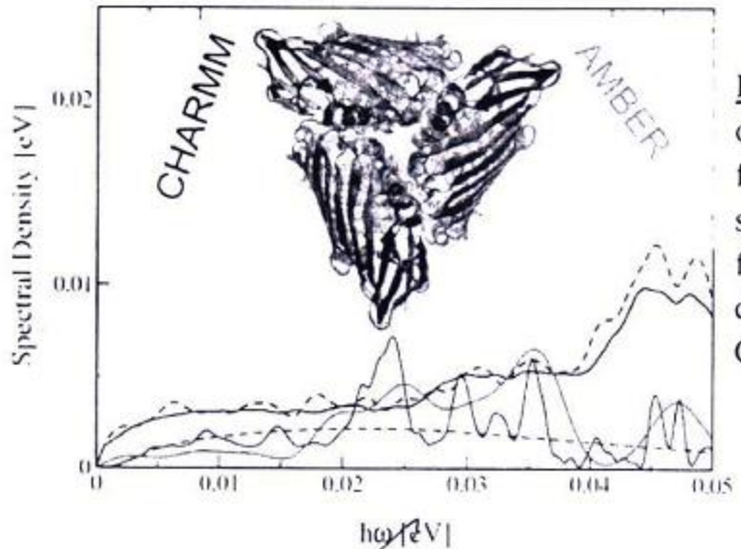

Figure: FMO complex structure in the inset of overlayed CHARMM and AMBER force field averaged over the trajectory. The spectral density results of respective force field are presented along with experimental data. (*source:* Chandrasekaran et.al, J. Phys. Chem. B **2015**, 119, pp 9995.)