Joint CQSE and CASTS Seminar

Weekly Seminar
Jun. 17, 2016 (Friday)

TIME Jun. 17, 2016, 14:30 ~ 15:30
TITLE Multiscale Molecular Simulation of Solar Energy Harvesting
SPEAKER Dr. Chun-Wei Pao
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PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

In this talk, I will present our recent efforts in developing multiscale molecular simulation framework for simulating the organization of organic solar cells and photosynthetic membrane under different fabrication conditions/ambient conditions. Organic solar cells are one of the promising renewable energy sources because of their low production cost, mechanical flexibility, and light-weight. The nanomorphologies of organic solar cells are critical to device performance; however, correlations between device fabrication conditions and resultant nanomorphologies remain elusive, despite of recent advances in experimental characterization tools. We developed a multiscale molecular simulation framework which can simulate nanomorphology evolution of organic solar cells under thermal annealing and solution processing, thereby providing insights into nanomorphologies and fabrication conditions. In contrast to organic solar cells, photosynthetic membranes are fascinating solar energy harvesting "device" because of their tunable protein supercomplex organizations in response to fluctuations in ambient conditions, rendering tunable photosynthetic efficiencies. We developed a coarse-grained (CG) model of protein supercomplexes based on experimental EM images. Our CG model can successfully reproduce several ordered supercomplex superstructures of photosynthetic membranes, and demonstrated the thermal reversibilities of supercomplex organization under temperature fluctuations.