IOWA STATE UNIVERSITY
Department of Mechanical Engineering

Multiscale Simulation of Solar Energy Harvesting

Chun-Wei Pao
Research Center for Applied Sciences
Academia Sinicia (Taipei, Taiwan)

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Seminar host: Baskar Ganapathysubramanian

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, solution processing, and vacuum co-deposition processes, 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.

Chun-Wei Pao has served as an Associate Research Fellow for the Research Center for Applied Sciences at Academia Sinica in Taipei, Taiwan since 2014. His research fields include atomistic simulations of graphene defect properties, CVD graphene growth kinetics, multiscale simulations of bulk heterojunction organic photovoltaic cells, atomistic simulations of water/graphene interfaces, and molecular dynamics simulation of LiFePO4 or graphene-based supercapacitors. Pao holds his PhD and MA in mechanical and aerospace engineering from Princeton University. He also holds his MS in applied mathematics from the National Taiwan University in Taipei. In 2014, he received the Young Theorist Award from the National Center for Theoretical Sciences. Prior to his time with the Research Center for Applied Mathematics, Pao served as a Post-doctoral Research Associate for the Theoretical Division of Los Alamos National Laboratory in New Mexico.

This seminar counts towards the ME 600 seminar requirement for Mechanical Engineering graduate students.

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