Special Program in Applied Mathematics and Applied Mechanics

Can Computational Simulation Help Development of Advanced Organic Photovoltaic Cells?

2013 - 02 - 20 (Wed.)
15:00 - 17:00
308, Mathematics Research Center Building (ori. New Math. Bldg.)

Organic photovoltaic cells (OPVs) are promising renewable energy sources because of their low production cost, mechanical flexibility, and light weight comparing with their silicon-based counterparts. The photoactive layer of OPV comprises two different materials, namely, electron donor, and electron acceptor materials. Electron donors are usually conjugated semiconducting polymer such as P3HT, whereas electron acceptors are usually materials with high electron affinity such as PCBM or even inorganic nanocrystals such as TiO2. The electron donor/acceptor materials in the photoactive layer form an interpenetrating network of donor/acceptor domains, namely, bulk heterojunction (BHJ), to maximize charge carrier generation. The three-dimensional morphologies of the BHJ layer is critical for the performance of OPV, however, experimental characterization of the BHJ layer is never trivial. Therefore, computer simulations may become a powerful tool to complement with experiments. In this talk, both opportunities and challenges of computer simulations of advanced OPVs will be addressed. The computational tools developed for modeling OPVs can not only be applied to helping development of next-generation OPVs, but also can be applied to helping the development of novel organic light- emitting diodes (OLEDs) and organic thin film transistors.