Abstract

Trevor Smith, Ken Ghiggino, Pawan Goyal
Chemistry (UoM) and Computer Science(IIT KGP)
Doctor of Philosophy

Self Assembly Nano Particle Simulation and Modelling of Organic Photovoltaic Materials

by Mayank BHASIN

This work contributes in predicting effects of OPV materials in solar cell active layers through MD simulations. Through general coarse grained simulations, the rate of change of component solubility, demixing tendency, and the difference in interaction energies, were studied for nano-composite self-assemblies. Routes to form uniform, core-shell, Janus, and eccentric morphologies were established. Using atomistic simulations it was established that increasing P3HT chain length the stability of the nanocomposite (P3HT:PCBM/ICBA) decreases, whereas increasing PDI stability increases. Also addressed is why two specific members of the entire BXR series (benzodithiophene- X-thiophene-rhodamine) exhibit liquid-crystalline phase and highest PCE in solar cell usage, compared to the other members. These members exhibit optimum aggregation which is necessary for liquid crystalline phase formation.