Molecular dynamics study on morphology of P3HT:PCBM for organic photovoaltic application

Owing to the growing demand for energy and depletion of fossil fuels, organic photovoltaics (OPV) have gained considerable attention to become a potential energy resource. The ultra thin photovoltaic technology has captured major interest among the researchers due to their light weight,low production cost, durability, flexibility and ease of processing. The efficiency of OPV has increased from 1%, in conventional single layer devices, to 10% when the materials are mixed in bulk heterojunction (BHJ). The BHJ technology comprises of both donor and acceptor materials mixed together in the active layer. The thermal annealing protocol which is a cheap manufacturing process allows the donor and acceptor material to phase separate. Usually there are two limiting phenomenon that effect the charge separation efficiency, i.e., the extent of phase separation and the formation of nano structure which interpenetrates within the bulk heterojunction. Thus improving the morphology of Poly(3-hexylthiophene-2,5-diyl) (P3HT): [6,6]-Phenyl-C_{61} -butyric acid methyl ester (PCBM), one of the widely used combination of donor-acceptor materials used in organic photovoltaics, is important to acheive high charge separation efficiency. Using molecular dynamics simulations we study the effect of nanoparticles on the morphology of PCBM in P3HT for polymer-based solar cell applications.

P3HT-grafted silica nanoparticles (SiNP) effect the spatial arrangement of PCBM in P3HT. The addition of SiNP not only alters the morphology of PCBM clusters but also improves the crystallinity of P3HT. We exploit the property of grafted SiNP to self-assemble into a variety of anisotropic structures and the tendency of PCBM to preferentially adhere to SiNP surface, due to favourable interactions, to achieve morphologies with desirable characteristics for the active layer. We also observe that by tuning the grafting parameters of SiNP, it is possible to achieve structures ranging from cylindrical to sheets to highly interconnected network of strings. Next we studied the effects of adding anisotropic shaped SiNP on morphology of BHJ solar cells. We varied the weight fraction of P3HT:PCBM and studied the impact of various shapes of SiNP such as cube, cylinder, disk and octahedron on morphology of P3HT:PCBM and compared the results with its pure counterparts. We also studied the effect of incorporation of nanorods (NRs) to the BHJ of P3HT:PCBM. We varied NRs aspect ratio and type to study the morphological changes induced by the NRs on P3HT:PCBM during thermal annealing. Due to higher strength of van der Waals interaction between PCBM and NRs, the PCBM covers the surface of NRs. As the aspect ratio of NRs increases the crystallinity of P3HT increases. This is due to the local organisation of P3HT on the surface of NRs. NRs used in this study consists of oxides of two types of particles, silicon (SNR) and titanium (TNR). TNR offer higher crystallinity compared to SNR because of higher strength of interaction between P3HT and TNR. Moreover TNR acts as additional electron acceptor which can further increase the efficiency compared to SNR. We also optimised the weight fraction of all the three components in BHJ. Our results suggest that an equal weight fraction PCBM:SiNP leads to better morphology.

We quantified several morphological properties like surface area of contact between P3HT:PCBM, domain size, percolation of domains and crystallinity of domains due to the formation of different morphologies by these particles. The effective control of all the morphological parameters help in improving the charge generation, extraction and transport to electrodes, thereby improving the performance of BHJ solar cells. These changes in morphological properties of P3HT:PCBM can be used as a benchmark to study the ternary blend solar cells with enhanced power conversion efficiency.