MORPHOLOGICAL CHANGES OF ORGANIC PHOTOVOLTAICS: MOLECULAR DYNAMICS SIMULATION STUDIES

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Organic Photovoltaics (OPVs) are a promising device for harvesting solar energy. In OPVs, bulk heterojunctions are formed in the active layer, in which electron donors and acceptors are randomly mixed to increase the active area. However, phase separation tends to progress in the active layers with time, which hampers the long-term stability of OPVs as well as their quantum efficiency. Hence, controlling the morphology of the bulk heterojunction plays an important role in enhancing both the long-term stability of efficiency of OPVs.

So, we studied the effects of compositions of donors and acceptors on the morphological changes of the OPVs using molecular dynamics (MD) simulations of atomistic OPV models. In our models, donors were poly([2,6′-4,8-di(5-ethylhexylthienyl)benzo[1,2-b;3,3-b]dithiophene]{3-fluoro-2[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl}) (PTB7-Th) and poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione)) (PBDB-T). In addition, round-shaped [6,6]-Phenyl-C71-butyric acid methyl ester (PC70BM) and flat-shaped 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(5-hexylthienyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene (ITIC-Th) were used as acceptors. We observed that the morphology changes of OPVs are highly dependent not only on composition but also on the order of active layers.