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Molecular dynamics study of phthalocyanine and sulfonated-phthalocyanine and C60 interface CARLOS DIAZ, MARCO OLGUIN, TUNNA BARUAH, RAJENDRA ZOPE, UTEP — Organic photovolatics (OPV) hold promise as cheap large-area technology for power generation. The fundamental mechanism of power conversion in OPV is dominated by interfacial processes such as charge transfer and charge separation. The energetics and dynamics of these processes depend on the morphology of the donor and acceptor (DA) interfaces. In experiments, these DA complexes are usually deposited on metal surfaces using spin coating or similar technique. To understand the morphology of interface and growth of the OPV on surface, we use molecular dynamics simulations with various layers of phthalocyanine and sulfonated phthalocyanine molecules on a Ag(111) surface. We examine the effect of sulfonation on the morphology of thin films. By introducing the acceptor molecules such as C60 in various concentrations we examine the variation in the morphology of OPV films with the different forms of phthalocyanine surfaces. We then select a few configurations of the DA complexes from the molecular dynamics trajectories and determine the charge transfer energies and the transport gap at the quantum mechanical level. Finally, by averaging over the configuration we obtain insights into the charge transfer energetics and the energy level alignments at the organic DA interface.

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