Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Disorder effects on the charge separation pathway by intermixing of donor and acceptor molecules[1] KODA SHOHEI, FUJII MIKIYA, KOICHI YAMASHITA, The university of Tokyo, School of Engineering, Department of Chemical System Engineering, THE UNIVERSITY OF TOKYO, SCHOOL OF ENGIEERING TEAM, CREST, JST TEAM — The organic photovoltaics (OPVs) have recently attracted much interest as alternative energy sources. Though the power convergence efficiencies (PCEs) of OPVs have reached more than 11%, the PCEs are lower than those of Si solar cells. To improve the PCEs, we need to reveal a fine mechanism of charge separations between the electrons and holes at the interface of electron donating and accepting materials. The objective of this study is revealing the mechanism of the charge separation in the OPVs by investigation of a typical pair of donor and acceptor, i.e., P3HT and PCBM, respectively. To this end, we investigated the energy profile from exciton states to charge separated states in two types of atomistic interface. Namely, we prepared bilayer and intermix interfaces of P3HT and PCBM, which were made by conducting molecular dynamics simulations with 48 P3HTs and 144 PCBMs. Then, we calculated electronically excited states in those interfaces by applying semi-empirical quantum calculations and then revealed charge separation pathway reaching 4 nm of electron-hole distance. Finally, we discuss critical effects of charge delocalization on the charge separation pathway.

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Date submitted: 08 Nov 2016 Electronic form version 1.4