Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Packing effects in charge transfer dynamics in organic molecular heterojunctions consisting of TFB and F8BT MIKIYA FUJII, KOICHI YAMASHITA, Department of Chemical System Engineering, University of Tokyo and JST, CREST — Organic semiconductors have been widely investigated for photovoltaic and light emitting devices. Especially, further improvements for more efficient organic solar cells (OSCs) are desired. Thus, we explored computationally possibilities to make OSCs more efficient by adjusting the packing of molecular heterojunctions. We analyzed a molecular heterojunction that consists of poly(9,9-dioctylfluorene-co-N-(4-butylphenyl)diphenylenediamine) (TFB) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT). Geometrical optimization of TFB(monomer)/F8BT(monomer) complex was carried out with DFT-D/B3LYP/6-31G*. Excited states were also calculated with CIS/6-31G*. To analyze packing effects, we rotated TFB around a principal axis. Then, charge transfer dynamics is analyzed with a quantum master equation (QME) approach in each packing From the excited states calculations, it is clarified that the packing strongly affects the energy level of the charge transfer state only. This packing dependency arises from a packing dependency of the exciton binding energy that is Coulomb interaction between an electron localized to F8BT and a hole localized to TFB. From the QME approach, it is confirmed that qualitative different electronic relaxation dynamics occurs in each different packing.

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Date submitted: 26 Nov 2012 Electronic form version 1.4