Abstract Submitted
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Dynamical- and static-disorder effects on charge transport property of organic semiconductors[1] HIROYUKI ISHII, JST-PRESTO, University of Tsukuba, NOBUHIKO KOBAYASHI, University of Tsukuba, KENJI HIROSE, NEC — In comparison with inorganic materials, electron transfer energy of typical organic semiconductors is small in the range of 10 - 100meV, which is comparable to the magnitude of dynamical disorder of transfer energy originating from the thermal fluctuations of molecular motions. Furthermore, the static disorder inevitably exists in realistic organic devices and disturbs the transport of charge carrier. To clarify the influence of the dynamical and static disorders on the mobility, we employ a realistic static-disorder potential, which is deduced from the data obtained by electron-spin-resonance spectroscopy. We evaluate the carrier mobilities of pentacene and rubrene semiconductors under the realistic situation, using our time-dependent wave-packet diffusion method. [1] In this methodology, we carry out the quantum-mechanical time-evolution calculations of wave packets and the classical molecular dynamics simulations simultaneously. We clarify the relation between the charge transport property and these disorders. We will talk about these results in my presentation. [1] H. Ishii, K. Honma, N. Kobayashi, K. Hirose, Phys. Rev. B, 85 (2012) 245206. H. Ishii, N. Kobayashi, K. Hirose, Phys. Rev. B (to be published).

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