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Wave-packet approach to thermal fluctuation effects on charge transport of organic semiconductors[1] HIROYUKI ISHII, Institute of Applied Physics, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan., NOBUHIKO KOBAYASHI, Institute of Applied Physics, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan, KENJI HIROSE, NEC Corporation, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, Japan. — Organic materials are formed with weak van der Waals interactions between molecules. For typical organic semiconductors, the transfer integrals are small in the range of 10 - 100meV, which is comparable to the dynamical transfer integral modulations originating from the thermal fluctuations of molecular motions. Therefore the fluctuations provide important contributions to the understanding of the transport mechanism. To investigate such effects, we have developed a methodology to calculate the carrier transport coupled with inter- and the intramolecular vibrations of organic semiconductors based on the 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 evaluate the anisotropic mobility of organic semiconductors, such as pentacene crystals. We also clarify the change of temperature dependence of mobility from the thermal activated behavior to the power law behavior. I will talk about these results in my presentation. [1] H. Ishii, K. Honma, N. Kobayashi, K. Hirose, Phys. Rev. B, 85 (2012) 245206.

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Hiroyuki Ishii
Institute of Applied Physics, University of Tsukuba,
1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan.

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