

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Charge transport calculations of organic semiconductors by the time-dependent wave-packet diffusion method<sup>1</sup>** HIROYUKI ISHII, NOBUHIKO KOBAYASHI, University of Tsukuba, KENJI HIROSE, NEC corporation — Organic materials form crystals by relatively weak Van der Waals attraction between molecules, and thus differ fundamentally from covalently bonded semiconductors. Carriers in the organic semiconductors induce the drastic lattice deformation, which is called as polaron state. The polaron effect on the transport is a serious problem. Exactly what conduction mechanism applies to organic semiconductors has not been established. Therefore, we have investigated the transport properties using the Time-Dependent Wave-Packet Diffusion (TD-WPD) method [1]. To consider the polaron effect on the transport, in the methodology, we combine the wave-packet dynamics based on the quantum mechanics theory with the molecular dynamics. As the results, we can describe the electron motion modified by (electron-phonon mediated) time-dependent structural change. We investigate the transport property from an atomistic viewpoint and evaluate the mobility of organic semiconductors. We clarify the 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, N. Kobayashi, K. Hirose, Phys. Rev. B, 82 085435 (2010).

<sup>1</sup>This work was supported by a Grant-in-Aid for Scientific Research from the MEXT of Japan.

Hiroyuki Ishii  
University of Tsukuba

Date submitted: 11 Nov 2011

Electronic form version 1.4