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The mobility in molecular organic systems with energies given by a charge-induced dipoles interaction

C. Tonezer[(1)*] and J. A. Freire[(1)]

(1) Departamento de Física, Universidade Federal do Paraná, Curitiba/PR - Brazil, ctonezer@gmail.com

* Corresponding author

Abstract – We studied charge carrier transport in disordered molecular organic systems. In these systems the polarization energy is the main source of the energetic disorder. In our model we considered a random distribution of sites and used the energy of the charge-induced dipoles interaction as the site energies. To investigate the dependence of mobility with the applied field we computed the system mobility using a master equation model of a time-of-flight experiment.

In disordered organic systems the charge carrier transport happens by thermally activated hopping between localized electronic states. These states are positionally and energetically disordered. The charge carrier interaction with induced dipoles in the neighboring molecules in a disordered environment is one of the main sources of the energetic disorder, particularly in molecular organic systems, other sources of disorder include the charge carrier interaction with permanent dipoles (in the case of polar materials) and the dispersion in conjugation length (in conjugated polymers).

Our study has as main objective to understand the physical origin of the mobility dependence with the exponential of the square-root of the applied field, a dependence known as Poole-Frenkel dependence, observed experimentally in many different organic systems.

In a previous work [1] we established that positional disorder plus site energies given by charge-induced dipoles give rise to a short-ranged site energy distribution. In the present work we considered a system of disordered organic molecules based on a random distribution of sites, the site energies were taken as the charge induced-dipoles interaction energy, the polarization energy present in any organic system. With this model we computed the mobility field dependence using a master equation model for the time-of-flight experiment. We used the Miller-Abrahams rate to describe the hopping between sites.

References

[1] J.A. Frire, and C. Tonezer, J. Chem. Phys. 130 (2009) 134901.