The Effect of Spatial Disorder on Charge Transport in Disordered Organic Semiconductors: Monte Carlo Simulation

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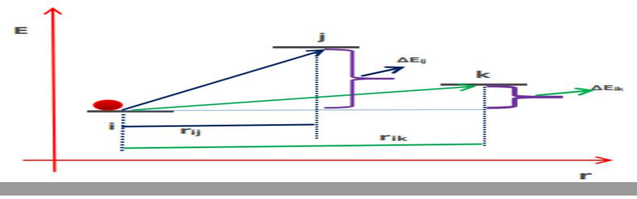
Introduction

Organic semiconductors are carbon–based molecular materials held together by weak interactions, such as van–der Waals forces. Disordered organic semi-conducting polymers can be used as active materials in electronic devices such as organic light-emitting diodes (OLEDs), organic field effect transistors (OFETs), organic solar cells. Charge carrier transport is one of the most important properties that determines the device applications. Thus, to design and synthesize better materials and further improve device performances. Understanding the transport properties in the active materials is very important.

We calculate the probability of hopping from occupied to unoccupied sites using Miller–Abrahams rate equation

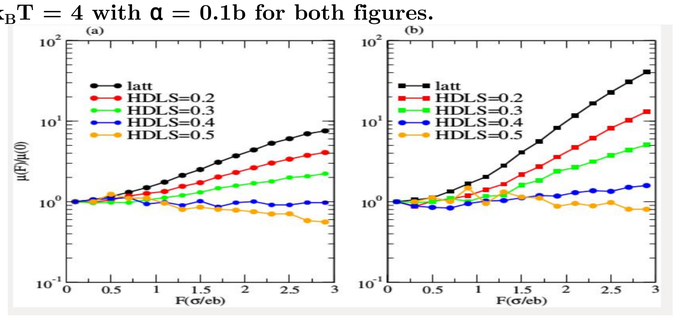
$$\nu_{ij} = \nu_o \exp(-2r_{ij}/\alpha) \exp\left(-\frac{\Delta E_{ij} + |\Delta E_{ij}|}{2k_BT}\right)$$



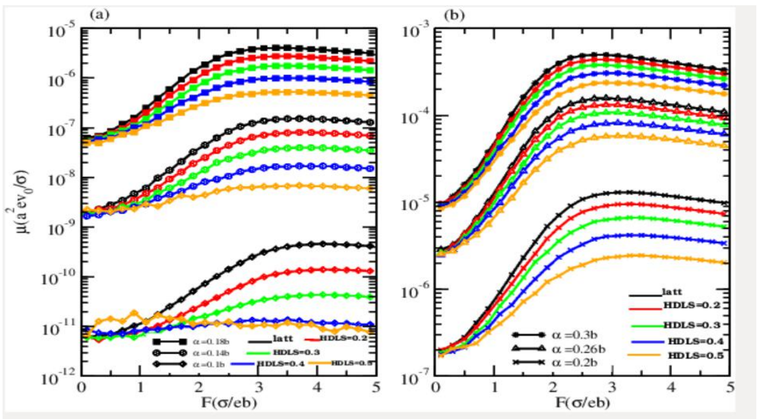
Mobility is the basic transport parameter. Charge carrier transport in most organic disorder semiconductors (ODSs) is performed by incoherent tunneling (hopping) of electrons or holes between localized states. The charge carrier mobility in ODSs depends on temperature, electric field, and disorders. In this work, we investigated the charge carrier mobility as a function of electric field and temperature using Monte Carlo simulation methods. We used lattice model with fluctuating lattice parameter and variable hopping distance. The results of our simulations show mobility as a function of electric field for different widths (fluctuations) of lattice parameter.

Simulation Results

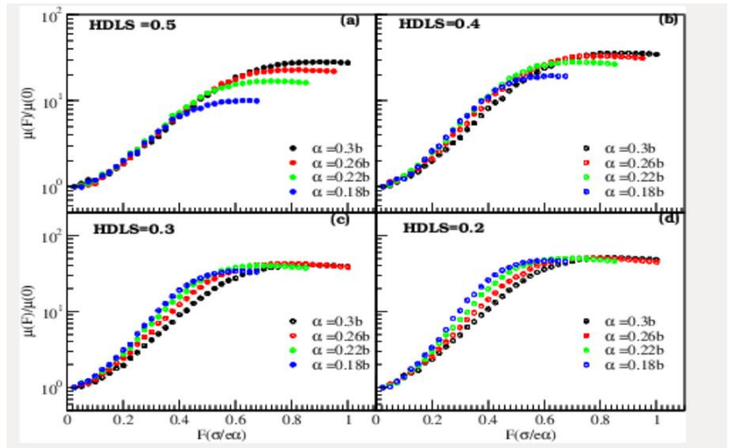
The carrier mobility versus electric field with fluctuating lattice parameter and variable hopping distance at (a) $\sigma/k_BT = 3$ and (b) $\sigma/k_BT = 4$ with $\alpha = 0.1$b for both figures.



Mobility versus electric field at $\sigma/k_BT = 4$ for different values of α/b and fluctuating lattice parameter with variable hopping distance.



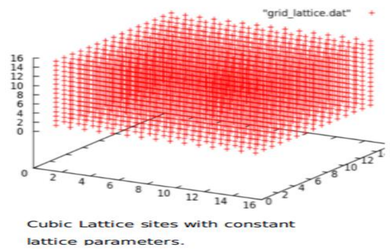
The carrier mobility as a function of electric field at $\sigma/kBT = 4$ for different values α/b and fluctuating lattice parameter with variable hopping distance.



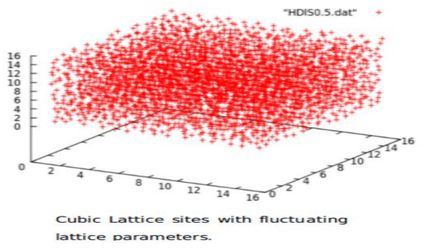
Methodology

We modeled our material as a three dimensional cubic lattice sites. The charge carriers are distributed randomly over the sites. The energy at different sites are uncorrelated and the distribution is assumed to be Gaussian, whose width characterizes the material's disorder.

$$g(E) = \frac{N}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\xi^2}{2\sigma^2}\right)$$

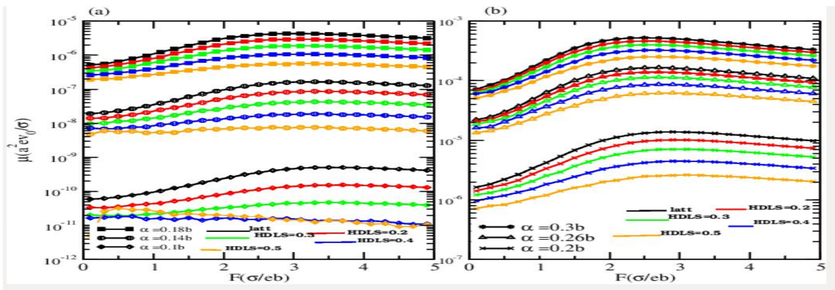


Cubic Lattice sites with constant lattice parameters.



Cubic Lattice sites with fluctuating lattice parameters.

Mobility versus electric field at $\sigma/k_BT = 3$ for different values of α/b and fluctuating lattice parameter with variable hopping distance.



Conclusions

- We found that the charge carrier mobility increases with electric field in case of lower values fluctuating lattice parameter and variable hopping distance of HDLS, whereas at higher values of HDLS the mobility differs from a regular grid.
- We showed that both the lattice constant and localization length are relevant for the mobility variation in case of cubic lattice sites with constant and fluctuating lattice parameter for lower values of HDLS, but in the case of fluctuating lattice system at higher values of HDLS the localization length is the only spatial parameter responsible for the mobility.

Acknowledgments

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References

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