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Use case: Charge carrier mobility study in pristine molecular layers

Introduction

The following use case shows an extensive investigation of the charge carrier mobility in pure α-NPD layers, including its dependence on temperature and electric field, using LightForge KMC with charge transport parameters derived from QuantumPatch for atomistic structures generated with Deposit.

Mobilities for α-NPD were calculated in five steps:

1. Single molecule parametrization using the Parametrizer
2. Generation of morphologies consisting of 1000 molecules with Deposit
3. Computation of electronic couplings (J), reorganization energies (λ) and orbital energies for both holes and electrons in the molecular structure from Deposit
4. Expansion of the molecular structure for better convergence in LightForge, using the Range Expander.
5. Simulation of charge transport in expanded structures for different temperatures and electric fields using LightForge, to extract temperature and field dependent charge carrier mobilities.

Detailed parameters for steps 1-3 are given below.

Expanding molecular structures for LightForge KMC calculations

The number of hopping sites (i.e. molecules) necessary to achieve convergence of the charge transport simulations in LightForge exceeds the capabilities of molecular simulations of e.g. Deposit (steps 1 to 3 above). Therefore, by analyzing the molecular structure from Deposit, the Range Expander generates a mesoscopic distribution of points is that exhibits the same density and nearest neighbor distance distribution as the center of geometry distances in the molecular structure.

Charge transport simulations with LightForge

For each connected pair in this expanded structure of hopping sites, Marcus rates for charge transfer are automatically calculated by LightForge, using the distance dependent distribution of electronic transfer integrals, energy levels and reorganization energies calculated with QuantumPatch. Based on these rates, transport simulations were

performed for different values of the electric field and at different temperatures. For investigating field dependence, different values for hole concentrations in the typical range for OLEDs were used. For each set of parameters (hole concentration, electric field, temperature), the charge carrier mobility is automatically calculated by LightForge using the cumulated charge carrier drift over time, electric field, volume and charge carrier concentration.

Fig. 1. presents a comparison of the calculated hole mobility with experimental data from [1]. As expected, high charge carrier concentration yields higher mobility, as more traps are filled. For the highest charge carrier concentration of n = 2 x 10^{-3}, KMC results agree well with experimental data.

The temperature dependence of the zero field mobility is displayed in Fig. 2. The zero field mobility is determined by extrapolating field dependent hole mobilities at different temperatures to zero electric field. In terms of both slope and absolute value, the calculated values show very good agreement with experimental measurements [2-4].

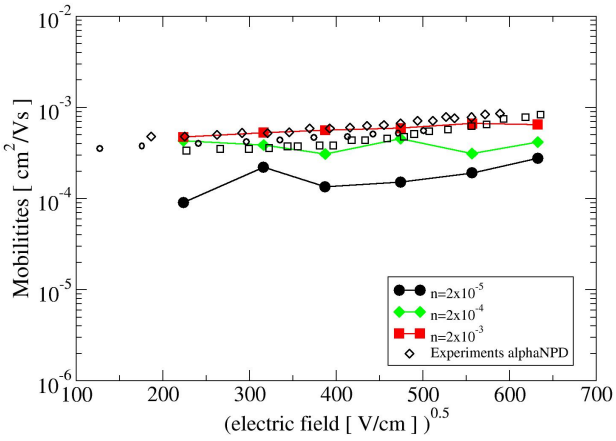

Figure 1: Field dependence of hole mobilities in α-NPD. Experimental values from [1]. The results will be published shortly in [5].

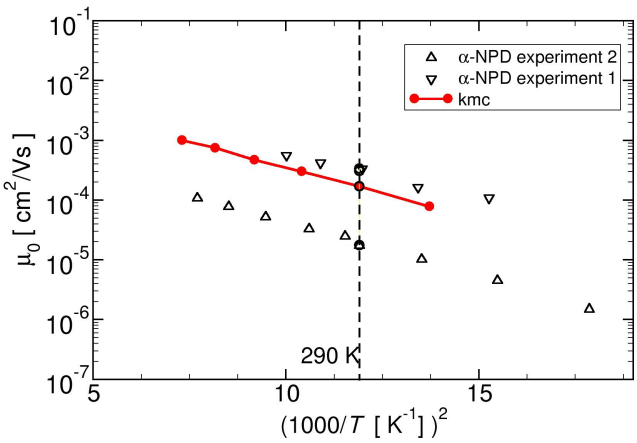

Figure 2: Temperature dependence of hole mobility (extrapolated to zero field) in α-NPD, in comparison with data from different experiments [2-4]. The results will be published shortly in [5].

Conclusion

LightForge can be used to perform predictive charge transport simulations in organic electronic layers. Charge carrier mobilities extracted from these simulations and their dependencies on temperature and electric field exhibit remarkable agreement to experimental data. Therefore, results from LightForge can be tabulated for different temperatures and fields as *ab initio* parametrization for Drift Diffusion simulations. This exemplifies how Nanomatch Software can be deployed to perform predictive simulations for computer aided design of materials and device setups in organic electronics.

Parameters used in the calculation:

Parametrizer:

Geometry optimization	DFT (b3-lyp, def2-SV(P))
Partial charges	DFT (b3-lyp, def2-SV(P))
Dihedral parametrization	Hartree-Fock (PM7)

Deposit:

Number of molecules	1000
Number of SA cycles	16
Number of steps per cycle	140.000
Initial temperature	4000K
Final temperature	300K

QuantumPatch:

	Neutral energy	Charged energy
No. of Mol in inner shell	200	200
No. of partial charge steps	7	7
Method	ridft, b3-lyp	ridft, b3-lyp
Hybrid mode	Off	On

[1] Toshinori Matsushima et al. “Optical, morphological, structural, electrical, molecular orientation, and electroluminescence characteristics of organic semiconductor films prepared at various deposition rates”. en. In: Thin Solid Films 520.6 (Jan. 2012), pp. 2283–2288

[2] Shigeki Naka et al. “Carrier transport properties of organic materials for EL device operation”. en. In: Synthetic Metals 111-112 (June 2000), pp. 331–333. issn: 03796779

[3] S. C. Tse, K. C. Kwok, and S. K. So. “Electron transport in naphthylamine-based organic compounds”. en. In: Applied Physics Letters 89.26 (Dec. 2006), p. 262102. issn: 0003-6951, 1077-3118

[4] C. H. Cheung et al. “Using thin film transistors to quantify carrier transport properties of amorphous organic semiconductors”. en. In: Applied Physics Letters 93.8 (Aug. 2008), p. 083307. issn: 0003-6951, 1077-3118

[5] F. Symalla “Modeling of charge and exciton dynamics in amorphous organic semicoductors”, Karlsruhe, 2017