Nanomatch
Hermann-von-Helmholtz Platz 1, Bau 640
76344 Eggenstein-Leopoldshafen
mail: tobias.neumann@nanomatch.com
T +49-721-608-26884
www.nanomatch.com

Use case: Calculation of charge carrier mobilities in pristine molecular layers

Introduction

The following use case demonstrates a very basic, but important application of the Nanomatch Software Stack: the calculation of charge carrier mobilities in pure α-NPD and ALQ_3 layers using Parametrizer, Deposit, QuantumPatch and the AnaMobi mobility solver (for more complex systems, e.g. doped layers or multi layer structures, AnaMobi needs to be substituted by LightForge KMC).

Mobilities for α-NPD were calculated in four 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 energetic disorder (σ) for holes using QuantumPatch for the molecular structure from Deposit
4. Calculation of the charge carrier mobilities for holes using AnaMobi based on the generalized effective medium model (GEMM).

Detailed parameters for each step are given below.

Results

QuantumPatch

The relevant results of QuantumPatch ($<J^2r^2>$, λ, σ) for holes in both materials are given in Tbl. 1. The energetic disorder, i.e. the standard deviation of the energy levels of electrons (or holes) in the material, has the strongest impact on the mobility.

Table 1: Microscopic electronic transport parameters of α-NPD and ALQ_3 calculated with QuantumPatch.

Material	$<J^2r^2>$ / eV^2A^2	λ / eV	σ / eV
α-NPD	1.44e-03	0.271	0.121
ALQ_3	1.12e-02	0.224	0.219

AnaMobi

Using the results of Tbl. 1, the charge carrier mobility was calculated using the analytic mobility solver AnaMobi. Comparison of calculated values to experimental data [1, 2] for hole mobilities is displayed in Fig. 1.

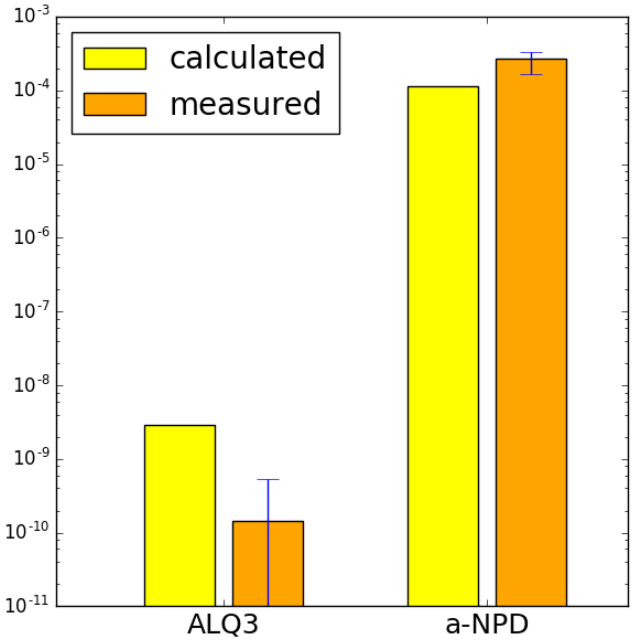

Figure 1: Comparison of analytic (calculated) and experimental hole mobilities in α-NPD and ALQ_3. Taking into account the experimental errors, the calculated results show a deviation of approximately half an order of magnitude for ALQ_3 and only a factor 2 in the case of α-NPD.

Conclusion

Calculating charge carrier mobilities in bulk material is a straight forward application of the Nanomatch Software Stack. As exemplified by two of the most prominent molecules in organic electonics, ALQ_3 and α-NPD, charge carrier mobilities are predicted within half an order of magnitude for reference values ranging over several orders of magnitude. Crucial to the reliability of the results is the correct calculation of microscopic transport parameters, such as electronic couplings and energy levels. This is achieved in QuantumPatch by taking into account the unique environment of each molecule on a full quantum mechanical level. The overestimation of the hole mobility of ALQ_3 is a expected to be a consequence of treating the molecules completely rigid throughout the deposition, leading to small energetic disorder and therefore higher mobility. Incorporation of internal degrees of freedom of rather rigid molecules such as ALQ_3 is currently being developed.

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] a) H. H. Fong, S. K. So, J. Appl. Phys. 2006, 100, 094502 b) S. Naka, H. Okada, H. Onnagawa, Y. Yamaguchi, T. Tsutsui, Synth. Met. 2000, 111, 331

[2] S. Tse, K. Kwok, S. So, Appl. Phys. Lett. 2006, 89, 262102