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Full *in silico* development of the novel compound Alq_2MHept

Introduction

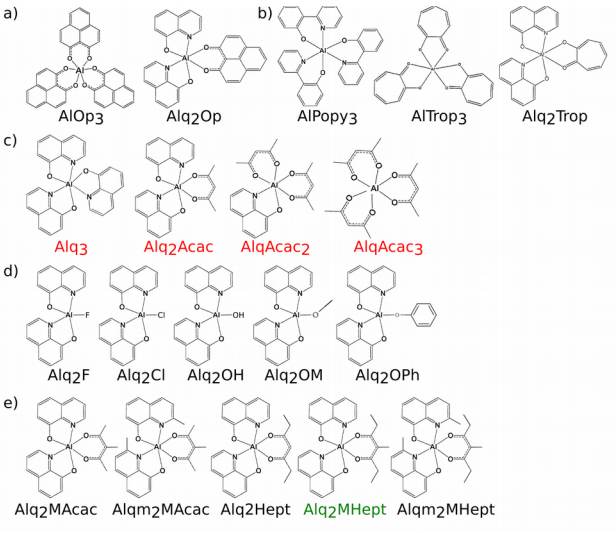
The following use case illustrates how innovation in organic electronics can be driven by computer aided design. We present the full *in silico* development of a novel electron transport material, Alq_2MHept, with a charge carrier mobility three orders of magnitude above the ETL material Alq_3. This test case exemplifies how the Nanomatch software stack is used to identify new compounds by predicting material properties with subsequent experimental verification of the most promising candidates, thereby minimizing costly experimental trial and error based R&D [1]. The results are also published in [1].

For 19 different ETL candidates derived from Alq_3 (including Alq_3 as reference system), electron mobilities were calculated in four steps:

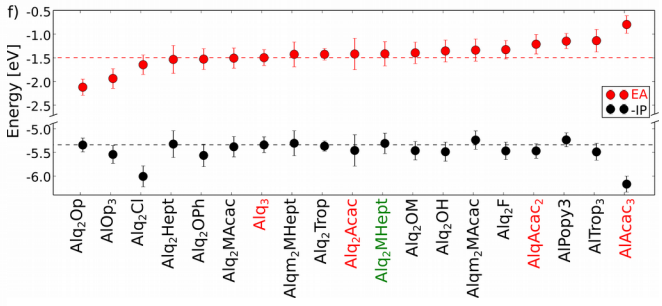
1. Single molecule parametrization using the PARAMETRIZER
2. Generation of morphologies consisting of 1000 molecules with DEPOSIT
3. Computation of ionization potentials (IP), electron affinities (EA), electronic couplings (J), reorganization energies (λ) and energetic disorder (σ) for electrons using 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.

Candidates and electron affinities



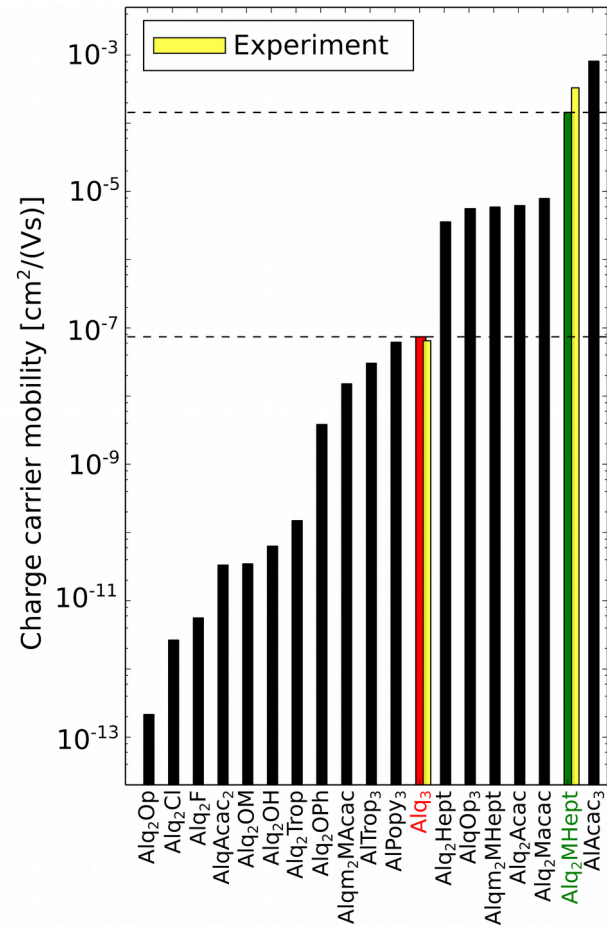
The compounds used for investigation are illustrated in the Fig. to the left. Starting with the known compound Alq_3, side groups were substituted or modified, resulting in 19 different structures.



1 While state-of-the-art ETL materials have mobilities of up to 3 orders of magnitude above Alq_3, this example was used to illustrate the general procedure of computer aided materials development by calculating specific quantities of interest for multiple candidates. This approach can be extended to other criteria than mobility, such as energy level shifts in specific materials or doping efficiency.

As molecules with low EA do not qualify as ETL material, values for IP and EA (f) of the molecules in the molecular layer were extracted from QUANTUMPATCH calculations as additional criterion.

Computed electron mobilities and experimental verification



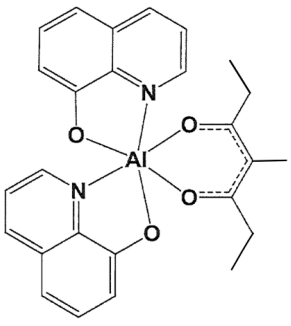
Computed electron mobilities of all 19 candidates are displayed to the left. While eleven materials performed worse than Alq_3 (red) and can be discarded immediately, seven materials show electron mobilities of at least two orders of magnitude larger than Alq_3. In particular, electron mobilities of Alq_2MHept (highlighted in green) and $AlAcac_3$ were calculated to be between three to four orders of magnitude above the value computed for Alq_3. Due to its low electron affinity, AlAcac2, however, is discarded as a potential ETL material, reducing the number of candidates from 19 to a single compound: Alq_2MHept.

The theoretical predictions of electron mobility were then validated by experimentally extracting zero field mobilities from conductivity measurements, performed only for Alq_2MHept and Alq3 (for reference). The experimental data (yellow bars in the left figure) show very good agreement with the theoretical results and confirm Alq_2MHept, depicted below, as an ETL material with a mobility three orders of magnitude above the original compound, Alq_3.

Conclusion

Using the Nanomatch Software Stack, a novel electron transport material was developed with minimized cost and effort. 19 ETL candidates were screened by computing electron mobilities and only the most promising compound, Alq_2MHept (fig. on the right), was used for further experimental investigation, along with Alq_3 as reference.

Using this computer based approach for materials development, experimental efforts (synthesis, purification, layer deposition and conductivity measurements) were reduced by almost one order of magnitude: from the full manufacturing and analysis of 19 materials to the investigation of only two compounds.



Chemical structure of Alq_2MHept.

Due to the scalability of the computational approach, the benefit of computer aided development of materials can be further increased, minimizing experimental efforts and therefore speed up materials development in organic electronics while reducing costs by orders of magnitude.

Parameters used in the calculation:

Parametrizer:

Geometry optimization	DFT (B3-LYP, def2-SV(P))
Partial charges	DFT (B3-LYP, def2-SV(P))
Dihedral parametrization	semiempirical (PM7)

Deposit:

Number of molecules	1000
Number of SA cycles	10
Number of steps per cycle	140.000
Initial temperature	4000K
Final temperature	300K

QuantumPatch:

	Neutral energy	Charged energy
No. of Mol in inner shell	100	100
No. of partial charge steps	7	7
Method	ridft, B3-LYP	ridft, B3-LYP
Hybrid mode	Off	On

References:

[1] P. Friederich et al., “Rational in Silico Design of an Organic Semiconductor with Improved Electron Mobility”.