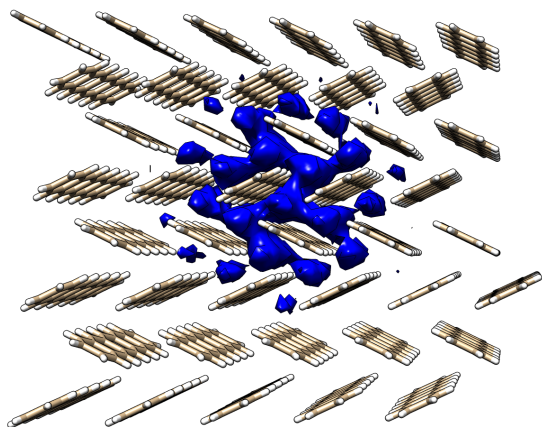


Charge transport in organic materials: Calculation of mobilities in polyacene single crystals

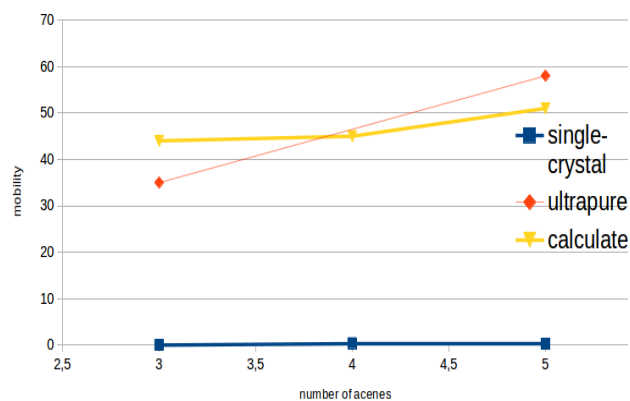
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The local molecular properties, local electron affinity[1,2] and local ionization energy[3] can be understood as scalar potentials embedded in 3-dimensional space which represents the interaction of charge carriers with a complicated quantum mechanical system. It is possible to perform quantum dynamics of an electron or hole using these energy maps as external potentials in the Hamiltonian operator. The crux is that this approach drastically reduces the number of entities that need dynamic treatment drastically and reveal information about conduction characteristics.



Hole in pentacene crystal (isovalue 0.00005)



values taken from [5],[6],[7],[8],[9]

We have performed periodic molecular-orbital calculations of polyacene single crystal structures of anthracene, tetracene and pentacene with the massively parallel program "EMPIRE"[4] based on experimental geometries. The orbitals and their energies are generated with NDDO-based semiempirical MO-theory to produce local electron affinities and ionization energies. With a linear term added to the Hamiltonian to represent a homogeneous field, imaginary time propagation of an excess charge carrier is simulated by stepwise matrix multiplication. Mobility values of different structures are calculated by the shift of the location expectation value. Compared to experimental data of mobilities on anthracene, tetracene and pentacene single crystals, we calculated a mobility of tetracene an order of magnitude higher $\sim 44 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$. We thus propose a theoretically attainable hole mobility of tetracene at least an order of magnitude higher than the current experimental value. The higher mobility is consistent with those found experimentally in the other acene crystals. The low experimental value found for tetracene is likely caused by impurities in the crystal.

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