Atomistic multiscale simulations of electronic transport in disordered organic materials

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It remains a challenge to understand and predict the charge transport in organic electronic materials due to a lack of a simple model that links the chemical structure of the material to its measurable macroscopic electrical properties. We will review our methodology that has been developed to calculate the charge carrier mobility in disordered conjugated polymers starting from the atomic structure of the material [1]. The key ingredients of the method are the charge patching method [2] which is an efficient method for constructing the single-particle Hamiltonian, the overlapping fragments method [3] that is used to diagonalize such a Hamiltonian and a multiscale procedure which is used to link the electronic structure calculation to macroscopic conductivity [1]. Applications of the methods to the calculation of the density of states, the DC and the THz mobility in several polymers [polythiophenes, polyfluorenes, poly(aryl–ethynylenes)] will be discussed [1, 4, 5] with special emphasis on insights that one obtains from such simulations.

References

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