Electron-vibration coupling : theoretical and numerical challenges

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Electron-phonon coupling constants for simulations of electronic transport in organic semiconductors

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Abstract

There is a strong interest to understand electronic transport properties of organic semiconductors based on conjugated polymers and small molecules due to their emerging applications in electronic and optoelectronic devices. In this talk, the calculation of electron-phonon (e-ph) coupling constants and their subsequent use in simulations of electronic transport in two main classes of organic semiconductors will be discussed.

Organic semiconductors based on conjugated polymers typically exhibit a largely disordered morphology which leads to strongly localized electronic wave functions. Charge transport in these materials then takes place by phonon-assisted hopping between these states. For accurate calculation of the wave functions, calculations of the systems larger than wave function localization length are necessary, which involves thousands of atoms. For systems of such size direct calculations of phonon modes and e-ph coupling constants based on density functional perturbation theory are not feasible. We will describe an approximate procedure for estimation of e-ph coupling constants in such systems. Phonon modes were calculated based on classical force field and e-ph coupling constants were calculated from the calculation of the change in single-particle Hamiltonian due to atomic displacements. These e-ph coupling constants are then used in a multiscale procedure which eventually yields the hole mobility in a disordered polymer material [1]. The results indicate that the mobility is not very sensitive to details of coupling to individual phonon modes [2].

In the second part of the talk, calculation of electronic transport in ordered materials where e-ph coupling could be relatively strong so that polaronic effects are important will be discussed. Typical examples of such materials are organic crystals [3] and ordered arrays of nanocrystals [4]. The approach is based on unitary transformation of the Hamiltonian to a polaronic basis where polaron-phonon interaction can be treated perturbatively. Application of the approach to model e-ph interaction Hamiltonians and numerical challenges of its application to realistic e-ph interaction Hamiltonians of crystals with several tens of atoms per unit cell will be discussed.

References

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Return to list