## Computational approaches for electronic properties of semiconducting materials and nanostructures

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### Abstract

Density functional theory (DFT) provides a reliable theoretical framework for studying the electronic properties of atoms, molecules, bulk materials, surfaces, interfaces, etc. However, due to its computational effort, the calculations based on DFT are typically performed only for relatively small molecules or for crystalline materials where periodicity of the structure can be exploited. There is a wealth of highly relevant systems which are currently beyond the reach of standard DFT calculations, such as, for example, disordered conjugated polymers, inorganic nanocrystals, and polycrystalline materials. To study these systems, one typically needs to do the calculation for a supercell containing thousands of atoms to get reliable information about the properties of the system.
The methods that can be used to study even such systems will be presented and computational aspects of the applications of these methods will be discussed.
Charge patching method (CPM) [1] is the method for the construction of electronic charge density of the system that avoids demanding self-consistent DFT calculations. It is based on the idea that electronic charge density in the neighborhood of an atom depends mainly on its local environment. Such an assumption is typically valid in semiconducting and insulating materials without any long-range charge transfer. The contribution of each atom to electronic charge density of the system is therefore extracted from the calculation of some small prototype system where atoms have the same environment as in the large system under study. Electronic charge density of the large system is then simply obtained by adding the contributions of each atom. With electronic charge density at hand, one gets the single-particle Hamiltonian by solving the Poisson equation for the Hartree potential and using the local density approximation formula for the exchange-correlation potential.
To study the electrical properties of the material, one does not need to calculate all the electronic states of the Hamiltonian but only these in the region near the band gap. Overlapping fragments method (OFM) [2] was developed to efficiently find these states. The method is in particular suited to study disordered conjugated polymers [3]. It is based on the divison of the system into fragments and the representation of the Hamiltonian in the basis of molecular orbitals of these fragments. It is typically sufficient to use only a few molecular orbitals of each fragment. This approach strongly reduces the size of the Hamiltonian matrix that needs to be diagonalized down to the size of several hundreds.
Finally, several applications of these methods in the studies of organic solar cell materials will be briefly presented.

[1] N. Vukmirovic and L.-W. Wang, J. Chem. Phys. 128, 121102 (2008).
[2] N. Vukmirovic and L.-W. Wang, J. Chem. Phys. 134, 094119 (2011).
[3] N. Vukmirovic and L.-W. Wang, J. Phys. Chem. B 115, 1792 (2011).