Simulation Insights into Electronic Properties of Disordered Organic Semiconductors

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Organic semiconducting materials exhibit complex atomic structures with a lack of periodicity that lead to charge carrier localization which, in turn, strongly affects electronic transport properties of these materials. To understand charge carrier localization and electronic transport in organic semiconductors, simulations that take into account the details of the atomic structure of the material are of utmost importance. Computational methods that can be used to simulate the electronic properties of organic semiconductors are reviewed and an overview of some results that have been obtained from such simulations is given. Using these methods the effects of static disorder, thermal disorder and interfaces between domains are investigated and the microscopic origin of these effects is identified. It is shown that in strongly disordered conjugated polymer materials the main origin of the localization of charge carrier wave functions is disordered long-range electrostatic potential. In ordered polymers, thermal disorder of main chains leads to wave function localization. In small molecule based organic semiconductors, grain boundaries introduce localized trap states at the points where electronic coupling is the strongest. It is also demonstrated that detailed atomistic simulations are necessary for quantitative and sometimes even qualitative description of charge mobility in organic materials.

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