Multiscaled simulation of functional organic materials

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Abstract

We applied multiscaled simulation methods to investigate the properties of functional organic materials.

Combining first principle calculations and Marcus theory, we developed a theoretical model to accurately predict the anisotropic hole mobilities of organic semiconductors. The parameters needed in this model are only organic crystal structures. To project the hole transport to conducting channel, the calculated hole mobities showed anisotropic. We applied this model to calculate the anisotropic hole mobilities of ruberene, pentacene, tetracene, 5,11-dichlorotetracene and hexathiapentacene and obtained comparable results to experiments.[1] We also used this model to explain the metallic conductivity of interface between organic semiconductors. [2]

We developed a multiscaled model to predict the quantum conversion efficiency of a dye sensitized solar cell (DSSC). The first principle calculations were used to predict the adsorption spectrum of organic dyes and mesoscopic simulation were used to predict electron diffusion in nanostructured TiO2 thin films. Differential equations were solved combining all above simulations and obtained quantum conversion efficiency of DSSC. The simulation results from our model show reasonable agreement with experimental results.[3]

References:

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[2] Wen, SH; Deng, WQ; Han, KL "Ultra-low resistance at TTF-TCNQ organic interfaces" Chem. Comm. 46, 5133-5135, 2010

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