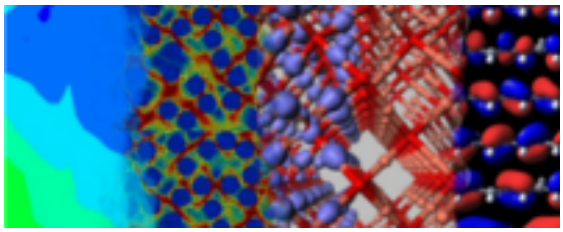

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Multiscale Modelling of Charge Transport in High mobility molecular semiconductor

Thursday, November 8, 2012 5:25 PM (10 minutes)

Recently, much attention has been paid to charge transport of high mobility molecular semiconductors [1]. Solution processed 6,13-bis(triisopropylsilyl ethynyl)- pentacene (TIPS-P) field effect transistors (FET) showed mobilities of up to 4.6 cm2/Vs [2] which is close to the performance of inorganic semiconductors. Until now most of the theoretical effort has been spent on a better understanding of the fundamental transport mechanism in these materials [3]. In this work we will present a multiscale approach to quantify the effect of anisotropy and structural defects on charge transport in high mobility organic materials. We prepared zone casted, large area 2D crystals of TIPS-P which show an anisotropic hole mobility in FET structures. Those TIPS-P crystals are used as a model system with which to test the capabilities of our simulation approach. In our multiscale approach charge transfer integrals and reorganization energies are calculated using semi-empirical quantum chemical methods. Either the Master equation or a Monte Carlo method is applied to estimate mobilities. Results are analysed in comparison with experimental data on TIPS-P FETs. We discuss how studies on this model system help to elucidate the role of anisotropy and structural disorder on charge transport and so help to develop design rules for high mobility molecular semiconductors. References

[1] Troisi A. Chem. Soc. Rev. 2011, 40, 2347-2358.
[2] Giri G, Verploegen E, Mannsfeld SCB, Athan-Evrenk S, Kim DH, Lee SY, Becerril HA, Aspuru-Guzik A, Toney MF, Bao Z. Nature. 2011, 480, 504-508.
[3] Geng H, Peng Q, Wang L, Li H, Liao Y, Ma Z, Shuai Z. Adv. Mater. 2012, 24, 3568-3572.

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