ATOMIC AND ELECTRONIC STRUCTURE OF GRAIN BOUNDARIES IN CRYSTALLINE ORGANIC SEMICONDUCTORS

Marko Mladenović, Igor Stanković, Nenad Vukmirović

Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, markoml@ipc.ac.rs

Organic crystalline semiconductors are very promising materials for electronic and optoelectronics devices, such as transistors, LEDs and solar cells [1]. Real organic semiconductors are polycrystals and therefore contain many contact interfaces (grain boundaries) between monocrystals with different crystalline orientations. Grain boundaries are believed to be bottlenecks to charge carrier transport in these materials [2].

We have developed a methodology for the investigation of the role of grain boundaries in polycrystalline organic semiconductors. The molecular structure is obtained using the united-atom description according to Transferable Potential for Phase Equilibria (TraPPE) methodology for the inter-molecular interaction [3]. A Monte Carlo algorithm is used for the minimization of the system energy and finding the equilibrium system structure [4]. The atomic structure of the material near the contact between two grains is calculated as a result of the energy minimization.

Electronic states near the grain boundaries are calculated using the charge patching method (CPM) [5]. Motifs for the CPM are generated from density functional theory (DFT) calculations [5]. CPM provides a similar accuracy as DFT but with a much smaller computational cost that allows us to calculate electronic states for systems composed of several thousand atoms, which is not feasible using DFT.

The methodology was applied to study the nature of electronic states introduced by grain boundaries in naphthalene crystals. The results obtained for the energies and the degree of localization of the wavefunctions will be presented and the consequences of the results for the device applications will be discussed.

This work was supported by a European Community FP7 Marie Curie Career Integration Grant (ELECTROMAT), the Serbian Ministry of Science (Project ON171017), Swiss National Science Foundation (SCOPES project IZ73Z0_ 128169), and FP7 projects (PRACE-1IP, PRACE-2IP, HP-SEE, and EGI- InSPIRE).

[1] S. Verlaak, P. Heremans, Phys. Rev. B 75 (2007) 115127
[2] A.B. Chwang, C.D. Frisbie, J. Appl. Phys. 90 (2001) 1342-1349
[3] M.G.Martin, J. I. Siepmann, J. Phys. Chem. B 102 (1998) 2569-2577
[4] M.P. Allen, D. J. Tildesley, Computer Simulation of Liquids, Oxford University Press, London, 1999.
[5] N. Vukmirovic, L.W.Wang, J. Chem. Phys. 128 (2008) 121102