Electronic structure of low-angle grain boundaries in naphthalene

Marko Mladenović, Nenad Vukmirović and Igor Stanković
Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Serbia
contact: marko.mladenovic@scl.rs

Introduction

- Organic semiconductors are promising materials for LEDs, transistors and solar cells
- Crystalline organic semiconductors form polycrystals
- Grain boundaries:
  - contact surfaces between different monocrystals
  - produce trap states for charge carriers
  - affect the performance of the devices
- We present a method for investigation of the role of grain boundaries in organic semiconductors
- Atomic structure: Monte Carlo algorithm

Model description

Two different monocrystals joined together

- Initial atomic structure
- DFT
- Final atomic structure
- Motifs
- Charge density
- Single-particle potential
- Folded spectrum method

- TraPPE [3, 4] potential for interaction between molecules
- Equilibrium at T = 300 K followed by slow cooling to 0 K

Electron charge density obtained by adding the motifs

Obtained from Poisson equation and LDA formula

Support:

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-2IP, PRACE-3IP, HP-SEE and EGI-InSPIRE).

Results

Angle between monocrystals is 5°

Atomic structure:
- Molecules at the grain boundary slightly change their orientations
- Nearly unchanged away from the grain boundary

Electronic structure:
- Three states with energies significantly higher than the other energies
- Wave functions of these states are localized on two molecules on the grain boundary with smallest mutual distances
- Remaining states are mostly delocalized

Discussion

- Grain boundaries in organic polycrystals:
  - have small impact on atomic structure
  - introduce localized states in the energy band gap of a material
- Localized states at the grain boundary are trap states for charge carriers
- In the devices which operate in low carrier concentration regime, such as LEDs and solar cells, traps reduce carrier mobility
- Traps broaden absorption and emission spectrum

References: