Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensend Matter Physics
of Charles University has a pleasure to invite you to attend the seminar

on 16 May 2019 at 13:00

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

Seminar room F052

RNDr. Petr Toman, Ph.D.

Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Charge transport in lamellar structure of linear conjugated polymers

The charge carrier transport in many linear conjugated polymers (e.g. polythiophene derivatives) proceeds predominantly by hopping among essentially parallel conjugated chain segments oriented perpendicularly to the nanofiber direction. While various previous charge transport models used for disordered organic solids are usually based on a cubic lattice of single-state point centers, in which the charge carriers may be localized, the charge carrier states in conjugated polymers are delocalized and their density of states creates a band-like structure. Thus, we combine a quantum mechanical calculation of the on-chain charge carrier states together with a semi-classical description of the inter-chain hopping.

The proposed model was used for calculation of the hole mobility in an active layer of the organic field-effect transistor (OFET), namely its dependences on the energetic disorder, hole concentration, and the longitudinal (between source-drain electrodes) and transverse (gate) electric field [1,2]. Obtained results among others predict qualitatively different transverse field dependences for the gate fields oriented either parallel or perpendicular to the local chain segment alignment. We believethese findings can be useful for macroscopic simulations of electrical characteristics of the OFETs and other electronic devices based on linear conjugated polymers. It is particularly important for analyses of these characteristics aimed to better understanding phenomena influencing the charge transport near the organic semiconductor–insulator boundaries, which are very important for the optimal and stable performance of organic electronic devices.

[1] P. Toman, M. Menšík, W. Bartkowiak, J. Pfleger, Physical Chemistry Chemical Physics 19, 7760 (2017)
[2] P. Toman, M. Menšík, J. Pfleger, Chemical Papers 72, 1719 (2018)