

Abstract of Presentation

Presentation Title(Should be no more than 20 words):

Structure-property relations for organic semiconductors: a theorist's approach

Abstract :

Conjugated materials offer the revolutionary prospect of producing semiconductor devices at low cost. Their performance is, however, limited by the morphological disorder which prevents efficient electronic coupling and reduces their charge carrier mobility. To improve the performance, clear structure-property relationships shall be formulated which would allow rational design of these compounds. An overview of the recent advances in theoretical modeling will be presented for several classes of organics materials, such as discotic liquid crystals and small aromatic molecules.

1. J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer, D. Andrienko, Phys. Rev. Lett., 98, 227402, 2007
2. J. Kirkpatrick, V. Marcon, K. Kremer, J. Nelson, D. Andrienko, J. Chem. Phys., 129, 094506, 2008
3. V. Marcon, J. Kirkpatrick, W. Pisula, D. Andrienko, Phys. Stat. Solidi B, 245, 820, 2008