Multiscale modelling of Organic Devices

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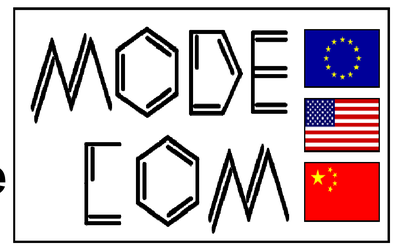
Modelling ElectroActive Conjugated polymers at the Multiscale



Abstract

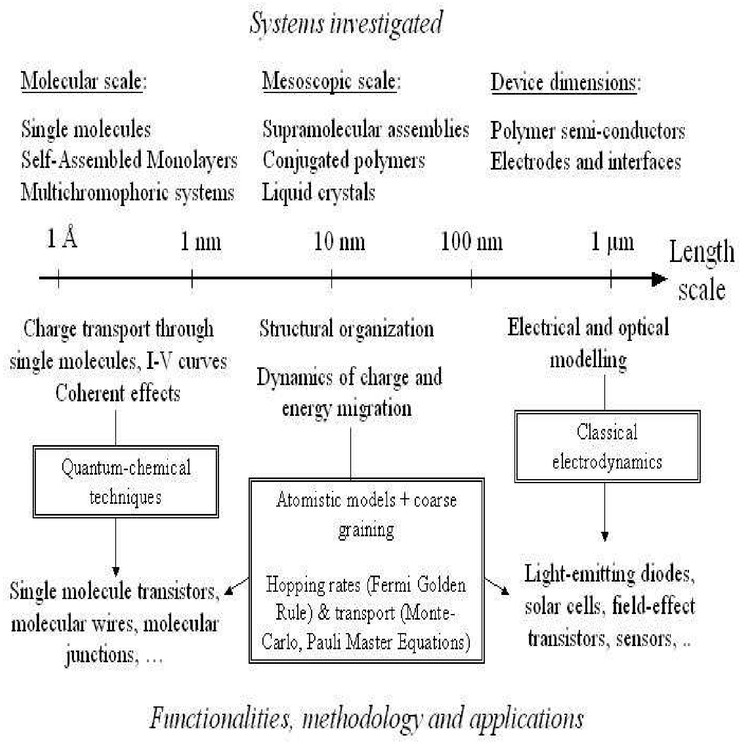
This poster describes the work of Modecom, a European Union Specific Targeted Research Project funded by the Framework 6 programme Oct 2006- March 2010.

Aims and Objectives

Our goals are:

i. to obtain accurate estimates of all basic microscopic parameters that control electron and energy transfer processes
ii. to develop theoretical models establishing a coherent connection between the microscopic parameters and the macroscopic description (verified by data from ultrafast spectroscopy, photoelectron spectroscopy and transport measurements)
iii. to determine reliable structure-transport property relationships that bridge the molecular scale, mesoscale and the macroscopic device scale.

This multiscale approach relies on powerful computational methods developed from quantum chemistry, condensed matter physics and statistical mechanics. We have shown how the organisation and structural properties of organic materials determine the transport properties of charge carriers and excitons, especially in device architectures, needed for technologies exploiting organic materials.



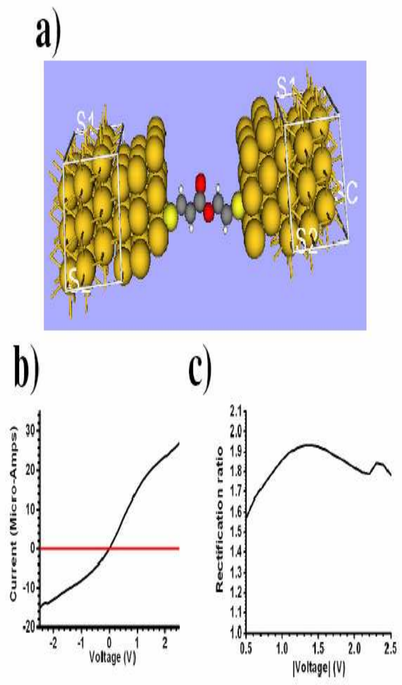
Examples of Modecom research below
For more information, see http://www.modecom-euproject.org

Possible applications of organic devices

Sony OLED TV

Flexible display

Workpackage 1: Calculations at the molecular scale



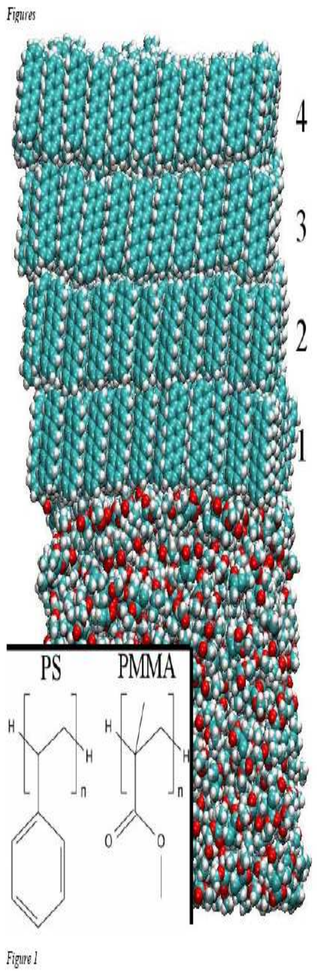
a) Single-molecule nanojunction with a molecule connected to gold electrodes via thiol groups

b) Calculated I/V curve for this junction

c) Rectification ratio: the ratio of the current in forward and reversed bias directions as a function of the applied voltage.

R. Stadler, V Geskin, J Cornil Phy. Rev B 78 113402 (2008)

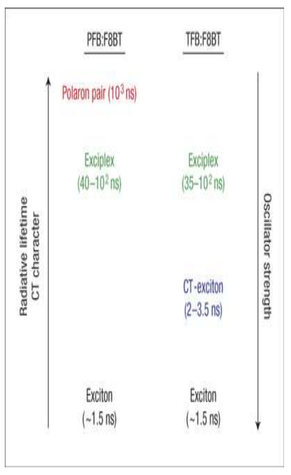
Workpackage 2: Supramolecular organization



Atomistic description of the pentacene/ polymethylmethacrylate dielectrics interface. The inset shows the chemical structures of the two polymers dielectrics studied.

N. G. Martinelli, M. Savini, L. Muccioli, Y. Olivier, F. Castet, C. Zannoni, D. Beljonne, J. Cornil, Adv. Functional Mater., early view (2009)

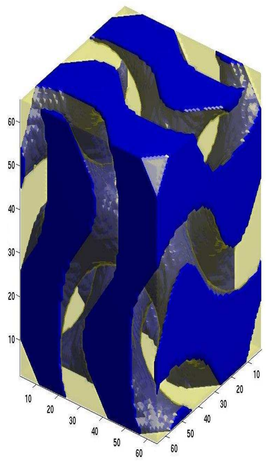
Workpackage 3: Dynamics of charge and energy transport at the mesoscale



The electronic excitations taking place at the heterojunctions of PFB:F8BT and TFB:F8BT (conjugated polymer) blends

Y-S Huang, SWestenhoff, I Avilov, P Sreearunothai, J M. Hodgkiss, C Deleener, R H. Friend, D Beljonne Nature Materials 7, 483 (2008)

Workpackage 4: Measurements and macroscopic modelling for polymer devices



Novel bicontinuous morphologies for organic solar cells

R G E Kimber. A. B. Walker, G. E. Schröder-Turk, D. J. Cleaver PhysChemChemPhys (2009)

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