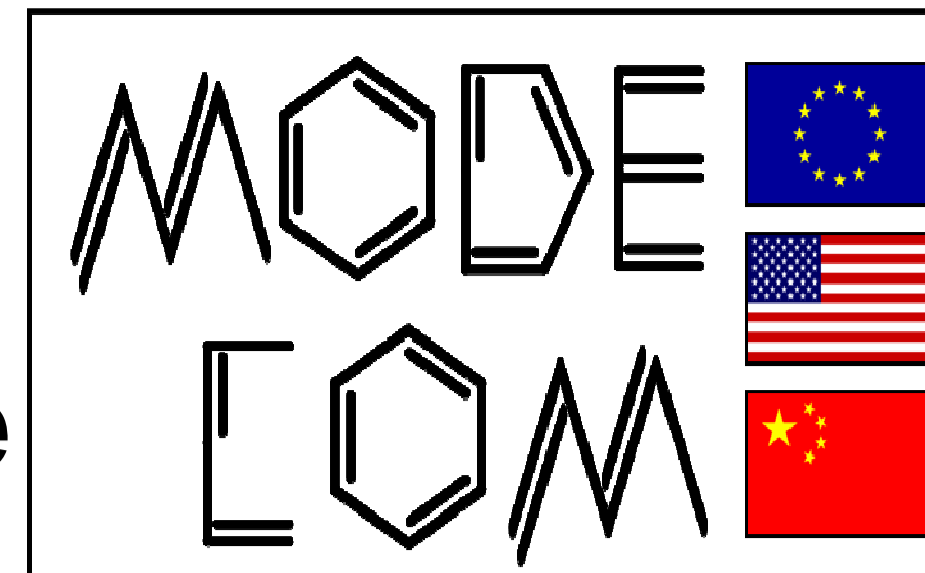


# Multiscale modelling of Organic Devices

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Modelling  
ElectroActive  
Conjugated  
polymers at the  
Multiscale



## Abstract

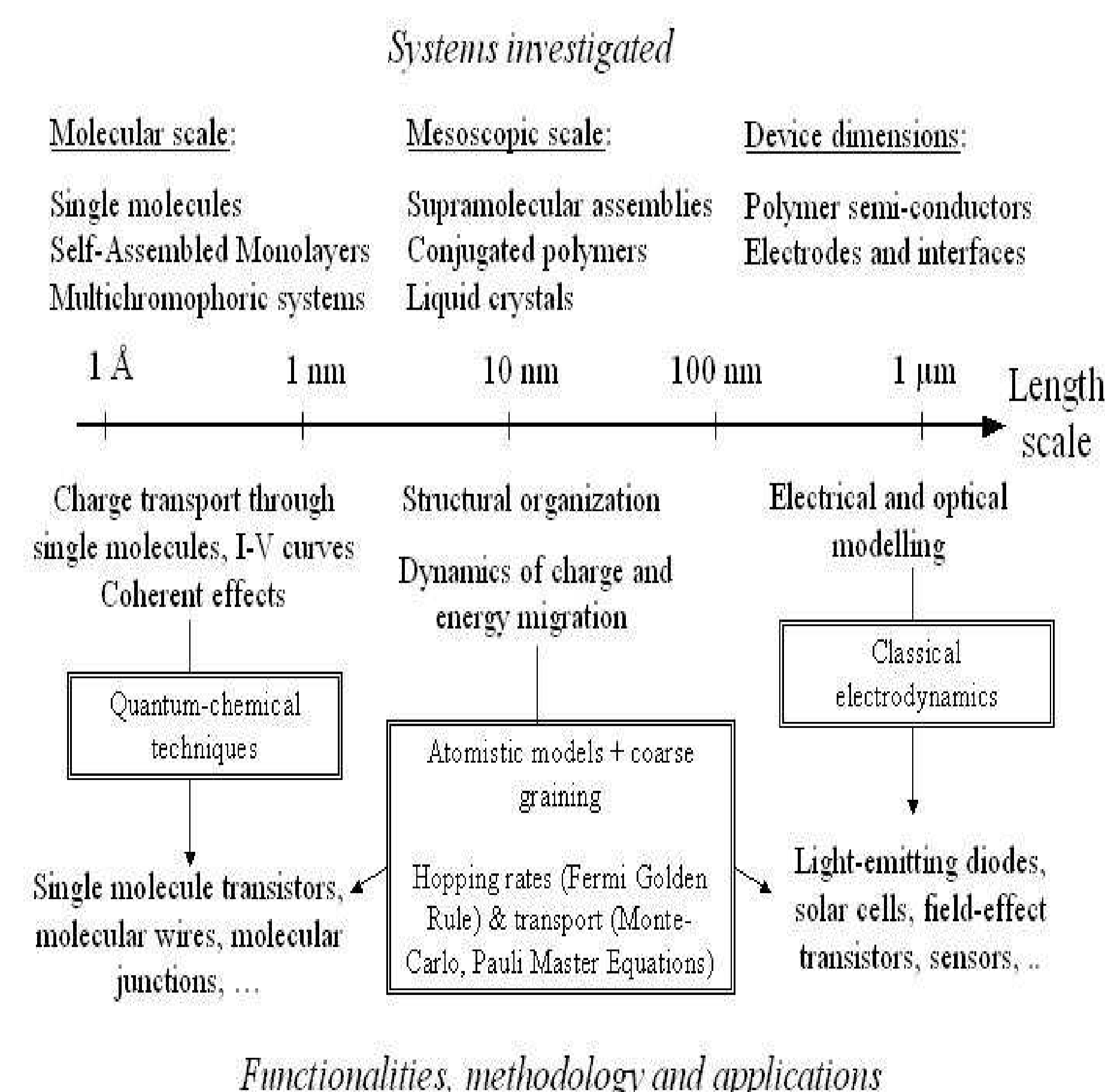
This poster describes the work of Modecom, a European Union Specific Targeted Research Project funded by the Framework 6 programme Oct 2006- March 2010.

## Aims and Objectives

Our goals are:

- to obtain accurate estimates of all basic microscopic parameters that control electron and energy transfer processes
- 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)
- 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

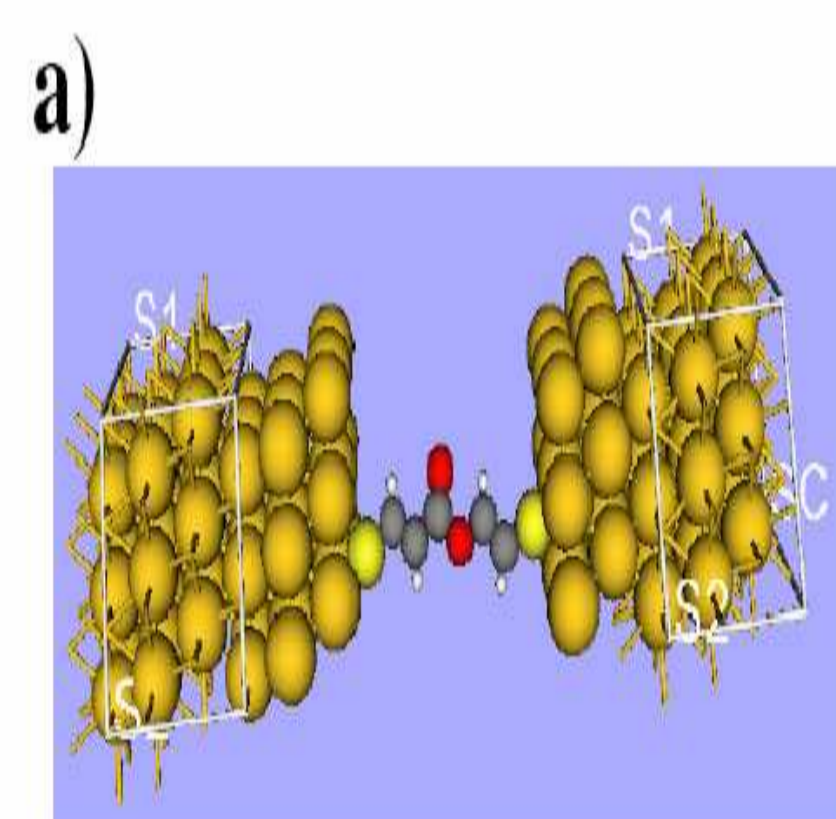


Sony  
OLED  
TV

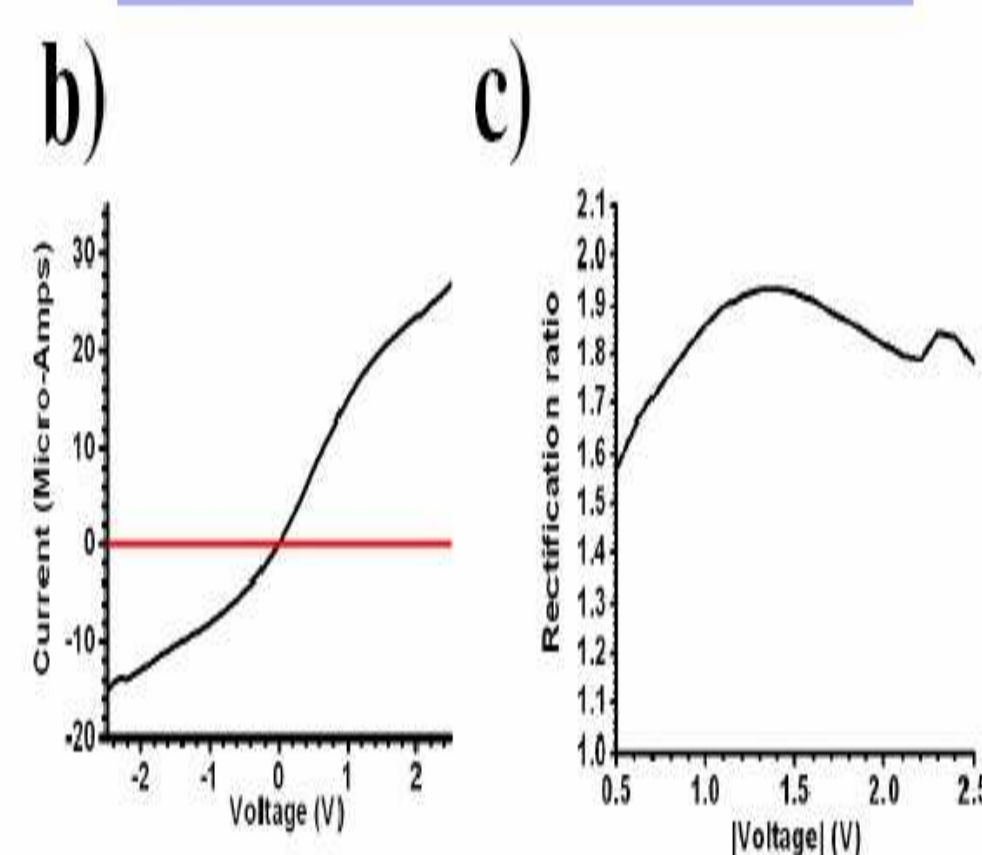


Flexible  
display

## Workpackage 1: Calculations at the molecular scale



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

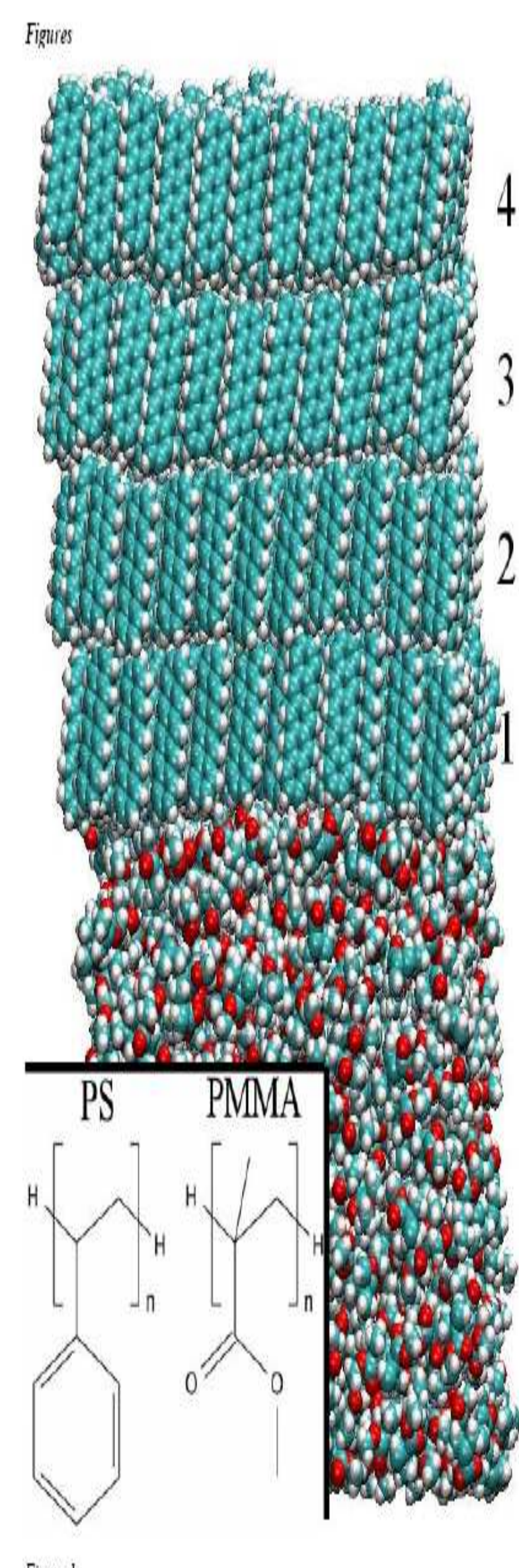


b) Calculated I/V curve for this junction

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

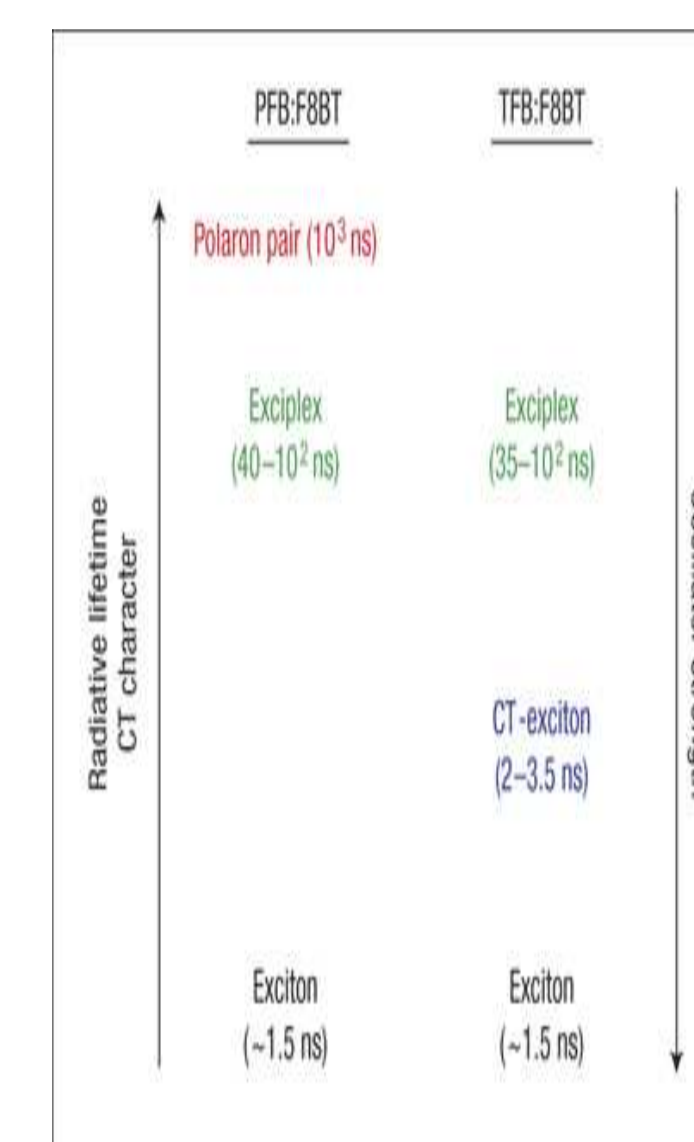
R. Stadler, V Geskin, J Cornil *Phy. Rev B* 78 113402 (2008)

## 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)

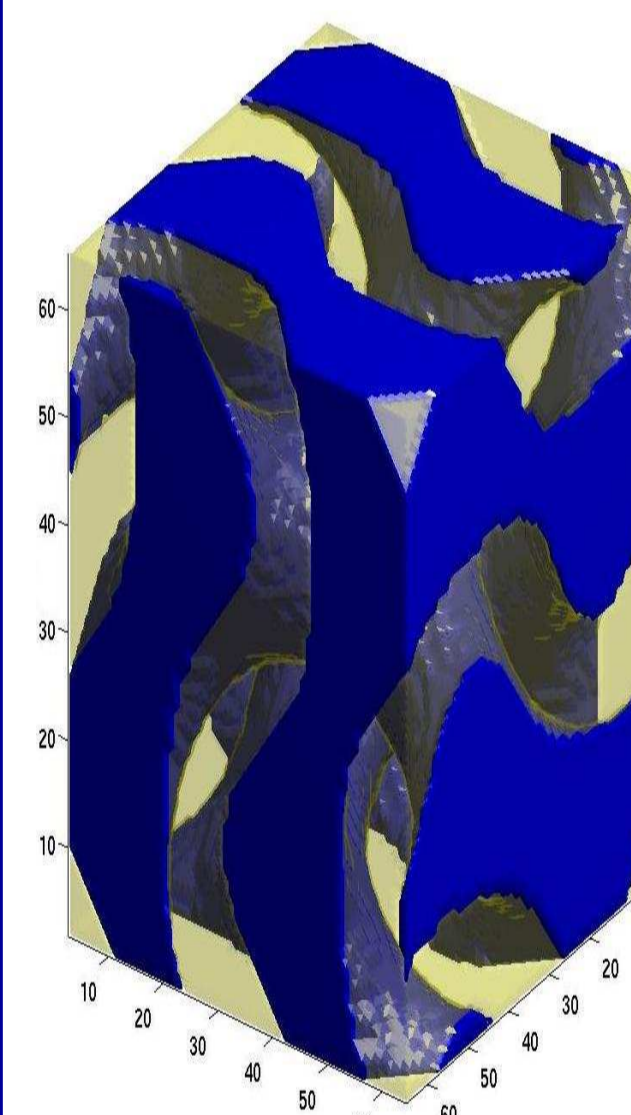
## Workpackage 3: Dynamics of charge and energy transport at the mesoscale



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)

## Modecom partners

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