



Modelling charge transfer in P3HT/PCBM/SWNT hybrid systems

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Introduction

Organic Photovoltaics & Delta SCF
P3HT/(PCBM)/(6,5)-SWNT heterojunctions

Experimental Data

Transient Absorption Spectroscopy on a P3HT/PCBM/SWNT blend

Results

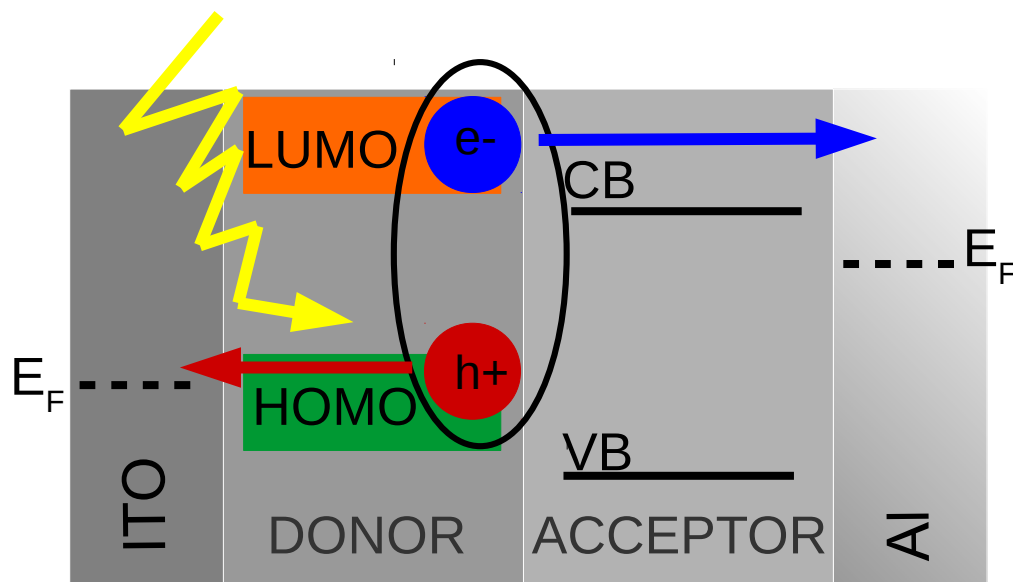
Kohn-Sham eigenvalues of ground state
Kohn-Sham eigenvalues E11 excited state from Delta SCF
Isosurfaces of E11 exciton from Delta SCF

Discussion

Introduction

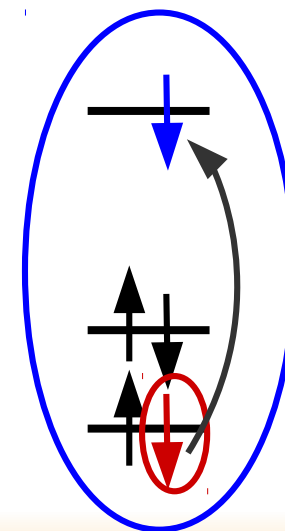


Working principle of an Organic Photovoltaic Device:
Type II heterojunction



Linear expansion Delta SCF [1]:

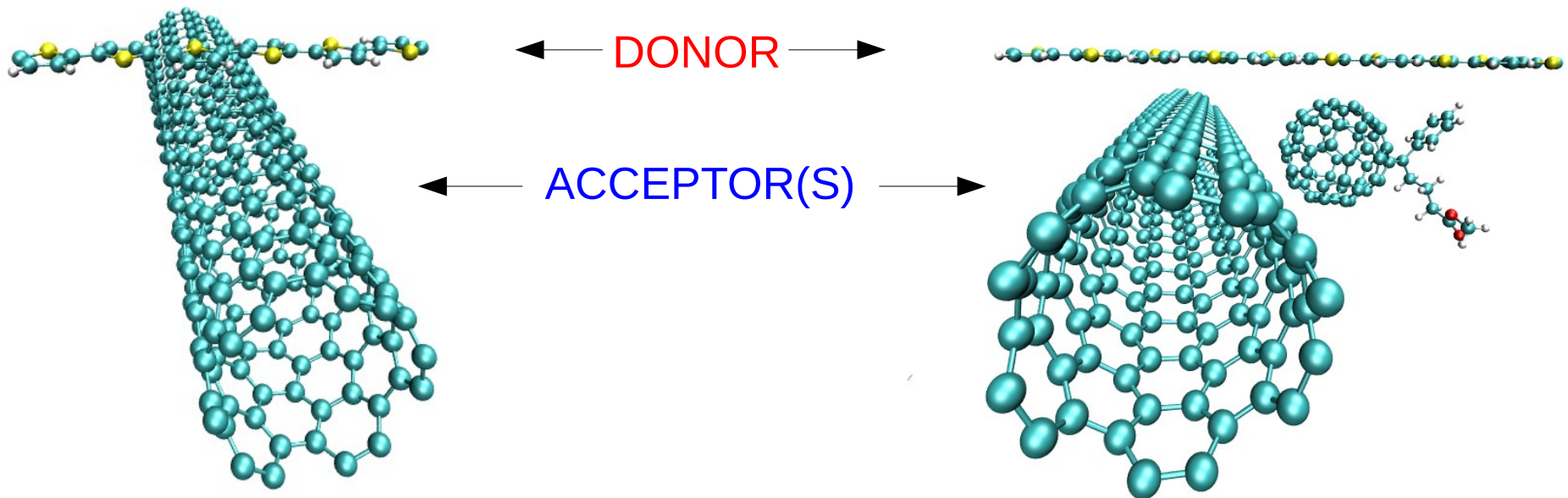
$$n(r) = \sum_n f_{N+1}(T, \varepsilon_n) |\varphi_n(r)|^2 - |\varphi_a(r)|^2$$



Introduction



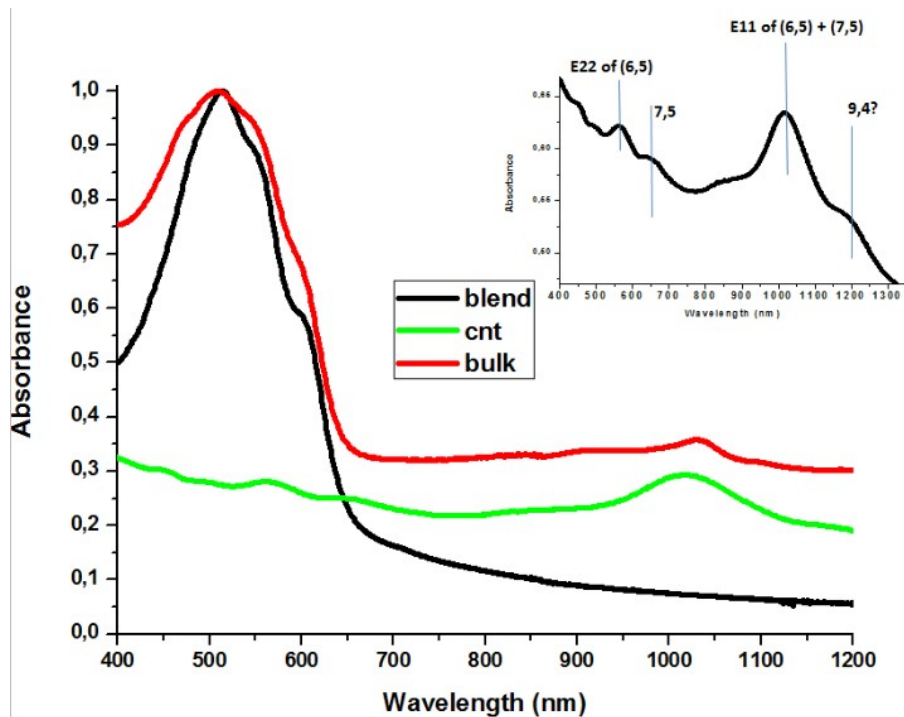
P3HT/6,5-SWNT & P3HT/PCBM/SWNT heterojunctions:



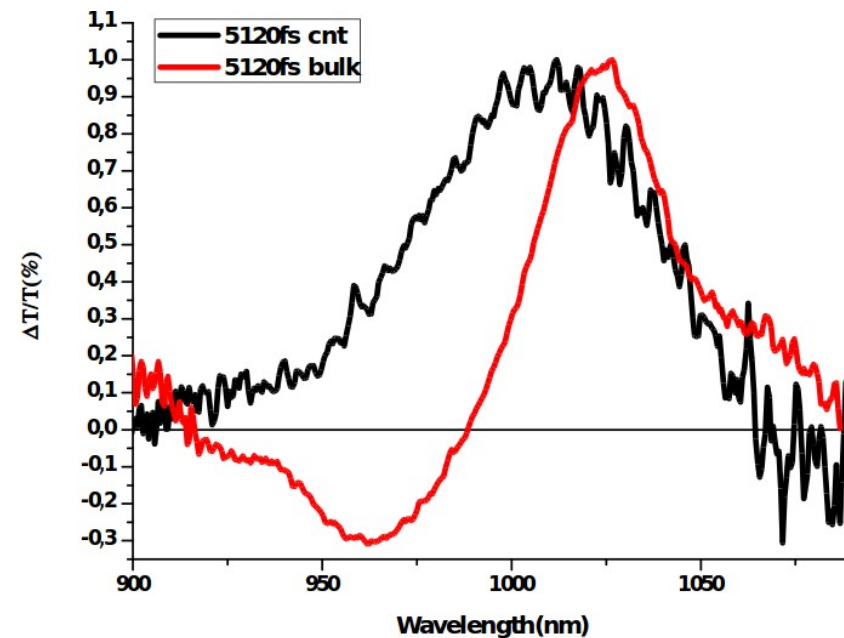
A
P3HT/(6,5)-SWNT

B
P3HT/PCBM/(6,5)-SWNT
(direct neighbors)

Experimental Data



Absorption spectra of SWNT sample (green), the P3HT/PCBM blend (black), P3HT/PCBM/SWNT bulk (red)[2].

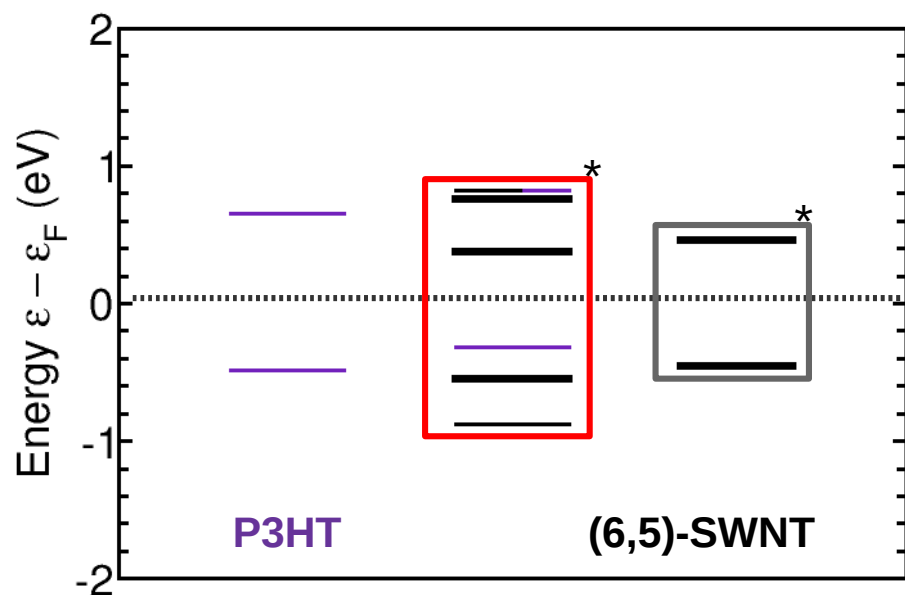


Transient absorption spectra of SWNT sample (black), P3HT/PCBM/SWNT bulk (red)[2].

Results



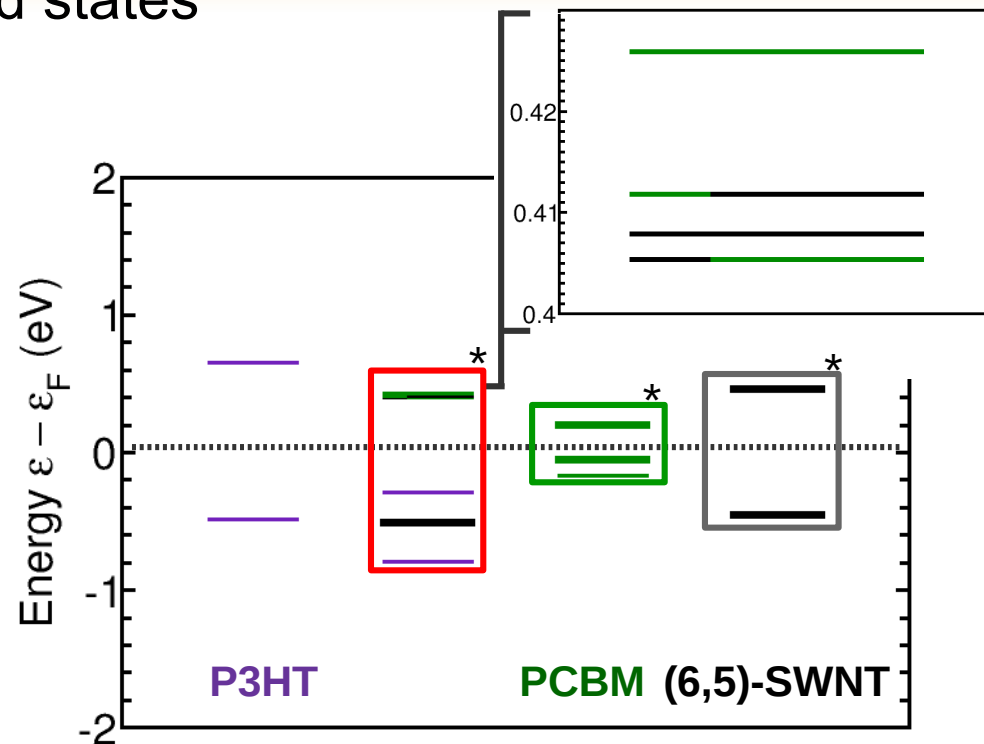
Kohn-Sham eigenvalues of the ground states



A P3HT/(6,5)-SWNT

Charge transfer:

P3HT \longrightarrow (6,5)-SWNT: 0.2 e^-



B P3HT/PCBM/(6,5)-SWNT

Charge transfer:

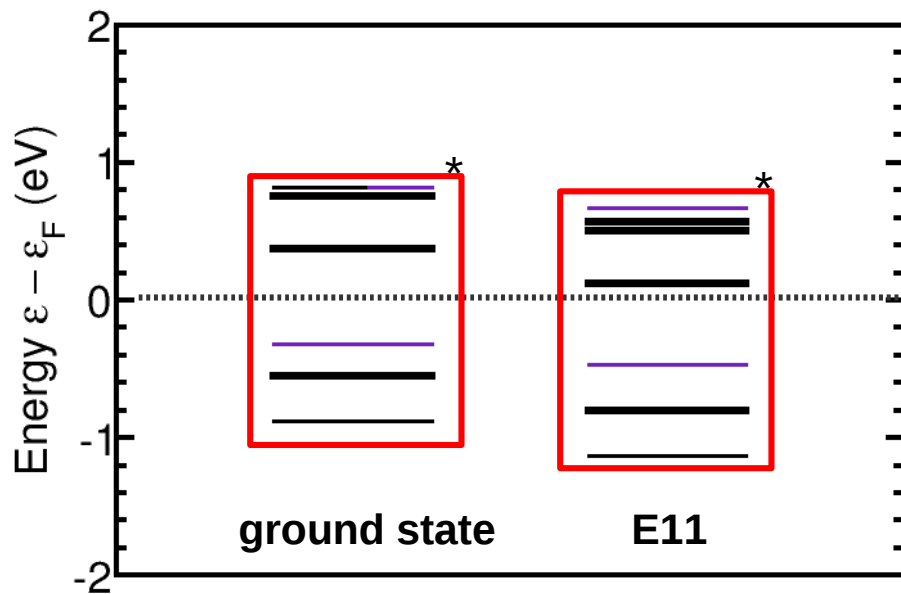
P3HT/(6,5)-SWNT \longrightarrow PCBM: 0.4 e^-

*only levels in in the energy range of the box are shown.

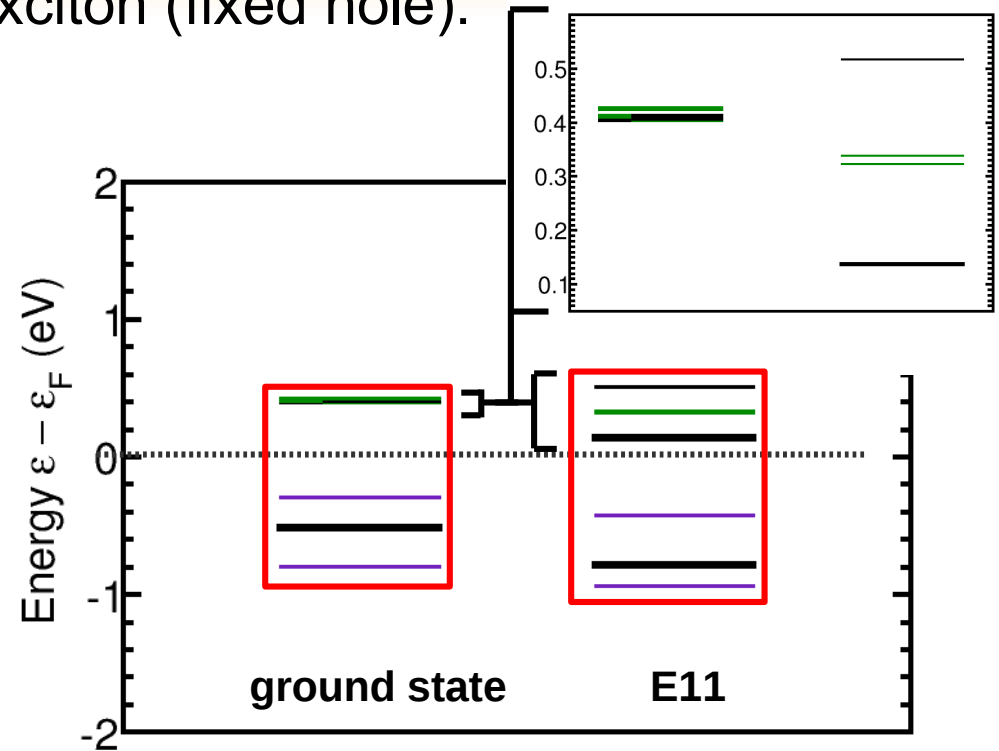
Results Delta SCF



Kohn-Sham eigenvalues of the E11 exciton (fixed hole):



A P3HT/(6,5)-SWNT



B P3HT/PCBM/(6,5)-SWNT

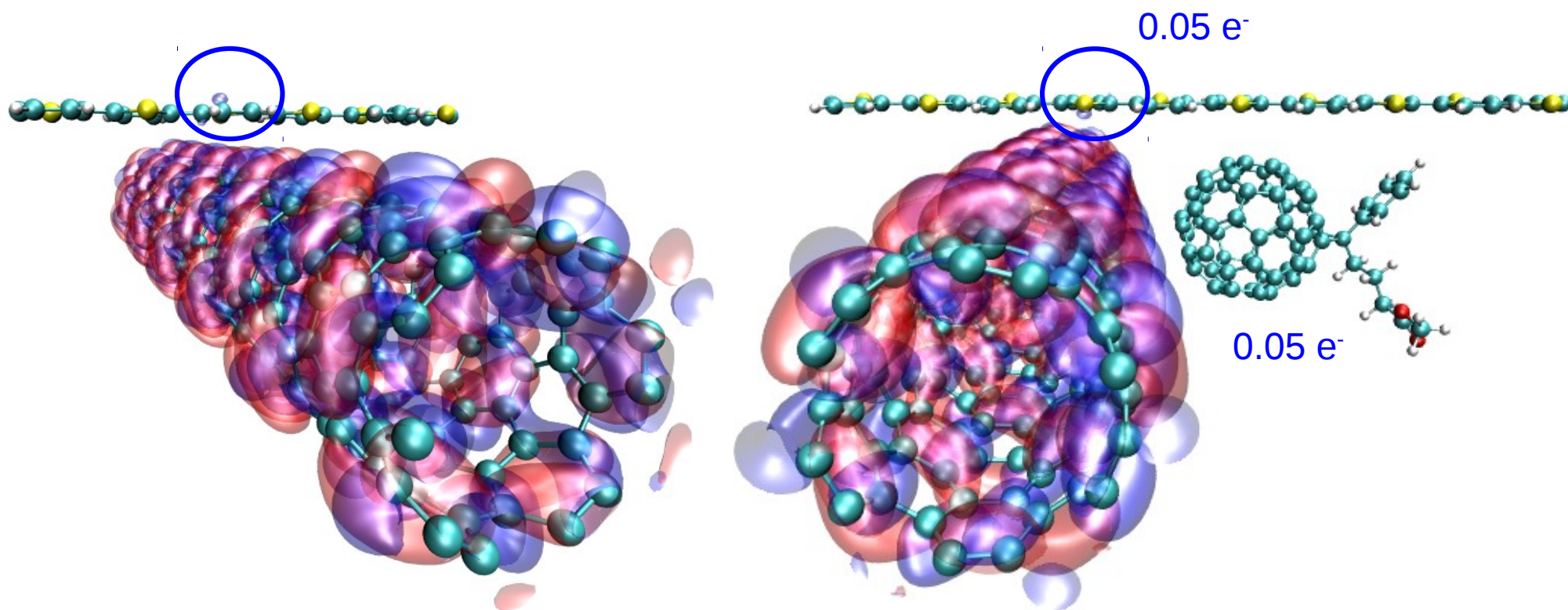
Charge transfer:
P3HT/(6,5)-SWNT \rightarrow PCBM: 0.4 e^-

*only levels in in the energy range of the box are shown.

Results Delta SCF



Isosurface of HOMO-1/LUMO of Delta SCF:



A
P3HT/(6,5)-SWNT

B
P3HT/PCBM/(6,5)-SWNT

Electron transfer of 10%

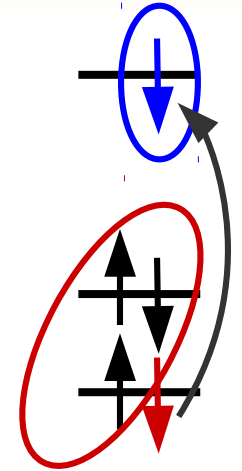


- full description of E11 Exciton:
Converging of the hole

$$n(r) = \sum_n f_{N-1}(T, \varepsilon_n) |\varphi_n(r)|^2 + |\varphi_a(r)|^2$$

hole transfer?

- photoinduced absorption?





Thank You!

