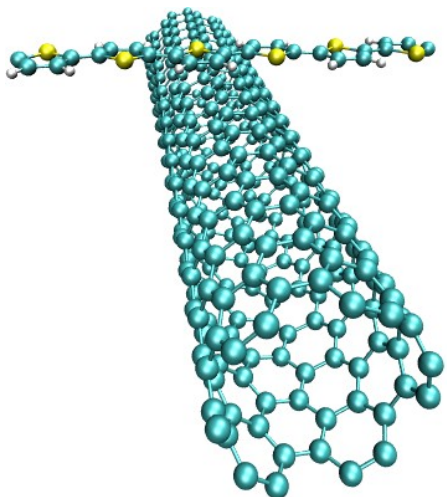




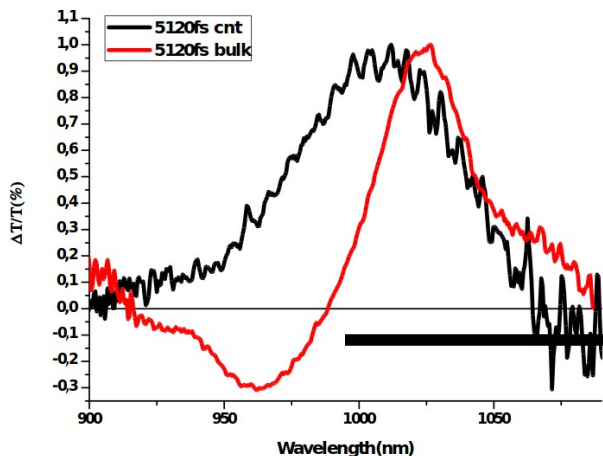
Multi-scale modelling of photoexcitation dynamics in medium-large systems

Livia Noemi Glanzmann (ESR/Er 4)

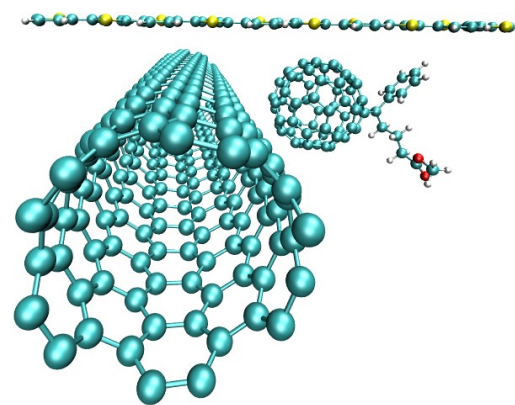
University of the Basque Country UPV-EHU



A
 P3HT/(6,5)-SWNT

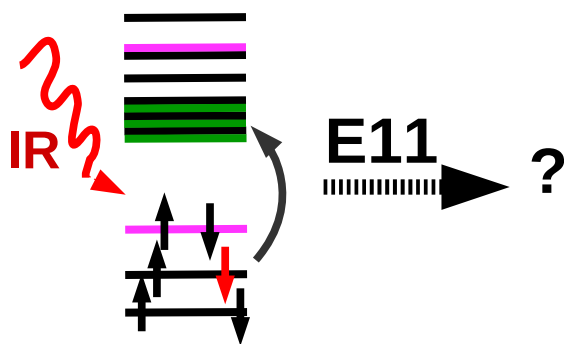


Transient absorption spectra of SWNT sample (black), and P3HT/PCBM/SWNT bulk (red)[1].
 [1] D. Figueroa del Valle, will be published.

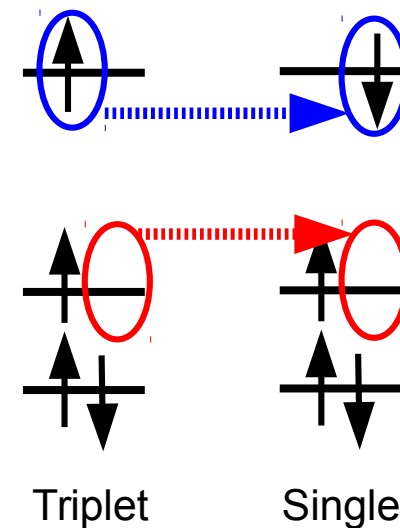


B
 P3HT/PCBM/(6,5)-SWNT

Modelling the E11 exciton via triplet state & DeltaSCF:

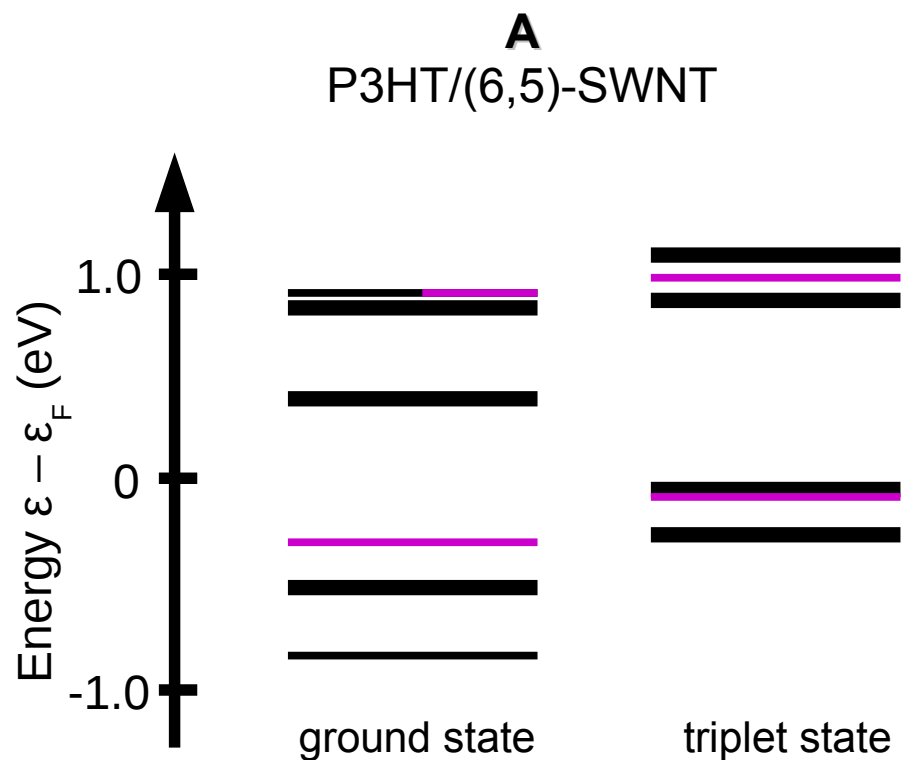


Ground state
 Type II hetero junction

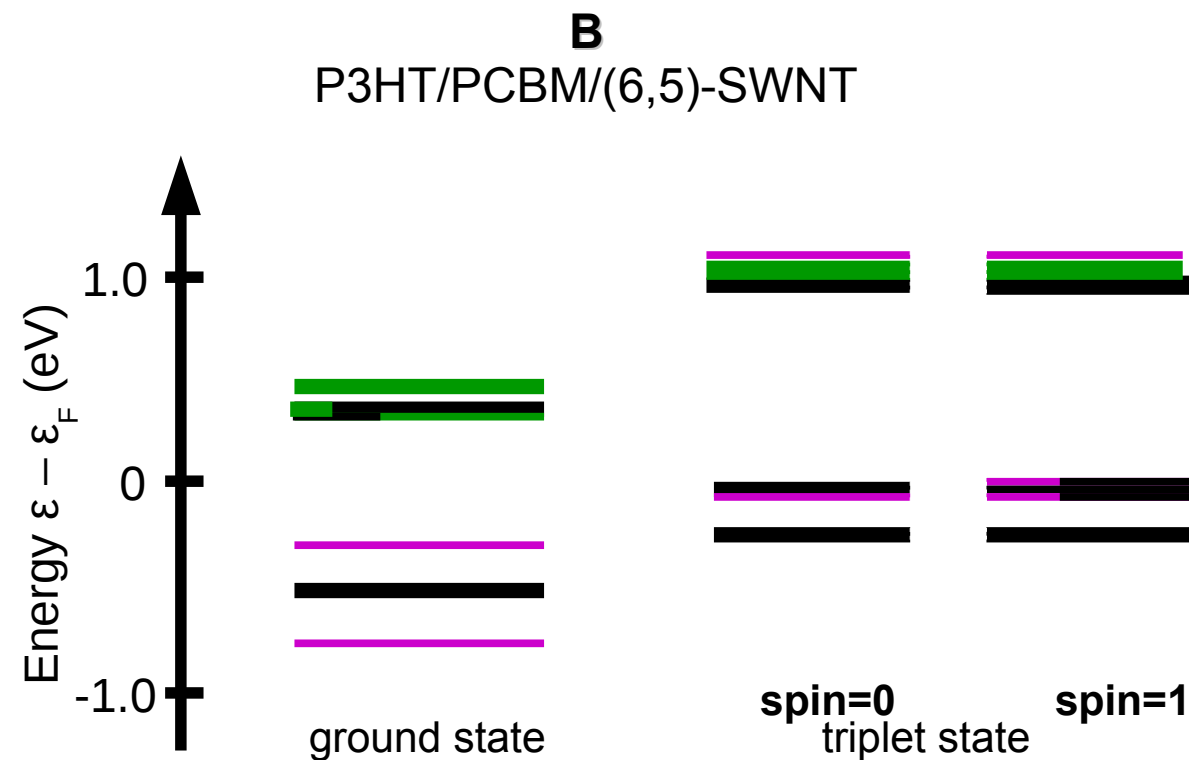


Triplet

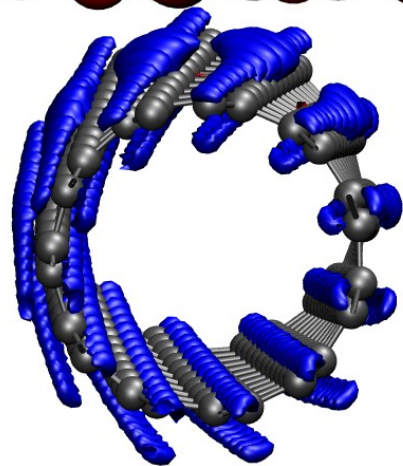
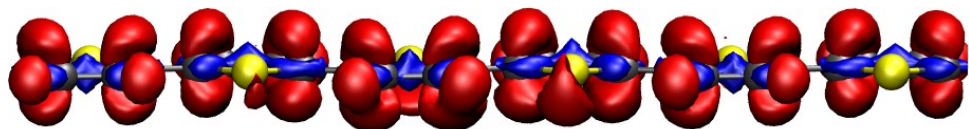
Singlet



Charge transfer ground state:
 P3HT +0.15 e (6,5)-SWNT -0.15 e
triplet state:
 P3HT +0.31 e (6,5)-SWNT -0.31 e



Charge transfer ground state:
 P3HT +0.22 e (6,5)-SWNT +0.17 e PCBM -0.39 e
triplet state:
 P3HT +0.45 e (6,5)-SWNT +0.04 e PCBM -0.49 e

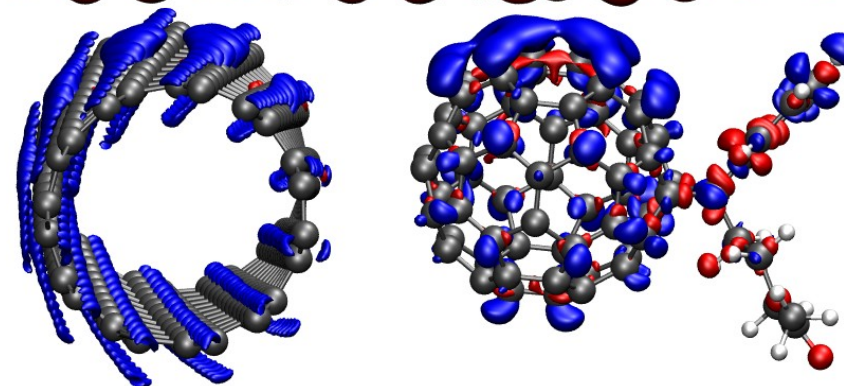
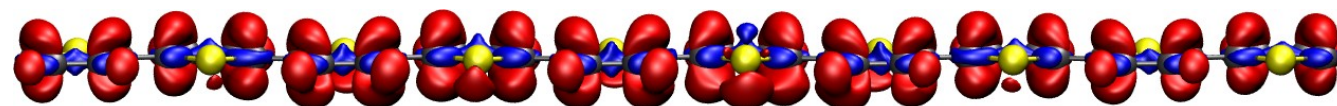


A
P3HT/(6,5)-SWNT

Difference in electron densities:
Triplet density – ground state density

=

electron and hole densities



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

Conclusion


- Charge redistribution \longrightarrow Polaron formation
- P3HT hole/e-donor – tube electron/e-acceptor
- Shifting of levels (less mixed levels)

Outlook

- Model the isolated tube exciton (reference)
- DeltaSCF
- Relaxing the triplet state
- Check for photoinduced absorption via RPA-TDDFT

- IIT Milano, 01/02/2015-25/04/2015, 3 months
- IMDEA, 2-3 months, still planned to do







- Deutsche Physikalische Gesellschaft-Frühjahrstagung, Berlin, 15/03-20/03/2015: Presentation



Universidad del País Vasco

Modelling charge transfer
in P3HT/PCBM/SWNT hybrid systems

Livia N. Glanzmann, Duncan J. Mowbray, and Angel Rubio

DPG-Frühjahrstagung Berlin
17/03/2015

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THANKS FOR YOUR ATTENTION!