Exitons in P3HT/SWNT/PCBM Heterojunctions

L. N. Glanzmann[1], D. J. Mowbray[1], and A. Rubio[1,2]

1 Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC, Universidad del País Vasco UPV/EHU, Av. Tolosa 72, E-20018 San Sebastián, Spain
2 Max Planck Institute for Structure and Dynamics of Matter, Hamburg, Germany

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

Introduction

Semiconducting single walled carbon nanotubes (s-SWNT) are known for their high charge carrier transport. Thus, they are promising electron transporting materials for photovoltaic (PV) active layers[1] of organic solar cells (OSCs). An increase in efficiency is found by adding s-SWNTs next to a donor (D) and acceptor (A) heterojunction such as P3HT and PCBM[1]. Pump probe spectroscopy is used to follow the exciton dynamics through these active layers. However, such multi-component spectra are difficult to interpret. To disentangle the various processes, we use the triplet state of the system to model the evolution of the lowest energy s-SWNT excited state (E11). Specifically, using the electron (spin majority channel) and hole (spin minority channel) density distributions for the triplet state, we find where electrons and holes are transferred within the active layer. Further, applying a non-equilibrium Green's function (NEGF) approach, we obtain the rate of D to A charge transport.

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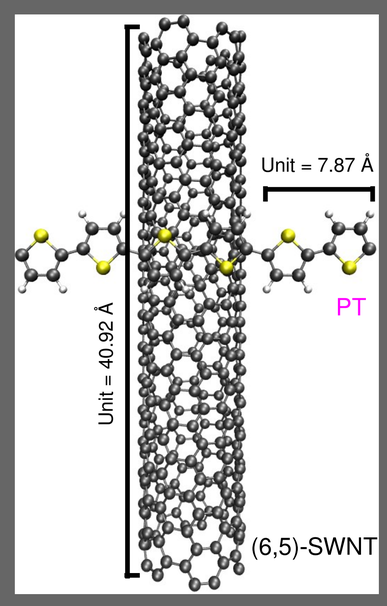
Methodology

All total energy calculations and structure optimizations have been performed with the DFT code GPAW[2] using a DZP LCAO basis set[3], and the PBE exchange and correlation (xc)-functional[4].

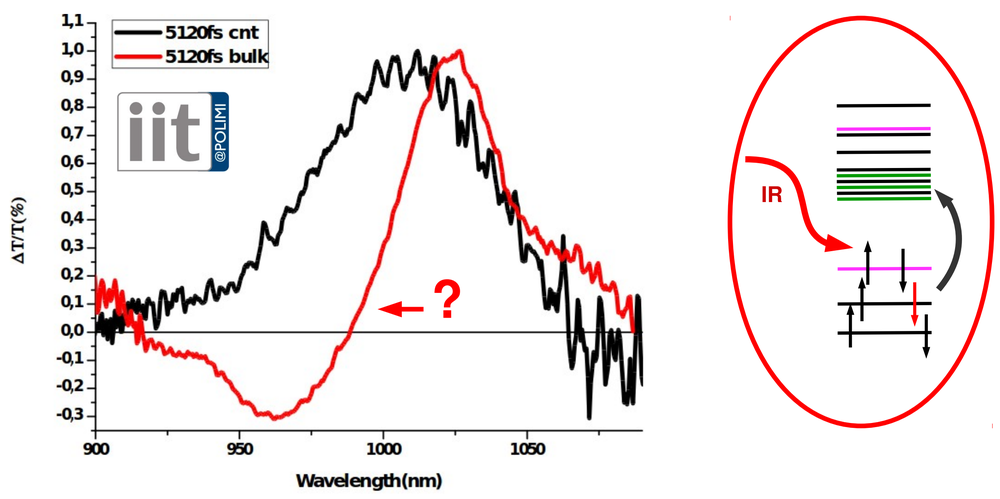
The system consists of a (6,5)-SWNT and a perpendicularly aligned planar s-trans polythiophene (PT) without side chains as a simplified model for P3HT. The relaxed molecules were positioned 3.4 Å apart.

The triplet state was calculated by fixing the total magnetic moment of the system to 2 μ_B.

The 4 terminal NEGF calculations were performed using our own implementation described in Ref 5.

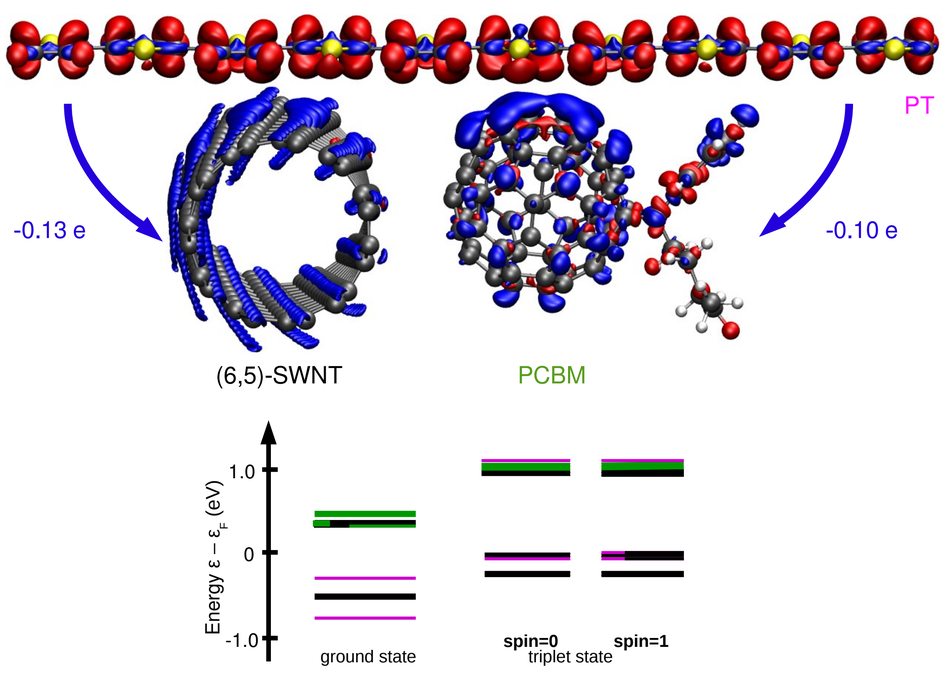


Triplet in P3HT/SWNT/PCBM heterojunctions

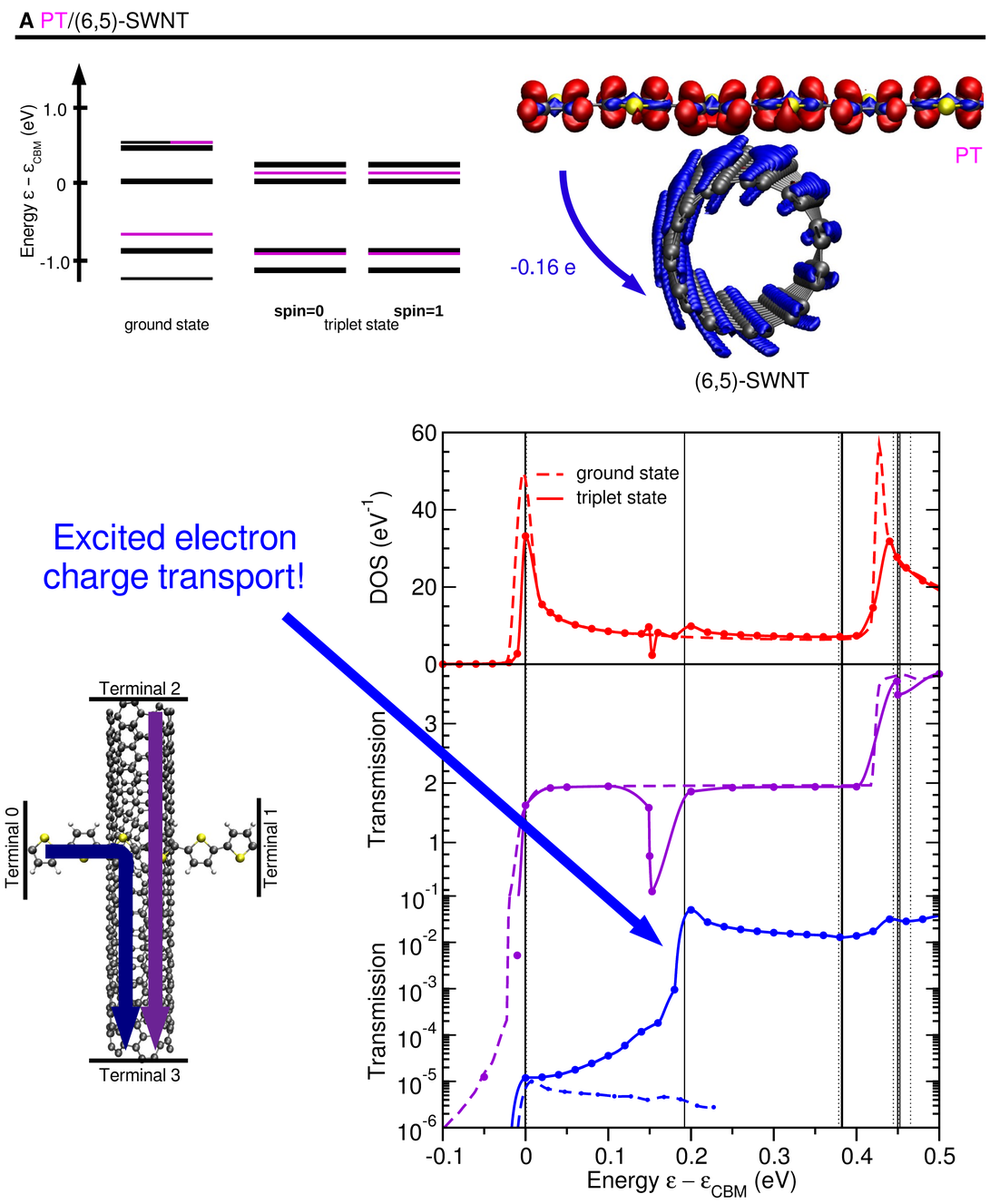


Transient absorption spectra of SWNT sample (black), and P3HT/PCBM/SWNT bulk (red)[1].

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



Transport through PT/SWNT heterojunctions



Conclusion

We find a significant increase in charge transfer from the PT to the SWNT/PCBM in the excited state. The hole transfer to P3HT may explain the negative photoabsorption peak measured for P3HT/SWNT/PCBM[1]. More importantly, we find the charge transport between PT and a (6,5) SWNT increases by four orders of magnitude when the system is in the excited triplet state. This may explain the observed increase in efficiency of photovoltaic devices upon including s-SWNTs at the electrode[1]. Our work provides a framework for describing quantitatively photoelectric processes in multi-component systems.

Acknowledgments

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References

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