Contribution submission to the conference Berlin 2015

Modelling charge transfer in Polymer/SWNT/PCMB hybrid systems — •Livia Glanzmann, Duncan Mowbray, and Angel Rubio — Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, Av. Tolosa 72, E-20018 San Sebastian, Spain

One way to increase power conversion efficiencies of organic photovoltaic devices (OPVs) is to optimize the electron donor (D) acceptor (A) materials. The level alignment of the frontier orbitals at the D-A heterojunction interface is important for an efficient charge transfer. Since the first heterojunction OPV, consisting of 3-alkylpolythiophene (P3HT) and Fullerene, several combinations of D-A materials were tested. As well, carbon nanotubes were introduced, which increased the efficiency of such multi-component systems. Still, the electronic processes within such systems are not well understood. To shed light on this subject, we simulate photovoltaic processes occuring in selected sets of P3HT-based-Polymer/SWNT or PCBM heterojunctions. As a first step, we create the excited states within the donor materials by performing TDDFT calculations and extract the electron density of the exciton. Then, we use the delta SCF approach to study the D-A electron transfer. On top, we calculate the probability of an electron passing the D-A interface and being transported through a nanotube by performing G0W0 calculations. All these results show the effect of certain types of D-A material, as well of their level alignment, on the efficiency of OPVs.

Part:	**CPP**
Type:	**Vortrag;Talk**
Topic:	**Organic Electronics and Photovoltaics (joint sessions DS/HL/O/CPP)**
Email:	**livia.glanzmann@gmail.com**