Organic Semiconductors Explored With Ab-initio Electronic Structure Methods

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Functional organic molecules form the basic building blocks for both low cost, large area and new nano-scale organic electronic devices, ranging from solar cells over light emitting diode displays to chemical sensors. It is becoming increasingly clear that if devices based on organic materials are ever going to have a significant relevance, one will need to achieve a fundamental understanding of their intrinsic electronic structure, and in particular of the properties of organic-organic and organic-inorganic interfaces. Here, insight from *ab-initio* electronic structure theory can provide valuable insights.

By discussing four exemplary cases, I will show how density functional theory (DFT) and many-body perturbation theory methods, i.e., the *GW* approximation for the quasi-particle band structure and the solution of the Bethe-Salpeter equation (BSE) for electron-hole pair excitations, shed light on the fundamental electronic and optical properties of organic molecules. Firstly, the relevance of van der Waals interactions for the bonding in these materials will be emphasized and results from the Langreth-Lundqvist functional will be presented. In the second example, a simple but powerful relation between the angleresolved photoemission intensity and spatial distribution of molecular orbitals will be established. This allows a very detailed comparison between theoretical predictions and photoemission experiments and thereby a benchmarking of exchange-correlation functionals in terms of orbital energies and ordering. Thirdly, the interface of a conducting polymer with graphene is studied by applying quasi-particle corrections at the G_0W_0 level. This model interface emphasizes that in order to obtain the correct level alignment at the interface, the band structure normalization arising from polarization effects, which are absent in the DFT approach, must be taken into account. Finally, optical properties of socalled nano-peapods calculated by solving the BSE for electron-hole pair excitations are presented. In these materials, which consist of organic molecules encapsulated inside of single-walled carbon nanotubes (SWCNT), the optically excited state gives rise to the formation of novel hybrid excitons, in which the SWCNT and the polymer are strongly coupled.