ELECTRONIC PROPERTIES OF PPP@ZnO FROM ALL-ELECTRON QUASIPARTICLE CALCULATIONS

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We investigate the electronic properties of poly(*para*-phenylene) (PPP) adsorbed on the non-polar (001) surface of rocksalt (*rs*) ZnO using all-electron density functional theory (DFT) as implemented in the *exciting* code [1] as well as the *GW* method to treat quasiparticle excitations within many-body perturbation theory. A comparison of the derived electronic band offsets at the interface with various mesoscopic alignment methods, such as the Shockley-Anderson approach [2] or the alignment via the electrostatic potential [3] shows the inadequacy of these methods for molecular adsorption even for physisorbed molecules with no charge transfer at the junction.

We discuss the influence of quantum confinement, charge transfer and molecular polarization as well as the impact of electron-phonon coupling on the electronic band discontinuities and the methodological implications for the *ab-initio* description of interface electronics.

Keywords: electronic structure theory; organic-inorganic heterostructures; hybrid systems; band-level alignment

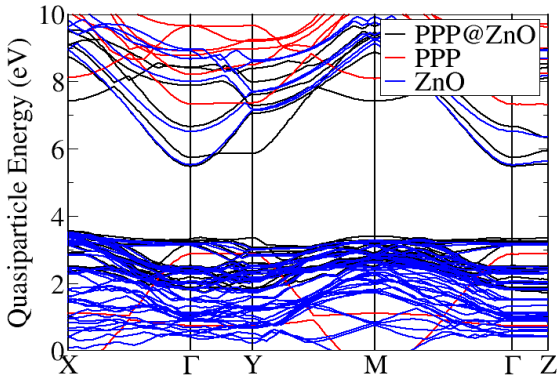

Fig. 1. QP band structure of PPP@*rs*-ZnO

References

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