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Electronic structure of PPP@ZnO from all-electron quasiarticle calculations BENJAMIN HÖFFLING, DIMITRI NABOK, CLAUDIA DRAXL, Humboldt Universität zu Berlin, CONDENSED MATTER THEORY GROUP, HUMBOLDT UNIVERSITY BERLIN TEAM — 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 well as quasiparticle (QP) calculations within the GW approach. A particular focus is put on the electronic band discontinuities at the interface, where we investigate the impact of quantum confinement, molecular polarization, and charge rearrangement. For our prototypical system, PPP@ZnO, we find a type-I heterostructure. Comparison of the band offsets derived from a QP-treatment of the hybrid system with predictions based on mesoscopic methods, like the Shockley-Anderson model or alignment via the electrostatic potential, reveals the inadequacy of these simple approaches for the prediction of the electronic structure of such inorganic/organic heterosystems. Finally, we explore the optical excitations of the interface compared to the features of the pristine components and discuss the methodological implications for the *ab-initio* treatment of interface electronics.

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