J. Yin, D. B. Migas, M. Panahandeh-Fard, S. Chen, Z. Wang, P. Lova, C. Soci, Charge Redistribution at GaAs/P3HT Heterointerfaces with Different Surface Polarity, J. Phys. Chem. Lett. **4**, 3303−3309 (2013).

Abstract/Аннотация

The nature of charged photoexcitations at the interface of highly delocalized inorganic crystals and more localized conjugated polymer systems is of great fundamental interest for a number of hybrid photovoltaic applications. Here we study the interaction between mainstream compound semiconductor GaAs and conjugated polymer P3HT by means of density functional theory simulations. When considering both nonpolar GaAs(110) and polar GaAs(111)B surfaces, we find that polarity of the GaAs surface strongly affects the electronic orbitals and charge redistribution: electrons are efficiently transferred to GaAs substrates, implying the formation of hybrid delocalized states at the interface. Furthermore, P3HT can act as an “acceptor” for GaAs(111)B via hole transfer from GaAs valence band states. Overall the intrinsic surface dipole moment of GaAs surfaces is enhanced by the charge displacement induced by adsorbed P3HT. These theoretical predictions correlate well with energy alignments derived by ultraviolet photoelectron spectroscopy and provide a robust methodology for the design of polymer/III−V heterointerfaces that optimize photovoltaic performance.