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Band offsets at semiconductor interfaces with hybrid functionals and the GW approximation[1] ROBERTO LONGO PAZOS, LEEOR KRONIK, JEFFREY NEATON — The ability to predict and understand how the electronic structure of a semiconductor is altered at an interface is important for many technological applications, carrier injection and confinement properties. While it is somewhat routine to compute band offsets at semiconductor interfaces with density functional theory (DFT) within standard approximations, mean-field Kohn-Sham band structures are well known to underestimate band gaps and neglect nonlocal correlations across the interface. Here, we use many-body perturbation theory within the GW approximation to compute band gaps and band offsets at a well-studied interface formed from two heterovalent semiconductors, GaAs and ZnSe, that have a small lattice mismatch. Comparing our results to calculations with standard DFT and hybrid functionals, we elucidate the quantitative importance of Fock exchange, and static and dynamic correlation effects, in developing an accurate picture of the electronic behavior at this interface, and in differentiating the interfacial electronic structure from that of bulk GaAs and ZnSe.

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Roberto Longo Pazos

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