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Exploring Level Alignment in Molecule-Metal Interfaces with Optimally-Tuned Range-Separated Hybrid Functionals ZHENFEI LIU, Lawrence Berkeley National Lab, DAVID A. EGGER, Weizmann Institute of Science, SIVAN REFAELY-ABRAMSON, Lawrence Berkeley National Lab, LEEOR KRONIK, Weizmann Institute of Science, JEFFREY B. NEATON, Lawrence Berkeley National Lab — Molecule-metal interfaces are ubiquitous in nanoscale functional materials and energy related applications. Characterizing the electronic structure at molecule-metal interfaces, especially the level alignment between molecular frontier orbitals and the Fermi level of the combined system, is crucial for understanding charge dynamics. Density functional theory (DFT) has been successful in computing binding geometries and adsorption energies, but much less successful in predicting level alignment. This is because the latter depends on quasiparticle excitation energies, typically believed to be outside the reach of DFT. In this work, we apply the recently developed optimally-tuned range-separated hybrid functional to the electronic structure of a model molecule-metal interface - benzene on graphite - and elucidate parameters leading to agreement with experiment and with many-body perturbation theory.

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