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Energy level alignment at hybridized organic-metal interfaces from a GW projection approach[1] YIFENG CHEN, Department of Physics and Centre for Advanced 2D Materials, National University of Singapore, ISAAC TAMBLYN, Department of Physics, University of Ontario Institute of Technology, Canada, SU YING QUEK, Department of Physics and Centre for Advanced 2D Materials, National University of Singapore — Energy level alignments at organic-metal interfaces are of profound importance in numerous (opto)electronic applications. Standard density functional theory (DFT) calculations generally give incorrect energy level alignments and missing long-range polarization effects. Previous efforts to address this problem using the many-electron GW method have focused on physisorbed systems where hybridization effects are insignificant. Here, we use state-of-the-art GW methods to predict the level alignment at the amine-Au interface, where molecular levels do hybridize with metallic states. This non-trivial hybridization implies that DFT result is a poor approximation to the quasiparticle states. However, we find that the self-energy operator is approximately diagonal in the molecular basis, allowing us to use a projection approach to predict the level alignments. Our results indicate that the metallic substrate reduces the HOMO-LUMO gap by 3.5 4.0 eV, depending on the molecular coverage/presence of Au adatoms. Our GW results are further compared with those of a simple image charge model that describes the level alignment in physisorbed systems.

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