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Covalently Bonded Aromatic Molecules on Gold using a GW Approach[1] ISAAC TAMBLYN, Dalhousie University, SU YING QUEK, Molecular Foundry, LBNL, STANIMIR A. BONEV, Dalhousie University, JEFFREY B. NEATON, Molecular Foundry, LBNL — Frontier molecular orbital energies dictate the nature of optical absorption, chemical reactivity, and charge injection at metal-organic interfaces. Recent work [1] on the conductance of benzenediamine-Au single-molecule junctions has shown that standard methods based on density functional theory fail to correctly position molecular orbital energies relative to the Au Fermi level, resulting in a pathological overestimate of the conductance for this class of systems. In this work, we use many-electron perturbation theory within the GW approximation to compute quasiparticle energies of aromatic molecules covalently bonded to a gold surface, taking particular care to assess dynamical screening beyond standard plasmon-pole approximations. We discuss results for benzene on Au(111) bonded via amine (-NH2) and thiol (-SH) link groups. These data are compared with more approximate model self-energy corrections applied to these systems [1], and also recent experiments. [1] Quek et al, Nano Lett. 7, 3477 (2007).

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