

Abstract Submitted
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Level alignment at covalently bonded metal-organic interfaces within the GW approximation JEFFREY NEATON, ISAAC TAMBLYN, Molecular Foundry, LBNL, SU YING QUEK, Institute of High Performance Computing (IHPC) and Physics and Applied Physics in Nanyang Technological University, STANIMIR BONEV, LLNL and Dalhousie University, PIERRE DARANCET, Molecular Foundry, LBNL — Accurate calculations of orbital energies for molecules chemisorbed on metal surfaces are important for understanding energy conversion, molecular scale transport, and charge transfer events at metal electrodes. Here, using density functional theory (DFT) and many-body perturbation theory within the GW approximation (GWA), we report the orbital energies of a well-studied molecule, benzene diamine (and derivatives), covalently bonded to aluminum and gold surfaces. For chemisorbed derivatives on Al surfaces, we predict a shift in the highest occupied molecular orbital resonance energy greater than 1 eV relative to the DFT result. We discuss our GWA results in the context of a model self-energy approach based on prior work [1], which can be applied to larger systems at greatly reduced computational cost.

[1] J. B. Neaton, M.S. Hybertsen, and S.G. Louie, PRL, 97, 216405 (2006)

Isaac Tamblyn
Molecular Foundry, LBNL

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