Abstract Submitted
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Electronic structure of metal-organic interfaces from first principles[1] ISAAC TAMBLYN, SU YING QUEK, Molecular Foundry, LBNL, STANIMIR A. BONEV, Dalhousie University, JEFFREY B. NEATON, Molecular Foundry, LBNL — Understanding electronic structure at hybrid metal-organic interfaces is crucial for the development and design of future nanoscale devices, particularly for many solar energy conversion applications. Using first-principles density functional theory and many-body perturbation theory within the GW approximation, we present calculations of molecular orbital energies of aromatic molecules covalently bonded to metal surfaces. Importantly, our parameter-free approach treats the metal slab and molecular adsorbate at the same level of theory, and includes exact exchange, as well as static and dynamical correlation effects. We explore the impact of variations in binding sites and molecular geometries for specific chemical link groups and surfaces, and compare directly with experiments where available.

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