

Abstract Submitted
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Microscopic Characterization of Organic/Metal Interfaces: a Combined DFT and Many-Body Perturbation Theory Study YAN LI, DEYU LU, GIULIA GALLI, University of California, Davis — Aromatic molecules and molecular assemblies have received widespread attention as possible components of molecular electronic devices. An essential prerequisite to understand their stability and transport properties is the microscopic characterization of the interface formed with metallic leads. We present a comprehensive, first-principles study of the interface of Au(111) and a representative aromatic isocyanide molecular SAM (phenylenediisocyanide). We provide predictions about the binding geometries, coverage and stability properties, which are in good agreement with experimental measurements. We also discuss the electronic properties of the organic/metal interface by including self-energy corrections through many-body perturbation theory (GWA), and surface polarization effects. Our results indicate that electronic structure calculations beyond DFT are required to make an accurate assessment of energy level alignments between SAMs and the metallic leads.

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