Abstract Submitted
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Atomic and Surface Interactions of Electrode Metals with a p-Type Organometallic Conductor[1] BHASKAR CHILUKURI, THOMAS CUNDARI, Department of Chemistry, Center for Advanced Scientific Computing and Modeling (CASCaM), University of North Texas, Box 305070, Denton, TX 76203-5070 — A computational study of the interaction of high and low work function electrode metal atoms (M' = Al, Au, Cu, La, Ni, Pd, Pt, Ru, Ni) used in electronic devices with cyclo-[Au(μ-Pz)]$_3$ trimer (T) (Pz = pyrazolate ligand), a p-type organometallic semiconductor is presented. Metal (M'$_M$) and ligand (M'$_L$) sites of the gold trimer are investigated as the possible sites of deposition for the metal atoms. Examination of metal binding, geometric and electronic properties suggest that these metal-based, p-type conductors will form stable interfaces with good electron transfer with typical source/drain electrode metals. Encouraged by the molecular simulation results, we performed periodic interface calculations of metal (001) and (111) surfaces with a monolayer of cyclo-[Au(μ-Pz)]$_3$ trimer using a plane-wave DFT approach. Structural and electronic properties of metal-trimer interfaces and implications for interface stability and electron transfer will be discussed.

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