Atomic and Surface Interactions of Electrode Metals with a p-Type Organometallic Conductor

BHASKAR CHILUKURI, THOMAS CUN-DARI, 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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