291g Electronic Structure and Electron Transport Characteristics of a Cobalt Complex

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The molecular and electronic structures and electron transport characteristics of a Co complex are investigated using first principle calculations. The Co complex belongs to the D2d point group with its two ligands perpendicular to each other. The central atom Co and its six donor N atoms form a distorted octahedron. In a low oxidation state, the bond length between Co and the pyrrole nitrogen (1.849 Å) is much shorter than the distance between Co and pyridine nitrogen (2.168 Å). While in a high oxidation, the bond length difference between Co and the pyrrole nitrogen (1.814 Å) and between Co and pyridine nitrogen (1.990 Å) are not as large as in the Co2+ complex. The HOMO energy of the low oxidation state is very close to the Fermi level of Au yielding a very low barrier, allowing hole-injection from Au anode to the molecule. On the other hand, the LUMO energy of the high oxidation state is close to Au Fermi level, allowing a low barrier electron-injection from Au cathode to molecule. These structural characteristics make the Co complex a good hole-conduction molecule. The density of states, transmission probability, and I-V characteristics are also evaluated using the Green's function approach.

Keywords: electron transfer, Green's function theory, DFT, cobalt complex, molecular electronics