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Chemisorption of Co-based cyanol pyridyl valence tautomers on Au(111)[1] WANDERLA SCOPEL, YIFENG CHEN, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University — Organic paramagnetic bistable molecules such as transition metal valence tautomers, where a magnetic transitions can be indiced by an external perturbation, are attracting considerable attention due to their potential utilization in molecular electronic and spintronic devices. Using calculations from first principle based on density functional theory we have investigated the chemisorbtion of Co-based cyanol pyridyl valence tautomer (VT) molecules on the Au(111) surface via a thiol head group. Among the possible adsorption sites on the Au(111) surface, we considered both the fcc hollow site and the bridge site, which are suggested to be the two lowest energy adsorption configurations in previous investigations. We have characterized the stability and the influence of the substrate bonding on the electronic and magnetic properties of the VT molecule. Moreover, by adding a top Au contact, we have studied the electron and spin transport properties of these systems.

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