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Electronic and transport properties of Cobalt-based valence tautomeric molecules and polymers YIFENG CHEN, Department of Physics, North Carolina State University, ARRIGO CALZOLARI, Istituto Nanoscienze CNR-NANO-S3, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University — The advancement of molecular spintronics requires further understandings of the fundamental electronic structures and transport properties of prototypical spintronics molecules and polymers. Here we present a density functional based theoretical study of the electronic structures of Cobalt-based valence tautomeric molecules Co^{III}(SQ)(Cat)L $Co^{II}(SQ)_2$L and their polymers, where SQ refers to the semiquinone ligand, and Cat the catecholate ligand, while L is a redox innocent backbone ligand. The conversion from low-spin Co^{III} ground state to high-spin Co^{II} excited state is realized by imposing an on-site potential U on the Co atom and elongating the Co-N bond. Transport properties are subsequently calculated by extracting electronic Wannier functions from these systems and computing the charge transport in the ballistic regime using a Non-Equilibrium Green's Function (NEGF) approach. Our transport results show distinct charge transport properties between low-spin ground state and high-spin excited state, hence suggesting potential spintronics devices from these molecules and polymers such as spin valves.

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