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Electronic transport in Co-based valence tautomeric conjugated polymers[1] MARCO BUONGIORNO NARDELLI, YIFENG CHEN, North Carolina State University, ARRIGO CALZOLARI, Istituto Nanoscienze CNR-NANO-S3, WANDERLA SCOPEL, North Carolina State University — Using first principle density functional theory (DFT) methods combined with maximally localized Wannier function (MLWF), real-space basis sets and a Green's function transport scheme within the Landauer ballistic transport regime, we investigated the electronic structures and electronic transport properties of a Co-based valence tautomeric (VT) conjugated backbone polymeric system. We found that GGA+U induced high-spin structure not in satisfactorily agreement with realistic circumstances from the computed Co projected density of states (PDOS). So we instead employed constrained magnetization calculations to induce the low-spin to high-spin magnetic transition computationally. Transport calculations showed that the high-spin structure is two orders of magnitude more conductive than the low-spin structure, thus supporting the vision that this kind of Co-based VT polymer can function as basis for switchable molecular spintronic devices. Finally, we will briefly discuss the chemisorption of this VT system on metallic substrates the spin transport properties of metal-molecule-metal configurations.

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