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Cobalt Bis(dioxolene) Valence Tautomers, from Molecules to Polymers¹ MARCO BUONGIORNO NARDELLI, University of North Texas, ARRIGO CALZOLARI, Istituto Nanoscienze CNR-NANO-S3, YIFENG CHEN, DANIEL DOUGHERTY, DAVID SHULTZ, North Carolina State University — Using first principles calculations we predict a complex multifunctional behavior in cobalt bis(dioxolene) valence tautomeric compounds. Molecular spin-state switching is shown to dramatically alter electronic properties and corresponding transport properties. This spin state dependence has been demonstrated for technologically-relevant coordination polymers of valence tautomers as well as for novel conjugated polymers with valence tautomeric functionalization. As a result these materials are proposed as promising candidates for spintronic devices that can couple magnetic bistability with novel electrical and spin conduction properties. Our findings pave the way to the fundamental understanding and future design of active multifunctional organic materials for spintronics applications.

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