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Magnetic Exchange Couplings from Local Spin Analysis[1] RAJENDRA JOSHI, BAYILEYEGN AKANIE ABATE, Science of Advanced Materials, Central Michigan University, JUAN PERALTA, Department of Physics and Science of Advanced Materials, Central Michigan University — We propose a method to calculate the magnetic exchange coupling parameters in transition metal complexes from a single spin-configuration. Our method uses constraint density functional theory and a local spin population analysis in combination to a non spin formalism to effectively extract the magnetic exchange parameter from the derivative of the electronic energy and spin pair correlation values. We show proof-of-concept calculations on the H-He-H systems and small transition metal complexes.

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