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Magnetic Exchange Couplings in Transition Metal Complexes from DFT[1] JUAN PERALTA, Dept of Physics and Sci of Adv. Mat. Program, Central Michigan Univ — In this talk I will review our current efforts for the evaluation of magnetic exchange couplings in transition metal complexes from density functional theory. I will focus on the performance of different DFT approximations, including a variety of hybrid density functionals, and show that hybrid density functionals containing approximately 30% Hartree-Fock type exchange are in general among the best choice in terms of accuracy. I will also describe a novel computational method to evaluate exchange coupling parameters using analytic self-consistent linear response theory. This method avoids the explicit evaluation of energy differences, which can become impractical for large systems. Our approach is based on the evaluation of the transversal magnetic torque between two magnetic centers for a given spin configuration using explicit constraints of the local magnetization direction *via* Lagrange multipliers. This method is applicable in combination with any modern density functional with a noncollinear spin generalization and can be utilized as a "black-box". I will show proof-of-concept calculations in frustrated Fe_7^{III} disk-shaped clusters, and dinuclear Cu^{II}, Fe^{III}, and heteronuclear complexes.

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