CORE-CM SEMINAR
Michigan State University

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Magnetic Interactions in Transition Metal Complexes from First-Principles

In this talk I will review our current efforts for the characterization of magnetic interactions in transition metal complexes from first-principles. Since for systems of practical interest, typically containing hundreds of atoms, density functional theory (DFT) is the only alternative for such calculations, I will first focus on the performance of different DFT approximations including a variety of modern density functionals. I will show that hybrid density functionals containing approximately 30% Hartree-Fock type exchange are in general among the best choice in terms of accuracy when compared to available experimental data.[1,2] I will also present a new computational method to evaluate exchange coupling parameters using analytic linear response theory. With this method we avoid the explicit evaluation of energy differences between different broken-symmetry spin multiplets, which typically becomes impractical for large systems. This new method is based on the evaluation of the magnetic torque between two magnetic centers for a given spin configuration using explicit constraints of the local magnetization direction via Lagrange multipliers[3] and it is applicable in combination with any modern density functional with a noncollinear spin generalization. I will show proof-of-concept calculations in small test systems, and in spin frustrated Fe^{III}_7 disk-shaped clusters.[4] Last, I will show our recent efforts for modeling spin dynamics using explicitly real-time evolution in the time-dependent DFT formalism.

[1] J.J. Phillips and J.E. Peralta, J. Chem. Phys. **2011**, 134, 034108.
[2] J.J. Phillips and J.E. Peralta, J. Chem. Theory Comput. **2012**, 8, 3147.
[3] J.J. Phillips and J.E. Peralta, J. Chem. Phys. **2013**, 138, 174115.
[4] J.J. Phillips, J.E. Peralta, and G. Christou, J. Chem. Theory Comput. **2013**, 9, 5585.

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Prof. Ben Levine - Host