

Representative Publications

"Antiferromagnetic Exchange Interactions from Hybrid Density Functional Theory," R.L. Martin, and F. Illas, *Phys. Rev. Lett.* 79, 1539 (1997).

"Magnetic Coupling in Ionic Solids Studied by Density Functional Theory," F. Illas and R.L. Martin, *J. Chem. Phys.* 108, 2519 (1998).

"Effect of Fock Exchange on the Electronic Structure and Magnetic Coupling in NiO", I. Moreira, F. Illas, and R. L. Martin, *Phys. Rev. B*, 65, 155102 (2002).

"Hybrid density functional theory and the insulating gap of UO₂", K. N. Kudin, G. E. Scuseria, and R. L. Martin, *Phys. Rev. Lett.* 89, 266402 (2002).

"Lattice defects and magnetic ordering in plutonium oxides: A hybrid density-functional-theory study of strongly correlated materials", I.D. Prodan, G. E. Scuseria, J. A. Sordo, K. N. Kudin, and R.L. Martin, *J. Chem. Phys.* 123, 14703 (2005).

"Spin-orbit splittings and energy band gaps calculated with the Heyd-Scuseria-Ernzerhof screened hybrid functional", Juan E. Peralta, Jochen Heyd, Gustavo E. Scuseria, and Richard L. Martin, *Phys. Rev. B* 74, 073101 (2006).

"Control of electronic and magnetic coupling via bridging ligand geometry in a bimetallic ytterbocene complex", C. N. Carlson, B. L. Scott, R. L. Martin, J. D. Thompson, D. E. Morris, K. D. John, *Inorganic Chem.* 46, 5013 (2007).

"Systematic Study of Modifications to Ruthenium(II) Polypyridine Dyads for Electron Injection Enhancement", Elena Jakibukova, Richard L. Martin and Enrique R. Batista, *Inorganic Chem.* 49, 2975 (2010).

"Pu Electronic Structure and Photoelectron Spectroscopy", J. J. Joyce, T. Durakiewicz, K. S. Graham, E. D. Bauer, D. P. Moore, J. N. Mitchell, J. A. Kennison, R. L. Martin, L. E. Roy, G.E. Scuseria, "International Conference on Strongly Correlated Electron Systems (SCES 2010), *Journal of Physics Conference Series*, 273, 012023 (2011).

"Localization of Electronic Excitations in Conjugated Polymers Studied by DFT", Iffat Nayyar, Enrique Batista, Sergei Tretiak, Avadh Saxena, Darryl Smith, Richard Martin, *J. Phys. Chem. Lett.* 2, 566 (2011).

"Determining Relative f and d Orbital Contributions to M-Cl Covalency in MCl₆²⁻ (M = Ti, Zr, Hf, U) and UOCl₅ Using Cl K-Edge X-ray Absorption Spectroscopy and Time-Dependent Density Functional Theory", S. G. Minasian, J. M. Keith, E. R. Batista, K. S. Boland, D. L. Clark, S. D. Conradson, S. A. Kozimor, R. L. Martin, D. E. Schwarz, D. K. Shuh, G. L. Wagner, M. P. Wilkerson, L. E. Wolfsberg, and P. Yang, *J. Amer. Chem. Soc.* 134, 5586 (2012).