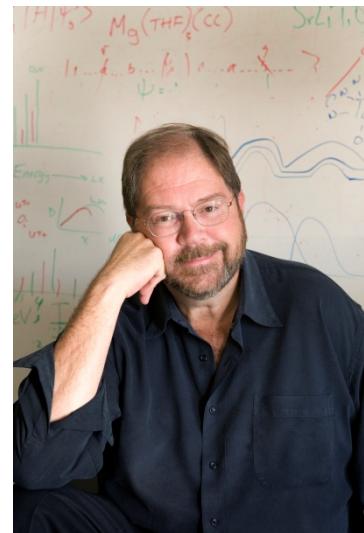


## Richard L. Martin

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Martin is a Los Alamos Laboratory Fellow. His research interests lie in the electronic structure theory of molecules and solids, especially transition metal and actinide chemistry, strongly correlated materials, charge and energy localization and transport in molecularly engineered electronic materials and devices, and homogeneous catalysis. He is a Fellow of the American Association for the Advancement of Science, and has co-authored some 200 peer-reviewed papers (h-index = 53, total citations 9,000+). Martin is a recipient of a DOE Award of Excellence, and has consulted with DuPont on computational co-design of organic light-emitting diodes.

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## 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).

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"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 MCl<sub>6</sub><sup>2-</sup> (M = Ti, Zr, Hf, U) and UOCl<sub>5</sub> 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).