CMQT
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Martin L. Kirk is Distinguished University Professor of Chemistry and Chemical Biology at The University of New Mexico. His research program focuses on (1) spectroscopic, synthetic, biochemical, and computational studies of pyranopterin molybdenum enzymes and models, (2) detailed magnetic, spectroscopic, and theoretical studies of spin containing molecular systems in the context of molecular electronics, and (3) optical generation of multiple spin qubits for quantum information science (QIS) applications. He has been a Research Fellow (7/03-1/04) at the Glenn T. Seaborg Institute at Los Alamos National Laboratories during a sabbatical leave and was Humphrey Symposium Lecturer at the University of Vermont, PROTRAIN Lecturer at Braunschweig Technical University (Germany), and the Highlands in Chemistry Lecturer at Virginia Tech. He was a National Science Foundation Postdoctoral Fellow (1990-1993, Stanford University) with E. I. Solomon, completed his Ph.D. in 1990 at The University of North Carolina at Chapel Hill with W. E. Hatfield, and obtained his B.S. in 1985 at West Virginia University performing undergraduate research with Naresh Dalal. He was guest Editor (with Prof. D. A. Shultz) for Molecular Spintronics: a web themed issue of *Chemical Communications* and an Editor of Molybdenum and Tungsten Enzymes; a three volume Metallobiology Series sponsored by the Royal Society of Chemistry. Prof. Kirk has served on the Editorial Board of *Inorganic Chemistry*, was a prior ACS Inorganic Division Chair of the Bioinorganic Subdivision, and a Chair of the Gordon Research Conference on Molybdenum and Tungsten Enzymes. He was a former Chair of UNM's Department of Chemistry and Chemical Biology and Adjunct Professor of Chemistry at New Mexico Institute of Mining and Technology. Prof. Kirk is currently a member of UNM's Center for High Technology Materials, Center for Computational Chemistry, Center for Quantum Information and Control, and a founding member of the Quantum New Mexico Institute.

The Role of Excited State Exchange Interactions in the Generation of Electron Spin Polarization

Excited state exchange interactions in radical-elaborated chromophores have a profound impact on excited state processes, including the generation of electron spin polarization. Our efforts have focused on determining excited state contributions to molecular bridge mediated electronic and spin coupling, understanding how complex open-shell excited state configurations promote long-range electron correlation, and developing new platforms for spin control of excited state dynamics in photoexcited donor-acceptor molecules. These new systems are particularly relevant to the emerging molecular quantum information science field, allowing for a deep insight into the optical generation and manipulation of spin qubits. In this lecture, we will focus on radical elaborated spin-bearing Pt Donor-Acceptor and Donor-*Bridge*-Acceptor ligand-to-ligand charge transfer complexes,

which have been used to control spin-dependent ground and excited state processes that include non-radiative lifetimes, magnetooptical activity, and ground state electron spin polarization. These molecules represent a new class of chromophore that can be photoexcited with visible light to produce an open-shell, charge-separated excited state where multiple spins are exchange coupled. Following photoexcitation, this excited state rapidly decays to the ground state by internal conversion, magnetic exchange-mediated enhanced intersystem crossing, and anisotropic exchange processes. This relaxation process generates excited state spin polarization that is transferred to the electronic ground state, leading to electron spin polarization of the pendent radicals that are covalently attached to the chromophore. Remarkably, exactly how this process generates electron spin polarization in these systems is still not well understood. We will present results that test theoretical hypotheses as they relate to how excited state pairwise superexchange interactions and energy transfer processes control the optical generation and manipulation of molecular spin qubits, and the nature of ground state spin relaxation processes in exchange coupled biradical systems.