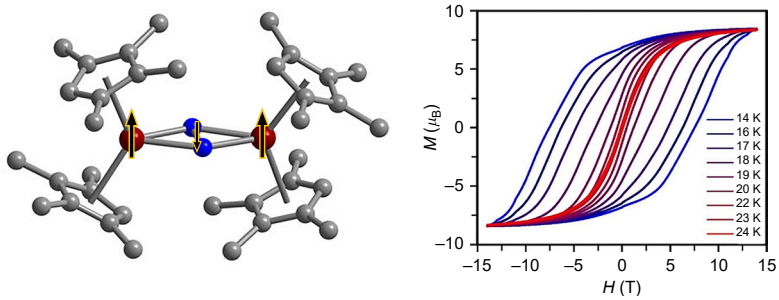
Single-molecule magnets (SMMs) are molecules that behave like nanoscopic bar magnets. They are interesting due to various potential applications in high-density information storage, molecular spintronics, and magnetic refrigeration. The challenge in realizing these applications lies in designing molecular magnets that have much higher operating temperatures than have been obtained currently.



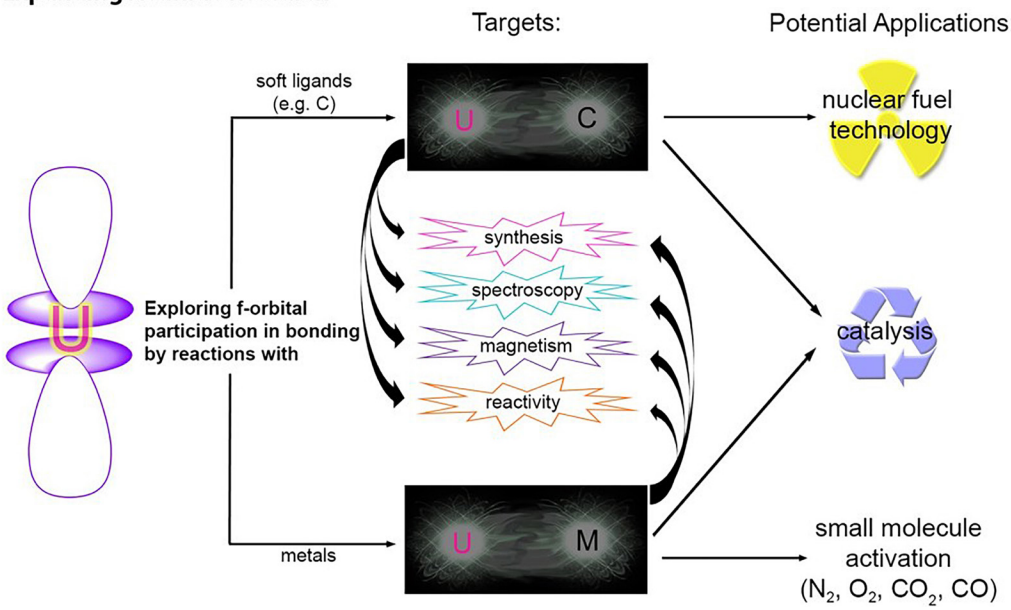
Structure of $[(CpMe_4H_2Tb)_2(\mu\text{-}N_2^{\bullet})]^-$ and magnetic hysteresis.

Lanthanide ions are particularly well-suited for the design of effective SMM because of their high magnetic anisotropic nature. This property inherently possessed by the lanthanide metals arise from unquenched orbital angular momentum and strong spin-orbit coupling. In order to suppress quantum tunneling relaxation processes that leads to a shortcut of the maximum spin-relaxation barrier and thus, a weaker magnet, a strong exchange coupling is required between the spins. Therefore, a promising route to increase operating temperature of single-molecule magnet is to design lanthanide complexes that simultaneously feature high-magnetic anisotropy and strong magnetic exchange coupling. As a means of achieving strong coupling, radical-bridging ligands with diffused spin orbitals are employed in order to penetrate the core electron density of the deeply buried 4f orbitals within lanthanide ions. We are exploring the utility of various redox-active ligands for the design of radical-bridged multinuclear lanthanide single-molecule magnets.

Uranium's rich chemistry lies in certain properties that results in chemical bonding and reactivity that are not seen with other elements. Uranium-ligand multiple bond compounds have been recognized as promising subjects of study for advancing uranium catalysis and actinide/lanthanide separation by shedding light on the extent of covalency in bonding of 5f orbitals. Covalency is expected to be more prominent when softer ligands are used such as C ligands rather than N or O ligands. Hence, investigating the electronic and reactivity properties of molecular uranium carbenes will improve fundamental knowledge that is crucial to the development of catalysts and new generation nuclear fuels.

Besides uranium carbenes, we will pursue uranium-metal bonds that are extremely rare. Such bonding moieties will uncover which 5f orbitals are involved. In particular, their chemical reactivity toward small molecules will be explored. In addition, the magnetism of all synthesized uranium complexes will be investigated since owing to a large magnetic moment, the high anisotropic nature, and the more diffuse 5f orbitals that promote magnetic exchange through better overlap, uranium represents a promising candidate for single-molecule magnetism.

Expanding Actinide Research



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517-353-1080

Selected Publications

Giant Coercivity and High Magnetic Blocking Temperatures for N_2^{3-} Radical-Bridged Dilanthanide Complexes Upon Ligand Dissociation, Demir, S.; Gonzalez, M. I.; Darago, L. E.; Evans, W. J.; Long, J. R., *Nat. Commun.* **2017**, doi:10.1038/s41467-017-01553-w.

Extraction of Lanthanide and Actinide Ions from Aqueous Mixtures Using a Carboxylic Acid-Functionalized Porous Aromatic Framework, Demir, S.; Brune, N. K.; Van Humbeck, J. F.; Mason, J.A.; Plakhova, T. V.; Wang, S.; Tian, G.; Minasian, S.G.; Tyliszczak, T; Yaita, T.; Kobayashi, T; Kalmykov, S. N.; Shiwaku, H.; Shuh, D. K.; Long, J. R., *ACS Cent. Sci.* **2016**, *2*, 253-265.

Radical Ligand-Containing Single-Molecule Magnets, Demir, S.; Jeon, I.-R.; Long, J. R.; Harris, T. D., *Coord. Chem. Rev.* **2015**, *289-290*, 149-176.

Exchange Coupling and Magnetic Blocking in Dilanthanide Complexes Bridged by the Multi-Electron Redox- Active Ligand 2,3,5,6-Tetra(2-pyridyl) pyrazine, Demir, S.; Nippe, M.; Gonza-lez, M. I.; Long, J. R., *Chem. Sci.* **2014**, *5*, 4701-4711.

Exchange Coupling and Magnetic Blocking in Bipyrimidyl Radical- Bridged Dilanthanide Complexes, Demir, S.; Zadrozny, J. M.; Nippe, M.; Long, J. R., *J. Am. Chem. Soc.* **2012**, *134*, 18546-18549.