HIGHLANDS IN CHEMISTRY SEMINAR SERIES



FEBRUARY 2, 2024

2:30PM ET

HAHN HALL NORTH 140

FACULTY HOST: NICK MAYHALL

SELVAN DEMIR

MICHIGAN STATE UNIVERSITY

"High-Performance Single-Molecule Magnets and Reactivity Studies with Organometallic Lanthanide Complexes"

Single-molecule magnets (SMMs) are molecules that possess an energy barrier to spin inversion, giving rise to slow magnetic relaxation and magnetic hysteresis. To realize their intriguing potential applications, ranging from molecular spintronics, quantum computing, to high-density information storage, spin-reversal barriers (Ueff) and magnetic blocking temperatures (TB) must be increased. Lanthanide ions are especially well-suited for the design of SMMs due to their large magnetic moments and magnetic anisotropy that originate from strong spin-orbit coupling of the 4f orbitals. To improve TB, we pursue multinuclear SMMs comprising strong magnetic exchange between lanthanides through the use of radical bridging and bismuth ligands, respectively, Fig. 1.1-8 We also devise unprecedented radical complexes with diamagnetic 89Y (I = $\frac{1}{2}$) to gain insight into the electronic structure and spin density distribution through spectroscopy and computations. The organometallic chemistry of the rare earth elements has been further advanced by first, employing dibenzocyclooctatetraene which led to unprecedented trismetallocene and sandwich complexes, respectively,9,10 and second, the isolation of the first guanidinate complexes featuring a weakly coordinated tetraphenylborate anion, Fig. 2.11 The latter compounds have ramifications for both magnet design and reactivity studies.





Fig. 1. Structures of the [Cp*₂Dy₂Bi₆]²⁻ dianion and the [(Cp*₂Dy)₂(μ-η²:η²-Bi₂•)]⁻ anion.



Fig. 2. Advancing dibenzocyclooctatetraene and guanidinate chemistry.