Electron (De)Localization in f-Element Systems: From Fundamental Questions to QIS Design Principles

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Chemistry Seminar on Understanding *f*-element Electronic Structure

**4:00 p.m. Monday Oct 4** *Via* Zoom

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Abstract: The La Pierre group studies how collective magnetic, physical, and chemical properties arise from electron (de)localization phenomena in f-element systems. Our studies include the development of solid-state and solution methodologies for the synthesis of novel lanthanide and actinide (Th - Pu)materials and complexes. These synthetic efforts are paired with synchrotron and neutron spectroscopies and physical property studies to break down the challenge of understanding the electronic structure of *f*-element systems. Particularly in solid-state systems, the *f*-elements present unique valence electronic structures due the near degeneracies engendered in these systems and strong electron correlation. Our efforts to-date have focused on the synthesis and analysis of systems governed by one of three phenomena: magnetic super-exchange (i.e. exchange coupled systems), multi-configurational electronic structures (ground state degeneracy including hybridization with ligand/band states), and mixedvalence metal ions (*i.e.* mixed f/d occupancy and mixed-oxidation states). Understanding and controlling the manifestation of these phenomena in molecular systems is crucial for understanding the interplay of these phenomena underpinning topological insulators such as SmB<sub>6</sub> and PuB<sub>6</sub> and superconductors such as CeCoIn<sub>5</sub> and PuCoGa<sub>5</sub>. In turn, the group has employed this expanded fundamental understanding of *f*-element electronic structure to construct components of quantum information technologies (e.g. qubits, single-molecule magnets).

About the speaker: Henry, also known by his nickname, Pete, was born in St. Louis, MO. During his undergraduate studies at Harvard University, he worked with Prof. Jared Shaw at the Broad Institute on the synthesis of antibiotics and with Prof. Masahiro Murakami at Kyoto University on main group organometallics. His graduate work, with Professors John Arnold, Robert Bergman, and Dean Toste at UC-Berkeley, focused on the development of a Zselective alkyne semihydrogenation catalyst. Following graduation, he studied ligand control of reactive low- and high-valent uranium complexes as a postdoctoral scholar with Prof. Karsten Meyer at FAU Erlangen-Nuremberg. He then worked as a Director's Postdoctoral Fellow at Los Alamos National Laboratory with Dr. Stosh Kozimor on ligand K-edge X-ray absorption spectroscopic studies of transuranic complexes. Since beginning his appointment at the Georgia Institute of Technology in 2016, his studies have been recognized by the Arnold and Mabel Beckman Young Investigator Award, the NSF CAREER Award, and the Ralph E. Powe Junior Faculty Enhancement Award. His group's research is also supported by the ACS Petroleum Research Fund and the DOE Heavy Element Chemistry Program.