Taking Inspiration From Bulk: Molecular Electrocatalysis and Magnetization Dynamics of Heterometallic Lanthanide – Transition Metal Complexes

The first part of the presentation will introduce our methodology towards improving molecular catalysts for energy relevant conversions. We strategically introduce redox-active and slightly acidic imidazolium moieties into the secondary coordination sphere of molecular CO2 reduction electrocatalysts. Results from systematic comparative studies will be presented that strongly suggest that mechanistic details of catalysis are altered for the new functionalized catalyst systems, resulting in improved catalytic metrics.

The second part of the seminar will discuss our strategies to study intramolecular interactions between transition metal (TM) and lanthanide (Ln) ions to generate novel spin systems that can display single-molecule magnet (SMM) properties. SMMs are very attractive candidates for the miniaturization of tunable information storage materials and quantum computing devices. Our work aims to generate heterometallic SMMs that feature either TM···Ln interactions or TM‑Ln bonding. I will present key results of our comprehensive structural and spectroscopic studies which have already led to the development of redox-switchable SMMs, new molecular platforms to facilitate strong magnetic coupling between Ln3+ ions, and hard SMM behavior.