Our 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 CO$_2$ reduction electrocatalysts. We will present results from systematic comparative studies that strongly suggest that mechanistic details of catalysis are altered for the new functionalized catalyst systems, resulting in improved catalytic metrics.

We will then 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 TMLn 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 Ln$^{3+}$ ions, and hard SMM behavior.

Hosted by Professor Smaranda Marinescu

*The scientific community is invited*