



Gesellschaft Deutscher Chemiker Ortsverband Bonn



Professor Dr. Demyan Prokopchuk Rutgers University-Newark Tuesday, May 21 at 5 pm (17 Uhr s.t.) in Hörsaal 2

Ligand Based C-H Bond Weakening for Synthesis and Electrocatalysis with Earth-Abundant Metals

The selective, efficient, and sustainable activation of carbon-hydrogen bonds continues to be a critical area of research. Current synthetic methodologies heavily rely on transition metal catalysts to mediate the reactivity of C-H bonds for making medicines, fuels, agrochemicals, and materials. Broadly speaking, we are interested in leveraging C-H bonds housed within chelating ligand frameworks to understand the fundamentals of C-H activation and discover new (electro)catalytic transformations. We have used an amine-rich cyclopentadienyl ligand (Cp^{N3}) coordinated to iron, which facilitates electrocatalytic H₂ production in the presence of exogenous acid. Although Cp ligands are classically viewed as unreactive "spectator" ligands, the H₂ production mechanism involves a crucial stereoselective *endo*-Cp^{N3} protonation step followed by ligand-to-metal proton transfer. In a separate endeavor, we are interested in understanding the magnitude of $C(sp^3)$ -H bond weakening when an alkane moiety interacts with a transition metal (i.e., agostic interactions). To achieve this goal, we use diamondoid pincer ligands coordinated to Ni and Pd, which provide unique insights into the thermochemical requirements for C-H activation with unactivated alkanes. Recent results in these areas of research will be presented.