“The Journey with 1,2,3-Triazole Ligands: Rational Design and Serendipity”

The research in Shi group focused on new synthetic methodology developed based on the mechanistic insight. One area is the application of functional 1,2,3-triazole (TA) as ligand in tuning transition metal reactivity for novel catalyst design and new transformations. These efforts have led to critical mechanistic insight on how 1,2,3-triazole regulates metal reactivity, offering unique reactivity for challenging chemical and material problems. Some recent results include triazole gold catalysis (TA-Au), triazole ruthenium metathesis catalyst library (TA-Ru), triazole as directing group in C-H activation (TA-Pd), new triazole-based metal complexes (Fe, Mn, Ni, Cu) etc.

The triazole gold catalysis led to the discovery of thermal stable gold catalysts and Lewis acid assisted TA-Au activation. More recently, the gold chemistry was further extended into redox catalysis and application of vinyl gold intermediates as nucleophiles using synergistic gold/iron dual catalyst to prevent out rapid protodeauration. The TA-Ru carbene complexes were proved as novel class of metathesis catalysts that tolerate higher temperature without decomposition, allowing C=C bond forming process as equilibrium for dynamic covalent chemistry (DCvC). These new catalytic systems have been applied into practical synthesis of important molecules toward biomedicinal and material applications.