Cu-Catalyzed C–N and C–O Bond-Forming Reactions Utilizing N^1,N^2-Diarylbenzene-1,2-Diamine Ligands

Prof. Michael J. Strauss

Cu-catalyzed coupling reactions represent an important alternative to well-established Pd-catalyzed approaches due to the differing reactivity and lower cost of Cu. Despite their promise, the realization of efficient Cu-catalyzed cross-coupling reactions has been hampered by the inefficient oxidative addition of aryl halides to ligated Cu-based catalysts. Anionic ligands have demonstrated the ability to lower the energy barrier to oxidative addition and enabled the development of coupling reactions between various classes of aryl halides and *N*- or *O*-centered nucleophiles. I will discuss the development of a new family of anionic ligands based on the N^1,N^2-diarylbenzene-1,2-diamine scaffold. This ligand design was initially guided by DFT calculations to (1) increase the electron density on Cu, thereby increasing the rate of oxidative addition, and (2) stabilize the active anionic Cu(I) catalyst via non-covalent interactions. A significant portion of this talk will focus on how the use of the catalysts derived from these ligands has improved the scope of Cu-catalyzed C–N and C–O coupling reactions while concomitantly using milder reaction conditions. I will also highlight how the modularity of this ligand scaffold has resulted in systematic improvements in reaction efficiency by using reaction outcomes and mechanistic insights as a guide. Collectively, the results to be discussed have established a new class of anionic ligands for Cu-catalyzed C– heteroatom bond-forming reactions in synthetically useful contexts.