

Pd-NHC Complexes: Whether in Solution or on Surfaces in Flow Beds, They Make Great Catalysts!

Considerable effort for almost half a century has been devoted to understanding how ligand steric and electronic properties modulate the reactivity of a metal centre in a large number of catalytic processes. This is confounded by the fact that many of these transformations have two or more steps in their catalytic cycles, which may mean that a favourable attribute in one step may act to disfavour another step. Many groups have worked diligently to develop methods to probe, and scales to grade ligand properties such that they can be used in, ideally, a predictive fashion to guide the development of new catalysts.

In this presentation our approach to rational ligand design in cross-coupling applications will be discussed and how this approach has been used to improve catalyst performance using Pd-NHC (N-heterocyclic carbene) complexes and, in some applications, to achieve high selectivity where isomeric coupling products are possible. Finally, the high catalytic performance and robustness of these Pd-NHC complexes will be demonstrated in flow chemistry applications using complexes that have been covalently tethered to the surface of different solid materials and loaded into pack-bed reactors for continuous manufacturing applications.