Transition metal catalyst discovery with high-throughput screening and machine learning

Heather J. Kulik[a]

[a]*Department of Chemical Engineering, Massachusetts Institute of Technology*
hjkulik@mit.edu

Computational chemistry has emerged as a leading tool for exploring large regions of chemical space, but many outstanding challenges remain to go from a feasible space to lead compounds that achieve a goal. This challenge is particularly daunting for the design of transition metal complexes due to the combinatorial challenges associated with their variable spin, oxidation state, and coordination number. At the same time, transition metal catalysis, especially at open shell transition metal complexes, represents one of the most fertile regions to explore with such computational techniques. I will describe our recent efforts in automation, high-throughput screening, and machine learning for the discovery of both selective catalysts and design rules. I will talk about how these approaches have allowed us to both identify new scaling relations in catalysis as well as ways to break those scaling relations. Such approaches are expected to enable the discovery and design of selective and active catalysts for challenging transformations (e.g., selective C-H activation). I will also describe our development of representations uniquely tailored for transition metal complex properties and how we obtain not just accurate predictions with machine learning models but also develop new chemical insights. Time permitting, I will describe our next steps in developing artificial intelligence engines that automate decisions that typically require advanced training to determine also when and how to carry out simulations.