Department of Chemistry Seminar Series
Spring 2023

Monday, April 10, 2023, 3:30 PM – **HPA1-O119 (Health Sciences)**

Design Principles for Catalyst Probe Reaction Systems

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The development of efficient, sustainable, and selective heterogeneous catalysts for nitro and azo-reductions, as well as photocatalytic oxidations, span importance in industry, agriculture, pharmaceuticals, and the environment. Thus, the development of robust, sustainable heterogeneous catalysts and elucidation of their mechanisms has become a critical area of research. Still, there are several significant challenges in these catalyst promoted reactions: (1) the current benchmark method for comparing catalytic activity does not account for chemoselectivity across different substrate patterns, (2) many of the most-active catalysts are based on precious metals which makes large scale implementation cost-prohibitive; (3) their structure-reactivity relationships are not well defined and, (4) the mechanisms of these probe reactions and impacting parameters are not well-elucidated, thus impeding the understanding-based design of better catalysts.

We address some of these limitations by providing an understanding-based approach to discover and investigate sustainable, earth-abundant catalysts for reduction of nitrophenols and azo-dyes. To improve the overall process of screening catalyst candidates, the limitations of the current screening protocol are presented; furthermore, an alternative, improved protocol is offered, assessed, and supported. We have produced a copper-oxide based catalyst supported on nickel foam that has reactivity for 4-nitrophenol reduction competitive with previously reported noble metal-based systems. This catalytic system was systematically studied to disentangle impact of surface defects, metal oxidation state, bandgap, size and surface properties. Finally, to better understand the active sites of supported nanocatalysts, we developed a methodology to investigate synergistic effects and permanently tune catalytic selectivity using selective area atomic layer deposition of an inert material.