

Insights into the Microenvironment of Catalysis: Water Oxidation and Selective C–H bond Functionalization

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Transition metal catalysis is a complex process, where each component of the reaction plays critical roles and compliments (and enhances) each-other's activities. The acquiring of atomistic-level fundamental knowledge on the roles of each component (including catalyst, substrate, ligand, base, additive, solvent, and oxidant) of the targeted catalytic transformation, under the utilized experimental conditions, is a monumental and greatly attractive research missions. Success in this endeavor requires true collaborative efforts between the scientists with complementary expertise (in analytical, physical, synthetic, and theoretical sciences), and will enable us to develop more effective, highly selective, environmentally friendly (i.e. green and sustainable), and economically viable (i.e. utilizing of important and accessible substrates, and inexpensive ligands and transition metals) societally critical technologies. In my talk, I will discuss our latest computational and experimental (*collaborative*) efforts on the:

Selective C–H Bond Functionalization. The C–H functionalization—defined as the transformation of “inert” C–H bonds into C–C, C–N, C–O, C–halogen and other C–heteroatom bonds—is a viable strategy for the synthesis of complex organic targets and efficient late-state modifications of advanced molecular scaffolds. A foremost challenge of this transformative research is to control site-selectivity of the reaction. In my talk I will briefly discuss our collaborative efforts that have led to discovery of new catalysts for effective site-selective functionalization of the most accessible non-activated secondary, tertiary, and primary C–H bonds.

Solar energy -to- chemical energy conversion. There are multiple concerns with respect to generation, storage, and utilization of energy on a global scale, which have emphasized the solar-to-chemical-energy conversion the most effective technology for the production and storage of solar fuel. The two prominent foci of this strategy are hydrogen production via water splitting and carbon-based fuel production via CO₂ reduction. We have launched considerable research on design of water oxidation catalysis and solar-to-chemical conversion systems. Currently, we have prepared several polyoxometalates-based (POM) water oxidation catalyst, such as $[\{Ru_4O_4(OH)_2(H_2O)_4\}(\gamma-SiW_{10}O_{36})_2]^{10-}$, $[Co_4(H_2O)_2(PW_9O_{34})_2]^{10-}$, and $[Co_4(H_2O)_2(VW_9O_{34})_2]^{10-}$. Some of these systems will be discussed in more details in my presentation.