Water: promoter or inhibitor of activity?

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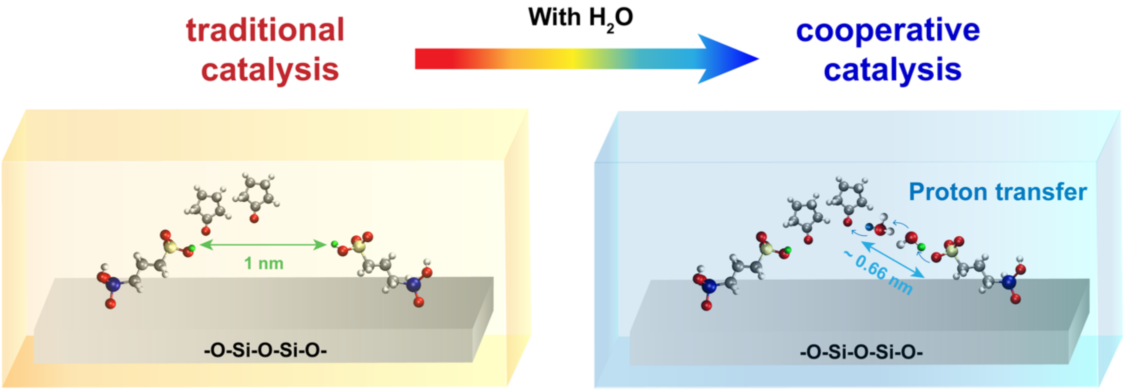

As one of the most ubiquitous and essential molecules in nature, water controls the catalytic activity of enzymes, which take advantage of its presence to achieve the required conformation and energy of the substrate during the reaction pathway. Recent experimental and computational studies show that these entropic and enthalpic roles of water are also relevant in reactions catalyzed by synthetic materials. The highly dynamic nature of interfacial water around active sites alters the reaction pathways, stability of the surface species, and reaction barriers. The effects of water are multifaceted and require a detailed understanding at the molecular–level for a proper description of the spatiotemporal dynamics of liquid–solid interfaces, which is essential to produce highly efficient catalysts for reactions of relevance for energy generation and chemical transformations, in a sustainable way.

This talk aims at introducing our current molecular level understanding of the water structure at the solid-liquid interface and how water influences the performance of a solid catalyst. By a combined study of the material synthesis, spectroscopic analyses, detailed reaction kinetics and theoretical calculations, we have investigated the relationship between the structure of water and the catalytic performance of solids in organic reactions that are relevant to biomass upgrading. For example, water can play an unexpected promotional role in crucial C–C bond forming reactions. The presence of water changes reaction kinetics by exerting remote-C=O bond polarization from a surface site to the reactant via a network of H-bonded water molecules. When the distance between the two acid sites is greater than a distance corresponding to about two water molecules, the efficiency of the bond polarization of the ketone by a remotely located acid site decreases significantly, and the presence of water no longer promotes the reaction. This work provides a quantitative assessment of how solvent molecules can bridge isolated active sites to enable cooperative catalysis, which offers an additional dimension for engineering catalysis at the nanoscale.

Bio

Dr. Gengnan Li is a Research Associate at Brookhaven National Laboratory. Gengnan obtained her PhD from East China University of Science and Technology with a degree in Materials Science and Engineering. She was a postdoc of Prof. Daniel E. Resasco at University of Oklahoma. She specializes in synthesizing nanostructured materials for sustainable energy applications. She is author of > 40 publications with > 759 citations; her h-index is 17.