CLINT
CRC 1452 Catalysis at Liquid Interfaces

Guest Colloquium of the CRC 1452
CLINT ~ Catalysis at Liquid Interfaces

Dynamics of solid-water interface and its impacts in heterogenous catalysis: a combined computational and experimental study

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The presence of water has been shown to enhance heterogeneous catalysis rates and selectivity. Here I discuss two case studies, water-enhanced hydrogenation and aldol condensation. Beyond what we reported previously for water-promoted C=O hydrogenation in furfural, in this presentation, I will highlight how the dynamics of the local water structures within the first solvation shell may affect the hydrogenation kinetics. Specifically, we find that the activation barriers correlate well with some collective variables that determine the local configuration and relative positions of surface hydrogen and water. In the second example, we show that water clusters around the acid site, which are introduced to a silica surface by grafting sulfonic acid groups, can form bridges with a ketone molecule located close to the activated carbonyl on another site and promote the C-C coupling. 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. Both examples provide a quantitative assessment of how solvent molecules can offer an additional dimension for engineering catalysis at the nanoscale.

1. Solvent-mediated charge separation drives alternative hydrogenation path of furanics in liquid water, Z. Zhao, R. Bababrik, W.H. Xue, Y.P. Li, N. M. Briggs, D.-T. Nguyen, U. Nguyen, S. P. Crossley, S. W. Wang, B. Wang, D. E. Resasco, Nat. Catal. 2, 431-436 (2019)
2. Bifunctional metal-acid sites on nickel boride catalysts: Phenol Hydrodeoxygenation and water-promoted C=C hydrogenation, G. Li, T. Salas, S.-T. Sun, B. Wang, M. R. Komarneni, D. Resasco, J. Catal. 431, 115384 (2024)
3. 1Water Confinement on Polymer Coatings Dictates Proton-Electron Transfer on Metal-Catalyzed Hydrogenations, P. Huang, Y. Yan, R. P. Martinho, L. Lefferts, Bin Wang, J. A. Faria, JACS Au 4(7), 2656-2665 (2024)
4. Optimizing the surface distribution of acid sites for cooperative catalysis in condensation reactions promoted by water, G. Li, Bin Wang, T. Kobayashi, M. Pruski, D. E. Resasco, *Chem Catal.* 1(5), 1065-1087 (2021)

Bio:
Bin Wang is a Professor, Conoco-DuPont Professor at the School of Sustainable Chemical, Biological and Materials Engineering at the University of Oklahoma. He is also a visiting scientist at the Lawrence Livermore National Laboratory and Max Planck Institute for Sustainable Materials. Before joining OU in 2014, he was a postdoctoral researcher in Department of Physics and Astronomy at Vanderbilt University. He received his Ph.D. in Chemistry from Ecole Normale Supérieure de Lyon supported by a Marie Curie Fellowship in 2011. His research is focused on computational simulations of nanoscale materials and their applications in catalysis, optoelectronics, and batteries. He received a US Department of Energy Early Career award, an ACS COMP OpenEye Outstanding Junior Faculty Award, and a Bessel Research Award by the Alexander von Humboldt Foundation. He has also been included in “Influential Researchers” by ACS I&EC Research and “Emerging Investigators” by the RSC Catalysis Science & Technology.