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Dr. M. Ali Haider has completed his M.S. and Ph.D. in Chemical Engineering at the University of Virginia (UVA). He joined the Department of Chemical Engineering at Indian Institute of Technology (IIT) Delhi as an assistant professor in 2013. He is a recipient of the Bioenergy-Award for Cutting Edge Research by the Indo-US Science and Technology (IUSSTF) Forum. He is currently working as a visiting scholar at the Catalysis Center for Energy Innovation at the University of Delaware. His research interests are focused on experimental and theoretical heterogeneous catalysis applied to the development of biorenewable chemicals.

Opportunities and Challenges in Molecular Heterogeneous Catalysis for Biorenewable Chemicals

Abstract

Importance of developing a molecular level understanding of catalyst functioning and reaction mechanisms to produce biorenewable chemicals is highlighted in two cases. For the first, phenol hydrogenation was studied over Pd nanostructures consisting of Pd octahedra, cubes and spheres. The reaction is widely used to produce precursors for polymers and has generated renewed interests in terms of understanding structure sensitivity, role of support, promoter and solvent, with an aim to develop methods for catalytic processing of lignin-derived phenolics. In general, irrespective of the solvent, or the support, Pd catalysts are known to produce partially hydrogenated cyclohexanone (which is generally thought of on the {111} facet) with high yield, as compared to the fully hydrogenated cyclohexanol. On Pd nanostructures aqueous phase hydrogenation of phenol was carried out. Mechanistic insight into the reaction mechanism was developed using density functional theory calculations. Contrary to the common belief, the results showed that {111} facet selectively yielded cyclohexanol, whereas {100} produced only cyclohexanone.

As the second case, a novel biomass-derived molecule was developed as a potential platform precursor to produce fuels, food additives, fragrances, polymers and pharmaceuticals. The proposed molecule, 6-amil- α -pyrone is a C₁₀, which is generally obtained from the fermentation of biomass and finds application as food additive. On ring-opening and decarboxylation, 6PP yielded C₉ linear ketones, at a relatively low temperature and without the requirement of an acid catalyst. The product obtained may be used directly as food-additive or transformed into jet and diesel range hydrocarbons fuels via aldol condensation. The overall process involves a unique integration of bio- and chemo-catalytic reactions. We envisage greater challenges related to catalyst deactivation by biogenic impurities to develop such a process. Theoretical simulations were utilized to understand the nature of bonded and non-bonded interactions of amino acids with the metal catalyst surface. A design of bimetallic alloy catalyst was proposed to overcome irreversible catalyst deactivation caused by sulfur containing amino acids.

Tuesday March 14th, 2017 | 2112 Learned Hall | 10:00 – 10:50AM