第366回触媒化学研究センターコロキウム

From description to prediction in Heterogeneous Catalysis

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Today's society needs to prepare itself for a more healthy future with food for all and sufficient energy and resources to fuel our growing prosperity. Catalysts will play a central role in the transition to a low-carbon economy. Catalysis itself is rapidly involving from a descriptive into a predictive science. In this lecture, I will highlight three examples of catalysis research done in Eindhoven. The first example concerns the prediction of optimum catalysts for the Fischer-Tropsch reaction by state-of-the-art computational modeling. I will show why the current catalysts are sub-optimal in performance. The second part of the presentation will be devoted to biomass conversion. The key mechanistic aspects of Lewis acid catalyzed conversion of glucose to fructose will be discussed. Theoretical models help to understand results obtained using Sn-containing zeolites and tungsten oxides. The final part of the lecture will be devoted to the upgrading of lignin which is most recalcitrant part of biomass. I will highlight how well-designed model experiments help to understand the mechanism of these complex conversion reactions. In this way, we are able to depolymerize lignin into a product with 60-90 wt% monomer yield in supercritical ethanol.
References: [1] I.A.W. Filot, R.A. van Santen and E.J.M. Hensen, Angew. Chem. Int. Ed. 53 (2014) 12746-12750. [2] G. Li, E.A. Pidko and E.J.M. Hensen, Catal. Sci. Techn. 4 (2014) 2241-2250. [3] X. Huang, T.I. Korányi, M.D. Boot and E.J.M. Hensen, ChemSusChem 7 (2014) 2276-2288.

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Professor Emiel Hensen holds a doctorate in the field of heterogeneous catalysis research from the Eindhoven University of Technology, After short stints at the University of Amsterdam (with Prof. Berend Smit) and Shell research, he returned to Eindhoven, where he serves as Professor of Inorganic Chemistry and Catalysis since 2009. The research of his group focuses on the fundamental aspects of catalyzed reactions relevant to clean and sustainable processes for the production of fuels and chemicals with the aim to identify active sites and understand reaction mechanism. His working approach is to combine advanced characterization methods with computational modeling and performance testing to guide the design and synthesis of nanoscopically organized and well-defined chemically functionalized catalytic solid materials. The materials explored include primarily highly structured porous materials containing reactive centers such as protons, metal ions and metal, metal oxide and metal sulfides clusters. Catalytic target reactions are hydrocarbon activation by Brønsted and Lewis acid as well as redox centers in zeolites and related mesoporous materials, hydrotreating reactions by metal sulfides, the Fischer-Tropsch reaction, conversion of biogenic molecules such as sugars and lignin, and metal-support cooperativity in selective oxidation. Hensen published about 250 papers in scientific journals and 15 contributions to multi-authored volumes. He currently acts as the chairman of the Netherlands Institute for Catalysis Research. He is recipient of prestigious national grants in the VENI, VIDI, VICI scheme and a TOP grant from the Netherlands Organization for Scientific Research