第364回触媒化学研究センターコロキウム

Biomass transformations over transition metals –Conquering complex reaction networks with DFT

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2015年5月27日（水）16:00–17:00

（創成科学研究棟3階セミナー室D）

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A sustainable future likely will include re-usage of carbon. One source of such carbon is biomass, i.e. plant matter and waste, which features a complex chemical composition that can vary notably. It is a huge challenge to find and to understand processes that convert these molecules into uniform target chemicals. In most cases many defunctionalization reactions, mostly of oxygen-based functionalities, have to be carried out. We explored computationally various catalytic reaction networks of (hydro-)deoxygenation and reforming reactions, starting from biomass-derived model molecules. We focused on differences between aliphatic alcohols (e.g. ethanol, propanol) and aromatic alcohols (e.g. phenol, guaiacol). Using results obtained from DFT plane-wave calculations on slab models, we discuss reforming and hydrodeoxygenation reactions of propanol on Pt [1-3] and compare the results to the situation on the more oxophilic transition metal Ru.[4] Moreover we illustrate the complex reaction network of aromatic oxygenates over transition metals on the example of the hydrodeoxygenation of guaiacol to phenol and benzene over Ru.[5] For the latter case, detailed insight on the experimental processes allows one to rationalize how the selectivity varies with hydrogen pressure.

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Professor Notker Rösch holds a doctorate in the field of theoretical chemistry, the first ever bestowed by Technische Universität München (TUM), Germany. After post-doctoral work in the USA at MIT and Cornell University (with Prof. Roald Hoffmann), he returned to TUM where he served as Professor of Theoretical Chemistry for three decades, now continuing his research as emeritus. In 2012 he started research activities in Singapore as head of the newly founded Catalysis Modelling Group at the Institute of High Performance Computing of the Agency of Science, Technology and Research. His main research field is quantum chemistry and the electronic structure of complex systems. He worked on DFT methods; his group at TUM developed the parallel DFT software ParaGauss, now in version 4.0. His current application work focusses on problems in heterogeneous and homogenous catalysis. Other research interests are metal clusters, zeolites, actinide environmental chemistry, and problems of biophysical chemistry. He published about 450 papers in scientific journals, 40 contributions to multi-authored volumes, a textbook, and an internet based practical for doing quantum chemistry calculations. As guest, Professor Rösch taught at various universities around the world, recently at Tsinghua University, Beijing. In 2005 the University of Sofia, Bulgaria, honored him as “Dr. honoris causa”. In 2012, TUM honored him with the Heinz Maier-Leibnitz Medal, its highest distinction for scientific achievements. In 2008 he was appointed Founding Director of the Catalysis Research Center of TUM; he continued to lead this institution until 2013.