第454回触媒科学研究所コロキウム

Chemistry automation to reduce expert bias and navigate the mechanistic maze towards rational catalyst design

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2023年6月20日（火）15:00—16:30
（創成科学研究棟　4階　会議室B・C）
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Catalysis plays a pivotal role in all chemical strategies towards novel more efficient and sustainable chemical conversion processes for the valorization of renewable feedstocks such as biomass and CO_2. Traditionally, catalyst development has predominantly relied on trial-and-error approaches. The grand challenge in the field is to make a step towards the rational design of efficient catalysts for a given chemical reaction. This on one hand requires a deep insight into the active site structure, the mechanism of their action, and evolution under operating conditions; and, on the other hand, accessible tools to swiftly and accurately probe the relationships between the catalyst systems' primary characteristics (e.g. chemical composition, conditions) and these complex phenomena defining their reactivity and catalytic behaviour.

In this talk, I will discuss our recent efforts in the automation of experimental and computational catalysis methodologies to resolve active site structures and get an insight into the challenging and rare-event chemistry of the catalyst deactivation pathways. The talk will be illustrated with our recent studies on relevant zeolite-based heterogeneous catalysts and homogeneous catalysts based on 3d transition metal complexes. Special focus will be on the formulation of the holistic view of catalyst performance and the introduction of dynamic descriptors of catalytic activity. With these examples I will emphasize the need for integration of the computational and experimental workflows as well as the introduction of new expert bias free and operando modelling strategies to construct representative and resolved molecular picture of complex catalytic phenomena, and pave the way towards accelerated discovery of durable and efficient catalyst systems.

Prof. Evgeny A. Pidko was trained physical chemistry at the Higher Chemical College of the Russian Academiy of Sciences in Moscow, Russia and received Ph.D. in computational catalysis with prof. Rutger van Santen from Eindhoven University of Technology, the Netherlands (2005-2008), where in 2011-2017, he was an Assistant Professor of Catalysis for Sustainability. He spent summer 2012 as a visiting professor in the group of Prof. Christophe Coperet at ETH Zurich to learn the art and science of synthetic organoemtallic chemsitry. In 2016 he obtained an ERC Consolidator grant "DeLiCat" to learn, understand and control the deactivation phenomena in hydrogenation catalysis. In September 2017, he moved to Delft Univeristy of Technology to become an Associate Professor and head of the Inorganic Systems Engineering group at the Chemical Engineering Department, where he was promoted to Full Professor in 2020. He is a member of the advisory boards of ChemCatChem and Catal. Sci. Technol. journals, and an editorial board member of Kin. Catal. and Mend. Commun. journals. He is an author of >230 publications on various topics of computational, physical, inorganic, supramolecular chemistry, catalysis, and chemical engineering. His research aims at understanding and development of catalytic systems for sustainable chemical processes including experimental and computational studies of the mechanisms and property-activity relationships in organometallic and molecular heterogeneous catalysis. Besides science, Evgeny enjoys diverse literature and music, cooking and spending quality time with his wife Svetlana and their kids Sasha and Stepan.

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454th Institute for Catalysis (ICAT) Colloquium