Abstract:

Over the last decade, computational chemistry has become one of the key components of catalysis research and has deserved a place in the catalysis toolbox next to common laboratory techniques such as FTIR, NMR or XRD [1]. The progress in fundamental understanding of catalytic phenomena currently relies largely on quantum chemical computations. State-of-the-art quantum chemical methodologies and, particularly, the density functional theory (DFT) methods have matured to the level that they can be nowadays routinely used not only to rationalize, but also to direct experimental catalysis studies. Accuracy is the corner stone of computational chemistry and it represents the key focus of this lecture. In this talk I will illustrate the problem of model definition in computational studies on industrially-relevant catalytic systems [2] and highlight the need for new operando modeling approaches to progress towards predictive modeling in catalysis. The discussion on the issues related to modeling accuracy, power and limitations of the available approaches and methodologies will be supported by representative examples from our recent research on heterogeneous catalysis for selective methane oxidation [3] and homogeneous hydrogenation catalysis [4]. During this talk, I will touch upon possible implications of the selective agreements between reductionism-dominated theories and highly complex catalytic experiments. I will emphasize the necessity of establishing a balance between the reductionist and systems approaches and the development of new operando modeling approaches to studying complex multicomponent reactive systems.

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**Biography:**

Evgeny Pidko (Moscow, Russia, 1982) received PhD from Eindhoven University of Technology in 2008, where in 2011-2017 he was an Assistant Professor of Catalysis for Sustainability. In 2016 he became a part-time professor of theoretical chemistry at ITMO University, St. Petersburg. Since September 2017 he is an Associate Professor and head of the Inorganic Systems Engineering group at the Chemical Engineering Department of Delft University of Technology. Evgeny Pidko serves as a member of the advisory boards of ChemCatChem and Catal. Sci. Technol. journals. He is an author of over 160 publications on various topics of computational, physical, inorganic, supramolecular chemistry, catalysis and chemical engineering. In his research he successfully combines experiments and theory to understand molecular mechanisms underlying the behavior of various chemical systems ranging from heterogeneous and homogeneous catalysis to inorganic functional materials and use these fundamental insights to guide the development of new more sustainable and efficient chemical technologies.