Karlsruher Institut für Technologie (KIT)

Institut für Technische Chemie und Polymerchemie
Helmholtz-Kolleg Energie-Relevante Katalyse
Freunde der Chemischen Technik e.V.

EINLADUNG

zu den Kolloquien des Instituts für Technische Chemie und Polymerchemie, des Helmholtz-Kollegs Energie-Relevante Katalyse sowie der Freunde der Chemischen Technik Karlsruhe e.V. im Wintersemester 2017/2018. Die Kolloquien finden

freitags, um 14.30 Uhr im Hörsaal 006, Gebäude 11.21, statt.

10.11.2017 **Prof. Dr. Vladimiro Dal Santo, Institute of Molecular Science and Technology, National Research Council (ISTM-CNR), University of Milan, Milan, Italy**

"(Photo)catalytic Materials for Hydrogen Generation and cleantech Applications"

01.12.2017 **Prof. Dr. Patrick Girauedeau, Interdisciplinary Chemistry, Synthesis, Analysis, Modeling (CEISAM), University of Nantes, Nantes (France)**

"Gradient-based NMR Spectroscopy on a benchtop Spectrometer: Applications to Reaction Monitoring and Authentication"

12.01.2018 **Prof. Dr. Kay Saalwächter, Fachgruppe NMR, Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle.**

"Stokes-Einstein and beyond: NMR Studies of Diffusion in crowded Solutions and under Confinement"

26.01.2018 **Prof. Dr. Evgeny A. Pidko, Inorganic Systems Engineering Group, Department of Applied Sciences, Delft University of Technology, Delft, The Netherlands – Theoretical Chemistry Group, Laboratory of Solution Chemistry for Advanced Materials and Technologies, ITMO University, St. Petersburg, Russia.**

"On the Validity of the "Single Site" Concepts in homogeneous and heterogeneous Catalysis: a Theory-Experiment Cross-Talk"

02.02.2018 **Dr. Dorothée Berthomieu, Institut Charles Gerhardt Montpellier, Chemistry Department of the CNRS, Montpellier, France.**

"Complementary Roles of theoretical Chemistry and Experiment to the understanding of Materials and heterogeneous Catalysis at the molecular Level"

Die Dozenten
des Instituts für Technische Chemie
und Polymerchemie

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(Photo)catalytic materials for hydrogen generation and cleantech applications

Vladimiro Dal Santo

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An overview of recent achievements in materials (heterogeneous catalysts, photocatalysts and photoelectrocatalysts) developed by "materials for hydrogen technology" research group at ISTM-CNR will be provided.

A series of case studies on low-loaded Ru catalysts for glycerol[1] and acetic acid[2] steam reforming, on Pt-Mn bimetallic catalysts for glycerol steam reforming and aqueous phase reforming[3]; on titanium and iron based photo(electro)catalysts, active in visible light, for water PEC splitting[4,5] and photooxidations[6], will be presented and discussed with the aim of highlighting the role of materials design and of nanostructures in obtaining active, stable and selective systems.

References

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On the validity of the "single site" concepts in homogeneous and heterogeneous catalysis: a theory-experiment cross-talk

Evgeny A. Pidko

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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]. The discussion on the issues related to modeling accuracy will be supported by representative examples from recent research of my group on zeolite catalysis for the production of biomass-derived aromatics [3] and homogeneous catalysis for CO_2 conversion [4].

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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. In his research he successfully combines experiments and theory to understand molecular mechanisms underlying the behaviour of various chemical systems ranging from heterogenous and homogeneous catalysis to inorganic functional materials.

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