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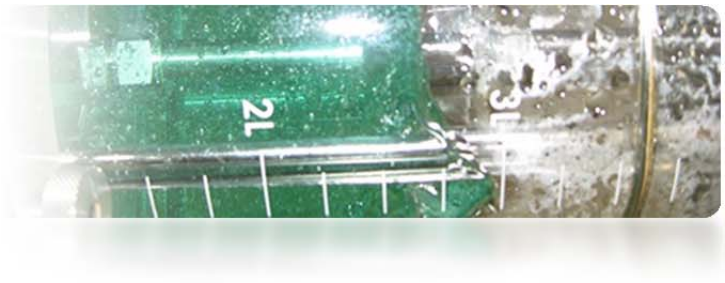
Chemical and Biomolecular Engineering



SEMINARS IN CHEMICAL AND BIOMOLECULAR ENGINEERING

Friday, January 22, 2016 10:00AM

PENTHOUSE → BH8500

Presented by

Prof. Philippe Sautet

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"Hetergeneous Catalysis: From First Principles to Multi-Scale Simulations "

Heterogeneous catalysis is at the core of sustainable chemistry, since it allows a fine control of chemical bond forming and breaking processes. For the optimal design of catalysts, a fundamental atomic scale understanding of the structure and electronic structure of the catalytic particle, in interaction with the support and with the reactant is of utmost importance. Computational chemistry today is a key method, to reach such an understanding at the molecular level of the structure of the active site and of the elementary processes occurring during the catalytic act.

However, modeling the catalytic reactivity of nanoparticles is challenging, because they expose a large number of potential active sites, and to make the task at all tractable fast methods for the calculations of adsorption energies are required. By exploring the adsorption on a large range of surface sites and transition metals, we propose a new way to quickly and accurately evaluate adsorption energies: the structure sensitive scaling relations, which are valid for all metals and for all surface sites.[1] Furthermore, for a highly affordable and reliable description of the size-dependent activity of the nanoparticles, a generalized coordination number is proposed as a leading descriptor for the adsorption strength.[3] This opens the way for a new class of activity volcano plots where the descriptor is not an energy but a structure-related quantity. Simple descriptors such as generalized coordination show a strong predictive potential, as shown in the design of optimal oxygen reduction reaction electro-catalysts.[3]

Computational chemistry also provides key insights into how the structure and reactivity of catalytic particles are affected by the interaction with the support and with the reactants. It shows how catalysts can be modified in realistic operating conditions.[4] Molecular reaction pathways can be explored, understanding how bonds can be formed and

broken. Finally I will show how the energetic information from the catalytic elementary reaction steps can be transferred to mesoscale, and then to macro scale simulations in order to understand reactivity in the gas flow around a catalytic grain.

References

1) F. Calle-Vallejo, D. Loffreda, M. T. M. Koper, P. Sautet, Nature Chemistry, 403-410 (2015)
2) F. Calle-Vallejo et al, Angewandte Chemie International Edition 53, 8316-8319 (2014)
3) F. Calle-Vallejo, J. Tymoczko, V. Colic, Q. H. Vu, M. D. Pohl, K. Morgenstern, D. Loffreda, P. Sautet, W. Schuhmann, A. S. Bandarenka, Science, 350, 185-189 (2015)
4) C. Mager-Maury, C. Chizallet, P. Sautet, P.Raybaud ChemCatChem 3, 200 (2011)

Philippe Sautet has studied at "Ecole Polytechnique" in Paris and defended his doctorate in Theoretical Chemistry at Orsay University (Paris XI) in 1989. He then entered CNRS at the Institute of Research on Catalysis in Lyon, where he developed and lead a group devoted to the applications of theoretical chemistry to heterogeneous catalysis. He spent a sabbatical at Berkeley University. After being the director of the laboratory of Chemistry at the ENS of Lyon for 8 years, he was director of the "Institut de Chimie de Lyon", a cluster of chemistry laboratories in Lyon, from 2007 to 2015.

His research interests are in the theory of the electronic structure at the interface between a solid surface and molecules and the modeling of elementary steps of heterogeneous catalysis. His work on the simulation of the atomic scale image of surfaces obtained with the scanning tunneling microscope brought him to international attention. He is worldwide recognized for his theoretical study at the molecular scale of catalysts and catalyzed reactions. He collaborates with several experimental groups in the field.

He has published over 270 scientific papers. The impact of his research is illustrated by more than 100 invited lectures at conferences and by a H factor of 54. He received the silver medal of CNRS in 2007, the Paul Pascal Prize of the French Academy of Science in 2008 and the Pierre Süe Grand Prize of the French Chemical Society in 2012. He was elected at the French Academy of Science in 2010. He is nominated in several councils or committees and is associate editor of ACS Catalysis, an international journal published by the American Chemical Society.