



The Gene and Linda Voiland School of
**Chemical Engineering and
Bioengineering**
2015 Seminar Series
Monday, March 2, 2015
12:10 p.m. Wegner G1



Karsten Reuter
Chair for Theoretical Chemistry and
Catalysis Research Center
Technische Universität München, Germany

Karsten received his Doctoral Degree in Theoretical Physics from the University Erlangen-Nürnberg in 1998. After postdoctoral stays at the Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin and the FOM-Institut for Atomic and Molecular Physics in Amsterdam, he headed an Independent Junior Research Group at the Fritz-Haber-Institut from 2005, combined with the position of a Privatdozent at the Free University Berlin. Since 2009 he holds the Chair of Theoretical Chemistry at the Technische Universität München (TUM), is an adjunct professor in the TUM Physics Department, and is affiliated to the TUM Catalysis Research Center. His research interests center on a quantitative multi-scale modeling of materials properties and functions, in particular on linking predictive-quality quantum-mechanical electronic structure calculations with more coarse-grained statistical and continuum approaches.

From Electrons to the Reactor: Multiscale Modeling of Catalytic Processes

As in many other areas of materials science, modern computational science is becoming a key contributor in the quest to quantitatively understand the molecular-level mechanisms underlying the macroscopic phenomena in chemical processing, which will ultimately enable a rational design of novel catalysts, energy suppliers and improved production strategies. Of particular relevance are hierarchical approaches that link the insights that modeling and simulation can provide across all relevant length and time scales. At the molecular level, first-principles electronic-structure calculations unravel the making and breaking of chemical bonds. At the mesoscopic scale, statistical simulations account for the interplay between all elementary processes involved in the catalytic cycle. At the macroscopic scale continuum theories yield the effect of heat and mass transfer, ultimately scaling up to a plant-wide simulation. A comprehensive control of catalytic and energy processes requires combining all of these facets and thus necessitates novel methodological approaches that integrate the various levels of theory into one multi-scale simulation. In my talk I will review our recent activities in this field, focusing in particular on current challenges in the development of error-controlled first-principles kinetic models of complex reaction networks [1], as well as on the integration of such first-principles microkinetic models into macroscale computational fluid dynamics [2,3].

- [1] M.K. Sabbe, M.-F. Reyniers, and K. Reuter, *Catal. Sci. Technol.* 2, 2010 (2012).
- [2] S. Matera and K. Reuter, *Catal. Lett.* 133, 156 (2009); *Phys. Rev. B* 82, 085446 (2010); *J. Catal.* 295, 261 (2012).
- [3] S. Matera, M. Maestri, A. Cuoci, and K. Reuter, *ACS Catal.* 4, 4081 (2014).