

# UniCat Seminar

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Lecturer: **Prof. Karsten Reuter**, Catalysis Research Center (CRC) and Chair of Theoretical Chemistry, Department of Chemistry, Technische Universität München

Title: ***Towards a First-Principles Chemical Engineering***

Abstract: 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 modelling 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 multiscale 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].

[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).

Find out more on Prof. Reuter on: <http://www.th4.ch.tum.de/>

Date: **Thursday, November 14<sup>th</sup>, 2013 at 5:00 pm**

Location: **TU Berlin, Gerhard Ertl Center, BEL Building, Marchstr. 6, 10587 Berlin, Meeting Room BEL 301**

Organizer: **Prof. Reinhardt Schomäcker (TUB)**

Coffee and tea will be served thirty minutes prior to the lecture start.

**Guests are cordially invited to attend!**

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat