

UniCat Colloquium

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Understanding Chemical Reactivity in Catalysis: The Challenge of Kinetics

In my talk, I will describe recent work aimed at modelling the mechanisms and kinetics of homogeneous catalytic processes. In recent years, we have become interested in trying to characterize not only individual reaction steps relevant to catalysis but also whole catalytic processes in a more quantitative way, including their kinetics. For example, we explored the plethora of mechanistic variants that can occur in the oxidative addition of aryl halides to Pd(0) compounds, as involved in many important cross-coupling catalytic cycles. Another recent highlight is the proposal of a mechanism involving a dimeric palladium complex in alkene cis-trans isomerisation.

The main focus of my presentation against this background will be recent work aimed at modelling the mechanism and kinetics of two important catalytic reactions: the Morita-Baylis-Hillman organocatalytic reaction, and the hydroformylation of alkenes with cobalt catalysts. In each case, the accurate treatment of electron correlation effects, conformational variability, entropy and solvation turns out to be important to get correct mechanistic understanding.

Wednesday, January 10, 2018 at 5:15 PM

TU Berlin, Institute of Chemistry
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall **C 264**

Prof. Dr. Schwarz (TUB)

Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!
Prof. Dr. Matthias Driess - Chair of the Cluster of Excellence UniCat - www.unicat.tu-berlin.de



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