unicat
Unifying Concepts in Catalysis

UniCat Colloquium

PROF. DR. JAMAL MUSAEV

Emerson Center for Scientific Computation, Emory University, Atlanta

Multi-Disciplinary and Collaborative Efforts toward the Novel Catalyst and Technology Design

I will briefly present our integrated and collaborative approaches to the:
(1) Solar-to-Chemical conversion including transition metal catalyzed water oxidation, designing of novel metal-to-metal charge transfer chromophores and novel methodology for interfacial electron transfer dynamics; and
(2) Transition metal catalyzed stereoselective C-H bond functionalization.
This talk will elaborate our efforts on understanding the transition metal catalyzed C-H bond alkylation and amination reactions.
I will analyze the factors (including nature of catalyst, auxiliary ligands, solvent, base and more) controlling the selectivity of these reactions and make intriguing predictions.
Presented joint computational-experimental findings allowed us to gain insights into the mechanisms and important elementary steps of the reaction and nature of active species, which were critical for predicting/designing of new catalysts for water oxidation and selective C-H bond functionalization, as well as for improvement of reaction efficiency and catalyst turnover number.

Tuesday, June 13, 2017 at 2:15 PM
C 074

Prof. Dr. Kaupp (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