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RCMS Research Center for Materials Science, Nagoya University

Theoretical Chemistry Colloquium

Sept. 11, 2013 (Wed), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Knowledge-based Catalyst Design: Transition Metal Catalyzed Water Oxidation and Stereoselective C-H Bond Functionalization

Dr. Jamal Musaev
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Abstract: *In the first part of my talk I will 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 methodology for interfacial electron transfer dynamics; (2) Designing of peptidedirected metal arrays as multi-electon transfer catalyst; and (3) Transition metal catalyzed C-H bond functionalization.*

In the second part of my talk, I will elaborate our efforts on understanding the di-Rh, di-Ru, (pybox)Ru catalyzed C-H bond alkylation and amination reactions. I will analyze the factors controlling the electivity of these reactions and make intriguing predictions. I will discuss our newly predicted Fe-catalyst for the C-H bond alkylation. Furthermore, we have recently discovered that monoprotected amino acid ligands (MPAA) can promote Pd(II)-catalyzed enantioselective C–H activation reactions with both pyridine and carboxylic acid directing groups. Computational investigations allowed us to gain insights into the mechanisms and important elementary steps of the reaction, nature of active species, a ligand coordination mode to the Pd(II) and transition state structure of the C–H activation step. The findings
were later supported by kinetic studies. Based on these new data we were able to improve reaction efficiency and increase catalyst TON.

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