

**演題：Multi-Disciplinary and Collaborative Efforts toward the Novel Catalysis and Technology Design: Insight into the C-H Functionalization and Water Oxidation Jungles**

**講師：Prof. Jamal G. Musaev**

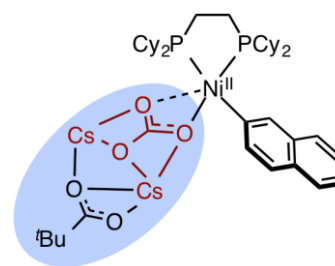
Cherry L. Emerson Center for Scientific Computation, and  
Department of Chemistry, Emory University, Atlanta, 30322, USA

日時：2016年6月20日（月）13:00~14:30

場所：北海道大学理学部7号館・2階219,220室

共催：北海道大学・触媒科学研究所，北海道大学「物質科学フロンティアを開拓する Ambitious リーダー育成プログラム」

At first, I will briefly present our collaborative approaches to the 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. Then I will elaborate in details of our latest efforts on understanding the transition metal catalyzed C-H bond alkylation and amination reactions. Our collaborative studies have revealed complexity, as well as key factors controlling reactivity and selectivity of the transition metal catalyzed C-H bond



functionalization. Namely, we have demonstrated unprecedented roles of base, auxiliary ligands and directing groups in the transition metal catalyzed C-H bond alkylation and amination. For example, it was shown that addition of Cs<sub>2</sub>CO<sub>3</sub> base to the reaction of Ni-dcype catalyzed C-H/C-O coupling of benzoxazole and naphthalene-2-yl pivalate, forms the Ni(dcype)(Naph)[PivOCs·CsCO<sub>3</sub>] cluster complex. Coordination of azole to the resulting cluster complex leads to an intermediate with a weak Cs-N(azole) bond, the existence of which increases acidity of the activated C-H bond and reduces C-H activation barrier. This emerging mechanistic knowledge was validated experimentally. Based on these findings we proposed the modified catalytic cycle for the Ni(cod)(dcype)-catalyzed C-H/C-O biaryl coupling of benzoxazole and naphthalene-2-yl pivalate.

**Prof. Jamal Musaev** is a Director of the Emerson Center for Scientific Computation and Adjunct Professor of Chemistry at Emory University. He is a founding member of the CCI-NSF Center for Selective C-H functionalization, and Emory's Bioinspired Renewable Energy Center. Dr. Jamal Musaev has over 35 years of experience in developing new computational techniques and applying them to elucidate the mechanism and controlling factors of various synthetic and enzymatic reactions. With over 350 peer-reviewed publications, 300 invited seminars, and numerous international and national awards, Dr. Musaev is regarded as an expert in the field of computational sciences. Currently, Dr. Musaev's group is studying the structure, stability and reactivity of various POMs, transition metal complexes, clusters and metalloenzymes with the aim to provide atomistic-level understandings of several state-of-art scientific and technological problems (such as water oxidation, C-H bond functionalization, etc.) and guide the design of new processes and improve existing ones. Dr. Musaev got his MS (in physics) degree from Azerbaijan State University (Baku, Azerbaijan) and PhD degree from USSR Academy of Science (Moscow, Russia).



「本講演は、大学院総合化学院『化学研究先端講義/総合化学特別研究第二』の一部として認定されています。」

連絡先：理学研究院化学部門 前田 理（内線：4921）