



ICReDD International Seminar Series

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Insights into the Microenvironment of Catalysis: Water Oxidation and Selective C–H bond Functionalization

Place: Hokkaido University, ICReDD building 4F
ICReDD Hall A

Time: Tuesday, July 16th, 2024
15:30-17:00



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Abstract: Transition metal catalysis is a complex process, where each component of the reaction plays critical roles and compliments each-other's activities. The acquiring of atomistic-level fundamental knowledge on the roles of each component of the targeted catalytic transformation, under the utilized experimental conditions, is a monumental and greatly attractive research missions. Success in this endeavor requires true collaborative efforts between the scientists with complementary expertise, and will enable us to develop more effective, highly selective, environmentally friendly, and economically viable societally critical technologies. In my talk, I will discuss our latest computational and experimental (*collaborative*) efforts on the: (A) Selective C–H Bond Functionalization and (B) Solar energy-to-chemical energy conversion.

Insights into the Microenvironment of Catalysis: Water Oxidation and Selective C–H bond Functionalization

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Transition metal catalysis is a complex process, where each component of the reaction plays critical roles and compliments (and enhances) each-other's activities. The acquiring of atomistic-level fundamental knowledge on the roles of each component (including catalyst, substrate, ligand, base, additive, solvent, and oxidant) of the targeted catalytic transformation, under the utilized experimental conditions, is a monumental and greatly attractive research missions. Success in this endeavor requires true collaborative efforts between the scientists with complementary expertise (in analytical, physical, synthetic, and theoretical sciences), and will enable us to develop more effective, highly selective, environmentally friendly (i.e. green and sustainable), and economically viable (i.e. utilizing of important and accessible substrates, and inexpensive ligands and transition metals) societally critical technologies. In my talk, I will discuss our latest computational and experimental (*collaborative*) efforts on the:

Selective C–H Bond Functionalization. The C–H functionalization—defined as the transformation of “inert” C–H bonds into C–C, C–N, C–O, C–halogen and other C–heteroatom bonds—is a viable strategy for the synthesis of complex organic targets and efficient late-state modifications of advanced molecular scaffolds. A foremost challenge of this transformative research is to control site-selectivity of the reaction. In my talk I will briefly discuss our collaborative efforts that have led to discovery of new catalysts for effective site-selective functionalization of the most accessible non-activated secondary, tertiary, and primary C–H bonds.

Solar energy -to- chemical energy conversion. There are multiple concerns with respect to generation, storage, and utilization of energy on a global scale, which have emphasized the solar-to-chemical-energy conversion the most effective technology for the production and storage of solar fuel. The two prominent foci of this strategy are hydrogen production via water splitting and carbon-based fuel production via CO₂ reduction. We have launched considerable research on design of water oxidation catalysis and solar-to-chemical conversion systems. Currently, we have prepared several polyoxometalates-based (POM) water oxidation catalyst, such as $[\{\text{Ru}_4\text{O}_4(\text{OH})_2(\text{H}_2\text{O})_4\}(\gamma\text{-SiW}_{10}\text{O}_{36})_2]^{10-}$, $[\text{Co}_4(\text{H}_2\text{O})_2(\text{PW}_9\text{O}_{34})_2]^{10-}$, and $[\text{Co}_4(\text{H}_2\text{O})_2(\text{VW}_9\text{O}_{34})_2]^{10-}$. Some of these systems will be discussed in more details in my presentation.

Musaev, Djamaladdin (Jamal) G.

Director, Cherry L. Emerson Center for Scientific Computation, Emory University



Professional Preparation:

Institution	Major/Area	Degree	Year
Azerbaijan State University, Azerbaijan	Quantum Physics	BS & MS	1978
USSR Academy of Sciences, Moscow, Russia	Quantum Chem	Ph.D.	1985
Institute for Molecular Sci., Okazaki, Japan	Quantum Chem	JSPS fellow	1991-93

Appointments: **1.** Director, Cherry L. Emerson Center, Emory University (2006-present); **2.** Adjunct Professor of Chemistry, Emory University (2015-present); **3.** Visiting Professor, Universitat de les Illes Balears, Palma de Mallorca, Spain, (Oct 2007); **4.** Visiting Professor The University of Tokyo, Japan (May 2002 – May 2003); **5.** Manager, Cherry L. Emerson Center, Emory University, (1993-2006); **6.** JSPS Research Associate, Institute for Molecular Science, Okazaki, Japan, (1991-1993); **7.** Senior Researcher, Inst. for New Chemical Problems, USSR Academy of Sciences, Chernogolovka, Moscow Region, Russia, (1986-1993); **8.** Junior Researcher, Inst. for New Chemical Problems, USSR Academy of Sciences, Chernogolovka, Moscow Region, Russia, (1981-1986); **9.** Visiting Scientist, Nesemyanov's Inst. of Organo-Element Compounds, USSR Academy of Science, Moscow, Russia, (1978-1981); **10.** Junior Scientist, Institute for Theoretical Problems of Chemical Processes, Azerbaijan Acad. of Science, Baku, Azerbaijan, (1978-1981).

RESEARCH INTERESTS:

1. Theoretical/Computational Studies of:

- Fundamental principles of transition metal-catalyzed nitrogen fixation, hydrocarbon oxidation, alkene/alkyne borylation, olefin polymerization;
- Solar-to-Chemical conversion, Water Oxidation Catalyst, Alternative energy;
- Stereoselective C-H bond functionalization (oxidation, amination, alkylation, etc.)
- Nano-scale materials with unusual physicochemical properties and reactivity.
- Mechanisms of enzymatic processes;

2. Development of Hybrid Computational Methods for interfacial charge transfer in complex systems.

HONORS/DISTINCTIONS

- IV Humanitarian Form (**under aspiration of the United Nation**): “Education and Science in the Context of Human Capital Development”, **2018**, October, Baku, Azerbaijan
- Editorial Board Member, *Organometallics*, (**2015-2018**)
- Japan Society for Promotion of Science (JSPS) Senior Fellowship, **2013**
- Turkish Scientific and Technological Research Council fellow, **2011**
- Visiting Professor: Universitat de les Illes Balears, Palma de Mallorca, Spain, (Oct. **2007**)
- Visiting Professor: The University of Tokyo, Tokyo, Japan (**2002**)
- Japan Society for Promotion of Science (JSPS) Fellowship (**1991-1993**)

PUBLICATIONS: 430+ papers, two Books, and six book chapters:

H-Index: **78** [*Seventy Eight* (Google Scholar)];

Total number of citations: 21550+;

PUBLICATION (see Publication List):

Lecture delivered: more than 325+ lectures were delivered at the Universities and R&D companies of USA, Japan, Canada, Russia, Germany, France, Spain, Italy, Sweden, Israel, China, Korea, Taiwan, Turkey, Azerbaijan,....

Synergistic Activities (*short list*):

- **Founding Member of the National Science Foundation (NSF, USA) funded “Center for Stereoselective C-H Functionalization”.** Center includes 14 top Universities of USA, 11 leading pharma Companies, 22 Principal Investigators and over 70 researchers. (see <http://www.nsf-cchf.com/>), Sept., 2009-2023
- **Member of the Catalysis Innovation Consortium (CIC).** CIC includes 20 top Universities of USA, 5 leading pharma Companies, 38 Principal Investigators (see <https://www.beyondcchf.org/>), Sept., 2023-current
- **Founder of the Emerson Center Lectureship Award with annual Symposium (2003-current).** Award Winners are World’s leading scientists. (see: <http://www.emerson.emory.edu/conferences/index.html>)
- **Organizer of the International (NATO) Symposium** “From Simplicity to Complexity in Chemistry and Beyond: Interplay Theory and Experiment” (with Drs. C. Hill (USA), A. Muller (Germany), V. Farzaliyev (Azerbaijan)), May 26-29, 2008, Baku Azerbaijan.
- **Organizer of the Symposium** “Theory and Computation for Complex Molecular Systems” within Pacificchem-2021, December, 2021, Hawaii.
- **Member of International Advisory Board:** “International Conference on Noncovalent Interactions”, 2019- present

Postdoctorals (past 5 years): Alex Kaledin (Emory), Brandon Haines (Westmont College), Manjaly John, Ajitha (India), LiPing Xu (Shandong Unver., China)

Scientific Reviewer of the dozens peer-reviewed scientific journals (such as Nature, Science, JACS; JPC; Org. Let.; Organometallics; Inorg. Chem.; J. Comp. Chem., Biochemistry, Angwante Chem., Phys.Chem. Chem. Phys., and more).

<u>Ad-hoc member of NIH reviewer panel,</u>	2008-2011
<u>DOE grant reviewer and panelist,</u>	2009-present
<u>NSF grant reviewer and panelist,</u>	2005-present