

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;
- Seleno-metabolism: Se-based anti-cancer drug design, Se transport mechanism, targeted drug delivery.

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:

390+ papers, two Books, and six book chapters:

H-Index:

75 [*Seventy Five* (Google Scholar), 68 (Web of Sci.)];

Total number of citations:

19000+;

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., 2012-current
- **Founding Member of the “Emory BioInspired Renewable Energy Center”.** (see <http://ebrec.emory.edu/>), Sept. 2006-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>)
- **Guest Editor:** *The Journal of Computational Chemistry*, 2019, v 40, # 1 and 2
- **Guest Editor:** *Chemical Physics*, 2019.
- **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** “The Interface of Computation with Chemistry and Biochemistry: Methods and Applications” within 55th Southeast Regional Meeting of the American Chemical Society (SERMACS-03), November 16-19, 2003, Atlanta, Georgia.
- **Organizer of the Symposium** “Theory and Computation for Complex Molecular Systems” within Pacifichem-2021, December, 2021, Hawaii.
- **Member of International Advisory Board:** “International Conference on Noncovalent Interactions” , 2019- present

Postdoctorals (past 5 years): A. Varela-Alvarez (AstraZeneca), Travis Figg (US Patent Office, Washington), MuthuKumar Kalliappan (Applied Materials), Alex Kaledin (Emory), Shentan Chen (China), Brandon Haines (Westmont College), Manjaly John, Ajitha (India), Rafal Roszak (Poland), LiPing Xu (Emory)

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
<u>ACS-PRF</u>	2000-present

Externally Funded research Projects

Current

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- Title:** “Solar energy-driven robust multi-electron-transfer catalysts for water splitting”.
Sponsor: Department of Energy (DOE (DE-FG02-07ER-15906))
Principal Investigator: Hill, Craig L. (Emory)
Role: Co-PI
Total award: ~\$1,180,000; Dates of project: 09/01/19 – 08/31/22
~\$390,000 for Musaev’s research
Number of person months per year devoted to project: 1 month

 - Title:** NSF-CCI; “Center in Catalytic Stereoselective C–H Functionalization”, Phase-III
Sponsor: National Science Foundation (CCI-NSF: CHE-1700982)
Principal Investigator: Davies, Huw (Emory)
Role: Co-PI
Total Award: \$20,000,000; Dates of project: 09/01/17 - 08/31/22
~\$1,050,000 for Musaev’s research
Number of person months per year devoted to project: 2.0 months

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Previous

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- Title:** Multidisciplinary Research for the Advancement of Filtration Materials:
in situ/operando Studies of Ambient Surface Chemistry
Sponsor: DOD-DTRA (W911NF-15-2-0107)
Principal Investigator: John R. Morris (Virginia Tech)
Total award: \$5,000,000 Dates of project: 9/1/14-8/31/19
~\$377,000 for Musaev’s research
Number of person months per year devoted to project: 1 month

 - Title:** “Principles of Selective O₂-Based Oxidation by Optimal (Binuclear) Catalytic Sites”.
Sponsor: Department of Energy (DOE, [Catalysis](#), DE-FG02-03ER15461)
Principal Investigator: Musaev, D. G. (Emory)
Total award: ~\$1,839,943.00: Dates of project: 09/01/03 – 08/31/14
Co-PI’s Hill, C. (Emory) and K. Morokuma (Emory)
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- Title:** “Acquisition of Computer Systems for Computational Chemistry and Chem. Physics”,
Sponsor: National Science Foundation- (MRI-R2) (CHE-0958205)
Principal Investigator: D. Lynn (Emory),
Role: Co-PI
Total award: \$368,000; Dates: 10/01/10-9/30/13

Total award: ~\$40,000; Dates: 03/01/08-02/28/10
 ~\$8,000 for Musaev's research

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11. **Title:** "Computational Methods for Catalyst Design. Development of Group 4 Metallocene Polymerization Catalysts Based on Theoretical Computation and Experiment."

Sponsor: Phillips Petroleum Company and NIST ATP project,

Principal Investigator: K. Morokuma (Emory),

Role: Co-PI

Total award: ~\$500,000; Dates: 9/30/95-9/29/98
 ~\$150,000 for Musaev's research

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12. **Title:** "Acquisition of IBM computer system",

Sponsor: IBM-SUR (Shared University Research Award)

Principal Investigator: K. Morokuma (Emory),

Role: Co-PI

Total award: ~\$625,000; Dates: Sept. 2000

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13. **Title:** "Acquisition of Computer Systems for Computational Chemistry and Chem. Physics",

Sponsor: National Science Foundation-MRI (CHE-0079627)

Principal Investigator: K. Morokuma (Emory),

Role: Co-PI

Total award: ~\$300,000; Dates: 10/01/00-9/30/03

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14. **Title:** "Acquisition of Computer Systems for Computational Chemistry and Chem. Physics",

Sponsor: Air Force Office of Scientific Research

Principal Investigator: K. Morokuma (Emory),

Role: Co-PI

Total award: ~\$213,569; Dates: 04/01/04 - 03/31/05

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15. **Title:** "Complexity and Simplicity in Chemistry and Beyond: Interplay Theory and Experiment."

Sponsor: NATO Scientific Council (For NATO workshop in Baku,
 Azerbaijan, May 26-28, 2008)

Principal Investigator: C. Hill (Emory),

Role: Co-PI

Total award: ~\$32,000; Dates: 03/01/08-02/28/09

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16. Multiple Deals with the vendors (IBM, SUN, SGI, Microwaves, Schrodinger Inc., etc.) Total: ~1 mil.