

## DJAMALADDIN ( JAMAL ) G. MUSAEV

*Principal Scientist and Director of the Emerson Center, Emory University*

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### POSITIONS HELD:

- **Director, Principal Sci.,** Ch. L. Emerson Center, Emory Univ., Sep. 2006-present
- **Visiting (European Comm.) Professor** Universitat de les Illes Balears, Palma de Mallorca, Spain, (Oct-Dec. 2007)
- **Principal Sci., Manager** Ch. L. Emerson Center, Emory Univ., March 2000- Sep. 2006
- **Visiting Professor** The University of Tokyo, Japan, May 2002 – May. 2003
- **Associate Scientist** Ch. L. Emerson Center, Emory Univ., 1993-March, 2000
- **Research Associate** Inst. for Molecular Science (IMS), Okazaki, Japan, 1991-93
- **Senior Researcher** Inst. for New Chem. Prob., Chernogolovka, Moscow, unt. 1993

### RESEARCH INTERESTS:

#### 1. *Theoretical/Computational Studies of:(on Catalysis, Enzymatic Processes, Drug Design):*

- Understanding of fundamental principles of transition metal-catalyzed (including nano-scale catalysts) nitrogen fixation, hydrocarbon oxidation,  $\sigma$ -bond (C-H, C-C etc) activation, alkene/alkyne boration, and olefin polymerization;
- Design of Solar energy-driven robust multi-electron-transfer catalysts for water splitting. Problems of Hydrogen production and storage.
- Search for new nano-scale materials with unusual physicochemical properties and reactivity.
- Elucidate mechanisms of enzymatic processes: Search for effective drugs against peroxynitrite toxicity. Application of nano-structures in biology.
- Seleno-metabolism: A search for effective Se-based anti-cancer drugs. Se transport mechanism in body.
- Understanding of fundamental principles and mechanisms of important metalloenzymatic catalysis such as oxidation (MMO, RNR), nitrogen fixation (FeMoco) and hydrogenation.

#### 2. *The development of hybrid methods applicable to nanoscaled systems.*

### RESEARCH GRANTS (CURRENT):

1. **Department of Energy (DOE):** “Principles of Selective O<sub>2</sub>-Based Oxidation by Optimal (Multinuclear) Catalytic Sites”. 09/15/06 – 09/15/09, Total award is ~\$936,000: Principal investigator (Co-PI’s are Drs. C. Hill and K. Morokuma)

2. **Department of Defense (DOD, Office of Naval Research):** “Fundamental Understanding of Propellant/Nozzle Interaction to Mitigate Erosion for Very High Pressure Missile Propellant Application”, Subcontractor (with MC Lin and S. Irle); Total Award is for Emory University **\$800,000**. Main Contractor is Penn State University (Prof. K.K. Kuo, The Mechanical Engineering Department), 07/01/2004-07/01/2009
3. **Department of Energy (DOE):** “Solar energy-driven robust multi-electron-transfer catalysts for water splitting” 09/01/07 – 08/31/10, Total award is ~**\$900,000**: Co-PI (together with Drs. C. Hill (PI) and T. Lian (Co-PI))
4. **NATO Scientific Council:** To organize NATO workshop in Baku, Azerbaijan, May 26-28, 2008, on “Complexity and Simplicity in Chemistry and Beyond: Interplay Theory and Experiment”, ~**\$32000** (together with Drs. C. Hill (USA), A. Muller (Germany) and A. Efendiev (Azerbaijan)).

#### **PUBLICATIONS:**

- **Author/co-author** of 210+ papers, 6 review article, and Chapters in 5 Books.
- **55+ papers** during the years of 2005-2007 and
- **Delivered scientific lectures** in more than 60+ Universities and R&D Companies of the USA, Germany, France, Spain, Japan, Canada, Sweden, Russia, and Israel.

#### **EDUCATION:**

- **B.S./M.S.** Azerbaijan State University, Baku, Azerbaijan, **1978**
- **Ph.D** Inst of General and Inorganic Chemistry, USSR Acad. of Sci., Moscow (one of the top Scientific Institutes of the USSR), **1985**

#### **HONORS:**

- Visiting Professor award from the European Committee: Universitat de les Illes Balears, Palme de Mallorca, Spain, (Oct. 2007)
- Visiting Professor award of the University of Tokyo, Tokyo, Japan (2002-2003)
- Japan Society for Promotion of Science (JSPS) Fellowship (1991-1993)
- Azerbaijan Republic Fellowship for Promotion of Science (1978 –1981)

**VISA STATUS:** USA Citizen (Naturalized in March 2002)

#### **Externally Funded Projects:**

#### **Current**

5. **Department of Energy (DOE):** “Principles of Selective O<sub>2</sub>-Based Oxidation by Optimal(Multinuclear) Catalytic Sites”. 09/15/06 – 09/15/09, Total award is ~**\$936,000**: Principal investigator (Co-PI’s are Drs. C. Hill and K. Morokuma)

6. **Department of Defense (DOD, Office of Naval Research):** “Fundamental Understanding of Propellant/Nozzle Interaction to Mitigate Erosion for Very High Pressure Missile Propellant Application”, Subcontractor (with MC Lin and S. Irle); Total Award is for Emory University **\$800,000**. Main Contractor is Penn State University (Prof. K.K. Kuo, The Mechanical Engineering Department), 07/01/2004-07/01/2009
7. **Department of Energy (DOE):** “Solar energy-driven robust multi-electron-transfer catalysts for water splitting” 09/01/07 – 08/31/10,  
Total award is ~**\$900,000**: Co-PI  
(with Drs. C. Hill (PI) and T. Lian (Co-PI))
8. **NATO Scientific Council:** To organize NATO workshop in Baku, Azerbaijan, May 26-28, 2008, on “Complexity and Simplicity in Chemistry and Beyond: Interplay Theory and Experiment”, ~**\$32000** (with Drs. C. Hill (USA), A. Muller (Germany) and A. Efendiev (Azerbaijan)).

## Pending

9. **BAA-DoD: Defense Threat Reduction Agency (DTRA)** “Multifunctional Nanomolecules underlying detecting and catalytically decontaminating materials” Requested award: ~**\$1,050,000**. Expected Period: 11/01/07-10/31/10, Co-PI (PI: Dr. Craig Hill).
10. **Azerbaijan-US Bilateral Grants Program (US Civilian Research and Development Foundation, CDRF):** “Designing of new non-metallocene based catalysts for synthesis of high-density polyethylene: Joint Experimental and Theoretical Studies.” Requested award: **\$50,000** .  
Expected Period: 01/01/08-12/31/10, Co-PI  
(Drs. Craig Hill (USA) and Akif Azizov (Azerbaijan)).
11. **Department of Energy (DOE)- Mid-Scaled Instrumental Grant:** “Acquisition of Computer Clusters to Support DoE Basic Energy Sciences Research at the Emory University Emerson Center for Scientific Computation”, Requested award: **\$600,000**. Expected Period: 01/01/08-12/31/10.

## Previous

12. **Department of Energy (DOE):** “Principles of Selective O<sub>2</sub>-Based Oxidation by Optimal (Binuclear) Catalytic Sites”. 09/15/03 – 09/15/06,  
Total award was ~**\$903,943.00**: PI  
(Co-PI’s Drs. C. Hill and K. Morokuma)
13. **National Science Foundation:** “Theoretical Studies of Structures and Reactions of Transition Metal Atoms, Ions, Complexes and Cluster Complexes” Total ward was **\$832,000** 07/01/98-06/30/06 Co-PI: (PI: K. Morokuma)

- 14. Phillips Petroleum Company and NIST ATP project**, entitled "Computational Methods for Catalyst Design. Development of Group 4 Metallocene Polymerization Catalysts Based on Theoretical Computation and Experiment" Participant are: Phillips Petr., Oklahoma State Univ., University of Minnesota and Emory University. Amount of funding for Emory was ~\$500,000 for 9/30/95-9/29/98. Co-leader from the Emory.
- 15. IBM-SUR grant** to Emerson Center: "Acquisition of IBM computer system", year of 2000, total amount was \$625,000; Co-PI (PI was Keiji Morokuma)
- 16. National Science Foundation** (Major Research Instrumentation Grant), "Acquisition of Computer Systems for Computational Chemistry and Chemical Physics", total award \$300,000 10/01/00-9/30/03; Co-investigator (PI: K. Morokuma)
- 17. Air Force Office of Scientific Research: Defense University Research Instrument Program:** "Computer Cluster for Computational Studies of Chemical Reaction Systems" \$213,569 04/01/04 - 03/31/05; Co-PI (PI K. Morokuma)
- 18. Various Deals with the vendors** (IBM, SUN, SGI, Microwaves, Schrodinger Inc., etc.) Total: ~1 mil.

#### **OTHER ACTIVITIES:**

- **Local Committee member** (coordinator of the scientific program) of the 9<sup>th</sup> Intern. Congress of Quantum Chemistry (9-14 June, **1997**, Emory University, Atlanta, USA).
- **Chair of the Organizing Committee** of the Intern. Symposium: "In the Frontiers of Quantum Chemistry and Chemical Reactions" (Emory University, 21-22 May **1999**).
- **Guest Editor**, Journal of Molecular Structure (THEOCHEM.), **1999**, Vols 461-462.
- **Local Committee Member** of the International Conference of ADHOC-2002, July, **2002**, Emory University
- **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 International (NATO) Symposium** "Complexity and Simplicity in Chemistry and Beyond: Interplay Theory and Experiment" (with Drs. C. Hill (USA), A. Muller (Germany) and A. Efendiev (Azerbaijan)), May 25-29, **2008**, Baku Azerbaijan.
- **Scientific Reviewer** of the dozens peer-reviewed scientific journals (such as JACS; JPC; Org. Let.; Organometallics; Inorg. Chem.; J. Comp. Chem., J. Mol. Str (Theochem), Biochemistry, Angwante Chem., Phys.Chem. Chem. Phys., and more).

**Current and Former Students/Postdocs:****Graduate Students:****Former:**

1. Dmitry Khoroshun (joint with Prof. K. Morokuma),  
Currently postdoc with Walter Thiel, Germany
2. Ilja Khavrutski, (joint with Prof. K. Morokuma),  
Currently postdoc with Dr. Andy McCammon (UCSD, San Diego)
3. Taraneh Nowroozi-Isfahani
4. Yukiko Sakimoto, (joint with Prof. K. Hirao, The University of Tokyo)

**Current:**

5. Hideaki Miyachi, (joint with Prof. K. Hirao, The University of Tokyo)

**Undergraduate Students:****Former:**

1. Mr. Robby Rahim (joint with Prof. K. Morokuma),  
Currently at Emory Medical School

**Postdocs:****Former**

1. Robert Froese, (joint with Prof. K. Morokuma)  
Currently, Scientific staff at Dow Chemical Co.
2. Max Holthausen (joint with Prof. K. Morokuma)  
Currently, at Philipps-Universität Marburg, Germany
3. Sergei Vyboishchikov (joint with Prof. K. Morokuma)  
Currently, Scientific staff at Girona University, Spain
4. Robert Szilagyi (joint with Prof. K. Morokuma)  
Currently, Faculty member at Montana State University
5. Maricel Torrent (joint with Prof. K. Morokuma)  
Currently, Scientific staff at Merck Co.
6. Ying-hong Sheng (joint with Prof. K. Morokuma)  
Currently, postdoc at Jackson State University

7. Marcin Hoffmann (joint with Prof. K. Morokuma)  
Currently at Poland
8. Petia Bobatova-Parvanova (joint with Prof. K. Morokuma)  
Currently at PNNL
9. Rajeev Prabhakar (joint with Prof. K. Morokuma)  
Currently, Faculty member at University of Miami
10. Yan Wang (joint with Prof. K. Morokuma)  
Currently, postdoct at Germany
11. David Quinonero (joint with Prof. K. Morokuma)  
Currently, Faculty member at Universitat de les Illes Balears, Spain
12. H. T. Chen (joint with Prof. M.C. Lin)  
Currently, scientific staff at Taiwan National Computing Center

**Current :**

1. Alexsey Kuznetsov (joint with Prof. K. Morokuma)
2. S. C. Xu (joint with Prof. M.C. Lin)