

ILJA V. KHAVRUTSKII

9500 Gilman Dr, La Jolla, CA 92093-0365; C: 858-366-3090, W: 858-534-2798, ikhavru@mccammon.ucsd.edu

Curriculum Vitae

EDUCATION

- Ph.D., Chemistry, Emory University, Atlanta, GA, 2004 (GPA 4.0)
Thesis: Computational study of the O-O bond activation and hydrocarbon oxygenation reactions in the catalytic cycles of the non-heme diiron enzymes and chiral Mn-Salen complexes
Research Advisor: Prof. Keiji Morokuma
- MS, Chemistry and Ecology, Novosibirsk State University, Novosibirsk, Russia, 1998
- BS, Chemistry, Ecology and Natural Sources Management, Novosibirsk State University, Novosibirsk, Russia, 1997

HONORS AND AWARDS

- Charles T. Lester Award, Emory University, 2003-2004 (\$6,000)
- Graduate Student Award, International Soros Science Education Program, 1999 (\$1,500)
- Undergraduate Student Award, International Soros Science Education Program, 1998, 1997 (\$750 each)

AFFILIATIONS AND MEMBERSHIPS

- United States Association for Computational Mechanics (USACM) and International Association for Computational Mechanics (IACM), Member since 2007
- American Association for the Advancement of Science (AAAS), Member since 2007
- NSF Center for Theoretical Biological Physics (CTBP), Affiliate since 2004
- American Chemical Society (ACS), Member since 2000

PROFESSIONAL SERVICES

- Reviewed papers for the following journals:
 - American Chemical Society: *Organometallics*, *Inorganic Chemistry*, and *The Journal of the American Chemical Society*
 - Wiley-VCH: *Chemistry – A European Journal*, and *Journal of Computational Chemistry*
 - American Institute of Physics: *The Journal of Chemical Physics*
- Managed numerous software and hardware for Morokuma group PC cluster
- Managed Morokuma group home page
- Contributed to a success of a research proposal to acquire a supercomputer worth \$214,000 via Defense University Research Instrumentation Program (DURIP) through AFOSR, 2003.

ACCOMPLISHMENTS

2007 – present. Research Associate at *Howard Hughes Medical Institute*, with Prof. J. Andrew McCammon; *University of California at San Diego*, Department of Chemistry and Biochemistry, La Jolla, CA

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2004 – 2007. Postdoctoral Research Associate with Prof. Charles L. Brooks, III; *The Scripps Research Institute*, Department of Molecular Biology, La Jolla, CA

- Studied the mechanisms of action of potential anticancer drug target proteins by means of molecular dynamics simulations
- Developed new forcefields for small molecules
- Studied mechanisms of protein folding using graph-theory techniques
- Developed Harmonic Fourier Beads (HFB) reaction path ensemble method for studying rare events in large systems
- Derived a novel free energy gradient theorem to compute free energy profiles
- Contributed the HFB code to the CHARMM simulation package

1999-2004. Graduate Research Assistant; *Emory University*, Department of Chemistry, Atlanta, GA

- Applied Density Functional Theory methods to study transition metal catalyzed reactions
- Developed novel electrostatic coupling scheme for ONIOM geometry optimization
- Developed a novel Perl-based toolset for complex optimization tasks with ONIOM method
- Applied ONIOM method to study non-heme diiron enzymes, Methane Monooxygenase and Ribonucleotide Reductase

1995-1999. Research Scholar; *Boreskov Institute of Catalysis (BIC)*, Research Group for Stereoselective Catalysis and Research Group for NMR and ESR Studies of Catalytic Processes

- Studied mechanisms of radical chain oxidation reactions of organic sulfides and epoxides catalyzed by transition metal-containing materials

1998-1999. Research Assistant; *Novosibirsk State University (NSU)*, School of Natural Sciences, Department of Chemistry, Novosibirsk, Russia

- Studied enantioselective sulfoxidation and epoxidation reactions catalyzed by chiral transition metal complexes
- Was actively involved in teaching Chemical Kinetics and Thermodynamics courses

TEACHING EXPERIENCE

1999-2003. Emory University

- TA, Foundation of Computational Chemistry (CHEM 511)
- TA, General Chemistry Lab (CHEM 141L/142L)
- TA, Inorganic Chemistry (CHEM 350)
- Trained several graduate students and postdocs to use ONIOM method for protein related computational studies
- Mentored an undergraduate student

1998-1999. Novosibirsk State University

- TA, Chemical Kinetics and Thermodynamics Labs

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SKILLS

- Areas of Expertise:
Electronic Structure Theory, Numerical Analysis, Chemical Kinetics and Thermodynamics, Statistical Physics, Molecular Dynamics, Inorganic Chemistry, Electrochemistry and Catalysis.
- Instrumentation:
ESR, NMR, UV/Vis, and FTIR Spectroscopies, Cyclic Voltammetry, GC (FID/ECD/MS), HPLC, Polarimetry.
- Computers:
OS: Unices (Linux, AIX, Mac OS X, IRIX), Windows.
Programming Languages: Fortran 77, C++, Perl, HTML.
Quantum and Molecular Mechanics Packages: Gaussian 98, 03; Gamess-US; Molpro; Turbomole; ACESII; Amber; CHARMM; Jaguar; Mopac.
Mathematical Packages: Matlab, Mathematica, MathCAD.
Visualization software: Molecule; Molekel; Molden; Molscript; Raster3D, Chem3D, VMD.
Misc. Software: AdobePhotoshop, ChemOffice, CorelOffice, MicrosoftOffice, EndNote, Origin, Gnuplot.

INVITED AND WELCOME TALKS

- 2007 (Jul).** The 9th U.S. National Congress on Computational Mechanics (USNCCM9), hosted by Prof. Sukky Jun (University of Wyoming), Prof. Ju Li (The Ohio State University) and Prof. Shaofan Li (UC Berkeley), San Francisco, CA.
- 2007 (Jul).** UC Berkeley, hosted by Prof. Martin Head-Gordon, Berkeley, CA.
- 2006 (Nov).** UC San Diego, hosted by Prof. J. Andrew McCammon, La Jolla, CA.
- 2006 (Nov).** UC San Diego, hosted jointly by Prof. Peter Wolynes and Prof. Jose Onuchic, La Jolla, CA.

PUBLICATIONS

I. PEER REVIEWED JOURNALS

1. in preparation
2. *Generalized Gradient-Augmented Harmonic Fourier Beads Method with Multiple Atomic and/or Center-of-Mass Positional Restraints*
Khavrutskii, I. V. and McCammon, J. A., *J. Chem. Phys.* **2007**, in press
3. *Gradient-Augmented Harmonic Fourier Beads Method for Quantitative Studies of Reaction Path Ensembles*

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- Khavrutskii, I. V.** and Brooks, III, C. L.; *J. Chem. Phys.* **2007**, *on-hold (times cited 1)*
4. *Harmonic Fourier Beads Method for Studying Rare Events on Rugged Energy Surfaces*
Khavrutskii, I. V.; Arora, K.; Brooks, III, C. L.; *J. Chem. Phys.* **2006**, *125* (17), 174108:1-7
(times cited 3)
 5. *Conformational Change of the Methionine 20 Loop of Escherichia coli Dihydrofolate Reductase Modulates Protonation of the Substrate Dihydrofolate*
Khavrutskii, I. V.; Price, D. J.; Lee, J.; Brooks, III, C. L.; *Protein Sci.* **2007**, *16* (6), 1087-1100 (times cited 1)
 6. *A Line Integral Reaction Path Approximation for Large Systems via Nonlinear Constrained Optimization: Application to Alanine Dipeptide and β -Hairpin of Protein G*
Khavrutskii, I. V.; Byrd, R. H.; Brooks, III, C. L.; *J. Chem. Phys.* **2006**, *124* (19), 194903:1-14 (times cited 5)
 7. *Computational Insights into the Mechanism of Radical Generation in B12-Dependent Methylmalonyl-CoA Mutase*
Kwiecien, R. A.; **Khavrutskii, I. V.**; Musaev, D. G.; Morokuma, K.; Banerjee, R.; Paneth, P.; *J. Am. Chem. Soc.* **2006**, *128* (4), 1287-1292 (times cited 5)
 8. *Cooperative Pull and Push Effects on the O-O Bond Cleavage in Acylperoxo Complexes of [(Salen)Mn^{III}L]: Ensuring Formation of Manganese(V) Oxo Species*
Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K.; *Inorg. Chem.* **2005**, *44* (2), 306-315
(times cited 4)
 9. *Does the Active Site of Mammalian Glutathione Peroxidase (GPx) Contain Water Molecules? An ONIOM Study*
Prabhakar, R.; Musaev, D. G.; **Khavrutskii, I. V.**; Morokuma, K.; *J. Phys. Chem. B* **2004**, *108* (34), 12643-12645 (times cited 10)
 10. *Epoxidation of Unfunctionalized Olefins by Mn(Salen) Catalyst Using Organic Peracids as Oxygen Source. A Theoretical Study*
Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K.; *Proc. Nat. Acad. Sci. USA* **2004**, *101* (16), 5743-5748 (times cited 5)
 11. *Axial Ligand and Solvent Effects on the O-O Bond Activation in Acylperoxo Complexes of [(Salen)Mn^{III}L]: Mn^{IV} versus Mn^V Oxo Species*
Khavrutskii, I. V.; Rahim, R. R.; Musaev, D. G.; Morokuma, K.; *J. Phys. Chem. B* **2004**, *108* (12), 3845-3854 (times cited 8)
 12. *Protein Effects on the O₂ Binding to the Active Site of the Methane Monooxygenase: ONIOM Studies*

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- Hoffmann, M.; **Khavrutskii, I. V.**; Musaev, D. G.; Morokuma, K.; *Int. J. Quant. Chem.* **2004**, 99 (6), 972-980 (*times cited 9*)
13. *Insights into the Structure and Reactivity of Acylperoxo Complexes in Kochi-Jacobsen-Katsuki Catalytic System. A Density Functional Study*
Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K.; *J. Am. Chem. Soc.* **2003** 125 (45), 13879-13889 (*times cited 20*)
14. *Structure, Stability, and Electronic and NMR Properties of Various Oxo- and Nitrido-Derivatives of [L(Salen)Mn(III)]⁺, Where L = None and Imidazole. A Density Functional Study*
Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K.; *Inorg. Chem.* **2003**, 42 (8), 2606-2621 (*times cited 29*)
15. *EPR detection and characterization of high-valent manganese complexes in MnIII(Salen) catalyzed aerobic olefin epoxidation*
Bryliakov, K. P.; **Khavrutskii, I. V.**; Talsi, E. P.; Kholdeeva, O. A.; *React. Kinet. Catal. Lett.* **2000**, 71 (1), 183-191 (*times cited 9*)
16. *Oxidation of methyl phenyl sulfide with molecular oxygen in the presence of isobutyraldehyde and transition metal monosubstituted heteropolytungstates.*
Khavrutskii, I. V.; Maksimov, G. M.; Kholdeeva, O. A.; *React. Kinet. Catal. Lett.* **1999**, 66 (2), 325-330 (*times cited 0*)

II. PUBLISHED PROCEEDINGS

ORAL PRESENTATIONS

Transition path and path ensemble optimization with gradient-augmented Harmonic Fourier Beads method.

Khavrutskii, I. V. and McCammon, J. A.; Abstracts of Papers, 9th U.S. National Congress on Computational Mechanics (USNCCM9), San Francisco, CA, Jul 23-26, **2007**, Mini-symposium on Recent Developments in Nanoscale Simulations: From Quantum to Coarse-Grained Modeling.

The enhanced harmonic Fourier beads method with novel free energy gradient approximation for quantitative studies of rare events via reaction path ensembles.

Khavrutskii, I. V. and Brooks, C. L., III; Abstracts of Papers, 233^d ACS National Meeting, Chicago, IL, March 25-29, **2007**, PHYS/COMP Capturing Complexity in Physical Sciences Simulation Symposium.

Conformational change of the methionine 20 loop of Escherichia coli dihydrofolate reductase modulates protonation of the substrate dihydrofolate.

Khavrutskii, I. V.; Price, D. J.; Lee, J.; Brooks, C. L., III; Abstracts of Papers, 231st ACS National

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Meeting, Atlanta, GA, March 26-30, **2006**, COMP

Protonation and push effects on the O-O bond cleavage in trans-acylperoxo complexes of [(Salen)Mn(III)L]: How to obtain reactive oxo species?

Khavrutskii, I. V., Rahim, R. R., Musaev, D. G., Morokuma, K.; Abstracts of Papers, 226th ACS National Meeting, New York City, NY, September 7-11, **2003**, INOR

Mechanism of the enantioselective epoxidation by [(Salen)Mn(III)L] oxo complexes

Khavrutskii, I. V., Rahim, R. R., Musaev, D. G., Morokuma, K.; Abstracts of Papers, 226th ACS National Meeting, New York City, NY, September 7-11, **2003**, INOR

New insights into the structure and reactivity of acylperoxo complexes in Kochi-Jacobsen-Katsuki (KJK) catalytic system. A density functional theory (DFT) study

Khavrutskii, I. V., Musaev, D. G., Morokuma, K.; 8th International Symposium on Activation of Dioxygen and Homogeneous Catalytic Oxidation, Emory University, Atlanta, Georgia, USA, June 2-7, **2002**

DFT theoretical study of acylperoxo complexes and their evolution in the Kochi-Jacobsen-Katsuki (KJK) catalytic system

Khavrutskii, I. V.; Musaev, D. G.; Morokuma, K.; Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, **2002**, INOR.

FULL PAPERS

Selective alkene epoxidation by molecular oxygen in the presence of aldehyde and different type catalysts containing cobalt

Kholdeeva, O. A.; Khavrutskii, I. V.; Romannikov, V. N.; Tkachev, A. V.; Zamaraev, K. I.; *Stud. Surf. Sci. Catal.* **1997**, 110 (3rd World Congress on Oxidation Catalysis, 1997, 947-955.

Selective aerobic epoxidation of olefins over NaY and NaZSM-5 zeolites containing transition metal ions

Kholdeeva, O. A.; Tkachev, A. V.; Romannikov, V. N.; Khavrutskii, I. V.; Zamaraev, K. I.; *Stud. Surf. Sci. Catal.* **1997**, 108 (Heterogeneous Catalysis and Fine Chemicals IV), 337-344.

ABSTRACTS ONLY

List available upon request

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REFERENCES

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Howard Hughes Medical Institute
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