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Olexandr Isayev, Ph. D.

Curriculum Vitae

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Case Western Reserve University*

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Education Background

- 2008 **Ph.D.**
Jackson State University, Department of Chemistry, Jackson, MS
- 2002 **M.S. with the Highest Honor (Red Diploma, summa cum laude)**
Dnepropetrovsk National University, Department of Chemistry, Ukraine
- 2001 **B.Sc. with the Highest Honor**
Dnepropetrovsk National University, Department of Chemistry, Ukraine

Workshops and Schools

- Aug 2008 **NRBSC Summer Institute**
San Diego Supercomputing Center, University of California, San Diego, CA
- Oct 2007 **NRBSC Workshop “Methods and Applications of Hybrid QM/MM Simulations to Biomolecular Systems”**
Pittsburg Supercomputer Center, Carnegie-Mellon University, Pittsburg, PA
- Aug 2007 **Summer Program “Classical and Quantum Approaches in Molecular Modeling”**
Institute for Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN
- Jul 2007 **13th SDSC Summer Institute “Reducing your Time to Solution”**
San Diego Supercomputing Center, University of California, San Diego, CA
- Nov 2006 **Workshop on “Quantum Simulation of Liquids and Solids”**
CECAM, ENS de Lyon, France
- Aug 2006 **Summer School on Computational Materials Science “Ab Initio Molecular Dynamics Simulation Methods in Chemistry”**
University of Illinois at Urbana-Champaign, Urbana, IL
- May 2006 **Workshop “New Developments for First Principles Molecular Dynamics Simulations in Condensed Matter and Molecular Physics”**
CECAM, ENS de Lyon, France

Work Experience

- 2009 – Present **Postdoctoral Fellow**
Department of Chemistry, Case Western Reserve University
- Autumn 2008 **Research Assistant**
Interdisciplinary Center for Nanotoxicity, Jackson State University
- 2002 – 2008 **Graduate Research Assistant**
Computational Center for Molecular Structure and Interactions,
Jackson State University
*Ph.D. thesis title “Theoretical study on nitroaromatic and related
compounds: properties, reduction and decomposition”*
- Summer 2006 **Visiting Research Assistant**
Equipe de Chimie et Biochimie Théoriques, Université Henri Poincaré,
Nancy, France
Theoretical modeling of formamide hydrolysis.
- 2003 – 2008 **System Administrator**
Computational Center for Molecular Structure and Interactions,
Jackson State University
*Configuration/management local computational clusters and
workstations. Porting/tuning scientific codes on our platforms.
Development/management of department’s web, mail and file servers.*
- 2004 **Teaching Assistant**
Department of Chemistry, Jackson State University
CHEM 141, general chemistry, chemistry lab.
- Summer 2001 **Summer Internship**
Computational Center for Molecular Structure and Interactions,
Jackson State University
Theoretical study on properties of nitroaromatic compounds.
- 2000 – 2002 **Research Associate**
Dnepropetrovsk National University, Department of Chemistry, Ukraine
*M.S. Thesis title “Synthesis, NMR spectra, and theoretical study on amides
with two bicyclic fragments”*

Awards and Honors

2009	IBM-Löwdin memorial Fellowship
2008	NBCR Summer Institute Scholarship
2006	Travel Award, NSF–Materials Computation Center (MCC), University of Illinois at Urbana-Champaign
2006	Best Professional Oral Presentation, 70 th Annual Meeting, Mississippi Academy of Sciences
2003	Honor for Outstanding Academic Leadership, Jackson State University
2001	Special Recognition Award, 10 th Conference on Current Trends in Computational Chemistry, Jackson, MS
2000	Prize winner of Ukrainian Chemical Olympiad for Students
2000	Prize winner of XI Mendeleev Competition for Student’s Research Projects, Moscow, Russia
1997	Award of Ministry of Education for Research Project of Young Scientists, Kiev, Ukraine

Research and Professional Activities

My research interests focus on connecting *ab initio* electronic structure methods with thermodynamic and kinetic properties of matter. I use state-of-the-art electronic structure methods in combination with a wide variety of techniques from quantum mechanics to molecular dynamics, to solve relevant problems in chemistry, biophysics, and materials science.

- Bonding, structural and electronic properties of ferrous/ferric centers with systems of biological and environmental interest.
- Hydration and dynamics of nucleic acid bases in water. Properties of liquid water.
- Reduction and decomposition of aromatic nitro compounds. Their ADMET and SAR properties.

☛ Chemistry under extreme conditions. Thermal decomposition in crystal nitramines.

(Full statement of research interests at http://www.olexandrisayev.com/Isayev_RI.pdf)

Minor code development and performance/functionality enhancements of existing molecular modeling codes. High performance computing, scientific visualization, graphics and animation.

During 2003-2008, I had been local committee member of Conference on Current Trend of Computational Chemistry (<http://cctcc.ccmsi.us>) and Southern School on Computational Chemistry (<http://sscc.ccmsi.us>).

In 2007 I participated on organization and leading CWCS workshop on Molecular modeling of biomolecules. (<http://cwcs.ccmsi.us>). Also in summer of 2007 I taught «Introduction to UNIX/Linux» class during CCMSI summer institute program at Jackson State University.

Reviewer: Structural Chemistry.

Technical Skills

Computational Chemistry & Molecular Modeling

Wavefunction based codes: Gaussian, GAMESS, NWChem, ACES II, AIM2000.

Plane-waves & hybrid codes: CPMD (including GROMOS QM/MM), Quantum Espresso, CP2K, Materials Studio.

Molecular modeling: NAMD, AMBER, GROMACS, Sybyl

IT & High Performance Computing (HPC)

Linux cluster design, construction, optimization and maintenance. Work with HPC vendors.

System administration under Windows 2000/XP/2003 and Linux environment.

Basic C/C++, Shell scripting, TCL, MPI.

Libraries: BLAS, ATLAS, LAPACK, MKL, ACML.

Math IDE: MATLAB, Origin, MathCAD.

Graphic & Design

Chemical Viz: VMD, gOpenMol, Molekel, Molden, Pymol, GaussView, ChemOffice, etc.

Scientific Viz: AVS/Express, POV-Ray, MATLAB.

Graphic/Design workflow: Adobe Photoshop, Illustrator, Corel Draw.

Web: (x)HTML, CSS, PHP, ASP, MySQL, file, web and mail servers.

Professional Publishing/Typography workflow: Adobe InDesign, Post Script, Acrobat.

List of Publications

1. O. Isayev, L. Gorb, J. Leszczynski. **Structure of Liquid Water from ab initio Molecular Dynamics at the Complete Plane Wave Basis Set Limit.** In preparation.
2. O. Isayev, L. Gorb, I. Zilberberg, J. Leszczynski. **Electronic Structure and Dynamics of Iron (II) – Nitrobenzene Complexes in Bulk Water.** In preparation.
3. O. Isayev, L. Gorb, M. Qasim, J. Leszczynski. **Ab initio Molecular Dynamics Study of the Initial Chemical Events in Nitramines: CL-20 under Extreme Condition.** *J. Phys. Chem. B*, 2008, **112**, 11005.
4. O. Isayev, A. Furmanchuk, L. Gorb, J. Leszczynski. **Efficient and Accurate ab initio Prediction of Thermodynamic Parameters for Intermolecular Complexes.** *Chem. Phys. Lett.*, 2008, **451**, 147.
5. O. Isayev, A. Furmanchuk, O. Shishkin, L. Gorb, J. Leszczynski. **Are Isolated Nucleic Acid Bases Really Planar? A Car-Parrinello Molecular Dynamics Study.** *J. Phys. Chem. B*, 2007, **111**, 3476.
6. O. Isayev, L. Gorb, I. Zilberberg, J. Leszczynski. **Electronic Structure and Bonding of {Fe(PhNO₂)₆}⁶⁺ complexes: A Density Functional Theory Study.** *J. Phys. Chem. A*, 2007, **111**, 3571.
7. O. Isayev, L. Gorb, J. Leszczynski. **Theoretical Calculations: Can Gibbs Free Energy for Intermolecular Complexes Be Predicted Efficiently and Accurately?** *J. Comp. Chem.* 2007, **28**, 1598.
8. O. Isayev, B. Rasulev, L. Gorb, J. Leszczynski. **Structure-Toxicity Relationships of Nitroaromatic Compounds,** *Molecular Diversity*, 2006, **10**, 233.
9. L. I. Kas'yan, D.V. Karpenko, A.O. Kas'yan, A.K. Isaev*. **Synthesis and Reactivity of Amines Containing Several Cage-like Fragments.** *Russian J. Org. Chem.*, 2005, **41**, 678.
10. Zilberberg, M. Ilchenko, O. Isayev, L. Gorb, J. Leszczynski. **Modeling the Gas-Phase Reduction of Nitrobenzene to Nitrosobenzene by Iron Monoxide: A Density Functional Theory Study.** *J. Phys. Chem. A*, 2004, **108**, 4878.

11. L. I. Kas'yan, A.K. Isayev*, A.O. Kas'yan, E.A. Golodaeva, D.V. Karpenko, I.N. Tarabara. **Amides containing two norbornene fragments. Synthesis and chemical transformations.** *Russian J. Org. Chem.*, 2004, **40**, 1415.
12. O.V. Krishchik, I.N. Tarabara, A.O. Kas'yan, S.V. Shishkina, O.V. Shishkin, A.K. Isayev*, L.I. Kas'yan. **Reaction of Endic Anhydride with Hydrazines and Acylhydrazines.** *Russian J. Org. Chem.*, 2004, **40**, 1140.
13. L. I. Kas'yan, E.A. Golodaeva, A.O. Kas'yan, A.K. Isayev*, **Amino Alcohols with Bicyclic Carbon Skeleton. Alternative Functionalization of Nucleophilic Reaction Centers.** *Russian J. Org. Chem.*, 2003, **39**, 1398.
14. A.O. Kas'yan, A.K. Isayev*, L.I. Kas'yan. **New N-(Arylsulfonyl)-5-aminomethylbicyclo[2.2.1]-hept-2-enes. Synthesis, ¹H and ¹³C NMR Spectra, and Chemical Reactions.** *Russian J. Org. Chem.*, 2002, **38**, 553.

* Name translation by Springer Science from Russian language.

Oral Presentations and Invited Talks

1. Theoretical insight into the nitroreductase mechanism. *237th ACS National Meeting*, Salt Lake City, UT, 2009 (Upcoming).
2. Ab initio and hybrid QM/MM simulations on massively parallel supercomputers: Experience at ERDC. *237th ACS National Meeting*, Salt Lake City, UT, 2009 (Upcoming).
3. Modern web technologies and Science 2.0. *Department of Chemistry, Jackson State University*, Jackson, MS, February 2009.
4. Transformation of nitrocompounds by nitroreductase. *Department of Pharmacy, University of Mississippi*, Oxford MS, November, 2008.
5. Transformation of nitrocompounds by nitroreductase. *236th ACS National Meeting*, Philadelphia, PA, 2008.
6. Convergence of Liquid Water Properties to the Complete Plane Wave Basis Set Limit. *8th Southern School in Computational Chemistry and Materials Science*, Jackson MS, 2008.
7. Structure of Liquid Water from ab initio Molecular Dynamics at the Complete Plane Wave Basis Set Limit. *235th ACS National Meeting*, New Orleans, LA, 2008.
8. An ab initio Molecular Dynamics Study of the Thermal Decomposition of CL-20. *235th ACS National Meeting*, New Orleans, LA, 2008.
9. Application of ab initio Molecular Dynamics to Study Nucleic Acids and Related Species. The Mississippi Center for Supercomputing Research, University of Mississippi, Oxford MS, 2007.

10. Toward Accuracy Free Energy Estimation from First Principles Simulations. Universite Henri Poincare, Nancy, France, 2006.
11. Structural Nonrigidity of Nucleic Acids Bases from ab initio Molecular Dynamics Simulations, *Psi-K micro-workshop*, CECAM, ENS de Lyon, France, 2006.
12. Car-Parrinello Molecular Dynamics Benchmark Performance on Altix 3700 High Performance Computing System. *70th Annual Meeting, Mississippi Academy of Sciences*, Vicksburg MS, 2006.
13. One-Electron Reduction of Nitrobenzene by Iron (II) Compounds. *Jackson State University*, Jackson MS, 2004.

Selected Poster Presentations and Contributions

1. Molecular Dynamics of Nitroreductase in Three States. *49th Sanibel Symposium*, St. Simons Island, GA 2009 (with L. Gorb, F. Hill and J. Leszczynski).
 2. Structural Nonrigidity of DNA Bases from First Principles. *Workshop on New Developments for First Principles Molecular Dynamics Simulations in Condensed Matter and Molecular Physics*, Lyon, France, 2006 (with A. Furmanchuk, L. Gorb, O. Shishkin and J. Leszczynski).
 3. Toward Chemical Accuracy of Gibbs Free Energy Evaluation for Weakly Bound Systems. *5th Congress of the International Society for Theoretical Chemical Physics*. New Orleans, 2005 (with L. Gorb, and J. Leszczynski).
 4. Reduction of Nitroaromatic Compunds: Theoretical Chemistry Approach. *2nd International Symposium on Recent Advances in Environmental Health Research*, Jackson, MS 2005. (with L. Gorb, and J. Leszczynski).
 5. Can Gibbs Free Energy for Intermolecular Complexes be Predicted Accurately? *14th Conference of Current Trends in Computational Chemistry*, Jackson, MS 2005 (with L. Gorb, and J. Leszczynski).
 6. Pathways of Nitrobenzene Reduction by Iron (II) Compounds. A DFT Study. *Gordon Research Conference on Computational Chemistry*, Holderness, NH 2004 (with L. Gorb, I. Zilberberg and J. Leszczynski).
 7. Theoretical Investigation of 1-Methyl-Cytosine Hydration. *13th Conference of Current Trends in Computational Chemistry*, Jackson, 2004 (with A. Furmanchuk, L. Gorb and J. Leszczynski).
 8. Quantum Chemical Investigation of NMR Chemical Shifts in Bicyclic Amines. *10th Conference of Current Trends in Computational Chemistry*, Jackson, 2001 (with S.I. Okovytyy, L.I. Kasyan, L. K. Umrikhina, V.V. Rossikhin).
- (Total number: 44)**

Misc

Languages	English – fluent; Russian and Ukrainian – native
Citizenship	Ukraine
Family Status	Married
References	Available upon request
Society Memberships	American Chemical Society (ACS) Association for Computing Machinery (ACM) National Geographic Society (NGS)
Hobby	Photography, graphic design, typography, hiking, ecotourism