CURRICULUM VITAE

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Division of Chemical Biology and Medicinal Chemistry, UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, 301 Beard Hall, Campus Box 7568, Chapel Hill, NC 27599
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APPOINTMENTS

Research Scientist
UNC Eshelman School of Pharmacy, University of North Carolina, Chapel Hill, NC — 2013–Present
Computer-aided design of novel materials, structure-property relationship (QSPR). Large-scale data mining of chemical information. GPU accelerated cheminformatics tools.

Sr. Scientist
Badger Technical Services, LLC; Environmental Laboratory, US Army ERDC — 2012–2013
Modeled thermodynamics of adsorption of organic pollutants on graphene. Involved in extensive collaboration with several experimental groups. Wrote successful proposals for internal funding and HPC allocations.

Postdoctoral Fellow
Department of Chemistry, Case Western Reserve University, Cleveland, OH — 2009–2012
Successfully identified novel mechanism of bacterial nitroreductase with *in silico* methods.
Studied structural changes of DNA nucleosome due to interaction with carbon nanotubes.
Developed method for prediction of redox potential for compounds of environmental interest.
Supervised research projects of graduate students.

Graduate Research Assistant
Department of Chemistry & Biochemistry, Jackson State University, Jackson, MS — 2002–2008
Developed novel method for prediction of thermodynamic properties of intermolecular complexes.
Predicted kinetics for thermal decomposition reactions in crystalline explosives.
Characterized hydration of DNA constituents and kinetics of proton transfer.

Visiting Research Assistant
Equipe de Chimie et Biochimie Théoriques, Université Henri Poincaré, Nancy, France — Summer 2006
Studied hydration of biomolecules with molecular dynamics.

System Administrator
Computational Center for Molecular Structure & Interactions, Jackson State University, Jackson, MS — 2003–2008
Deployed center's IT infrastructure including HPC clusters, servers and workstations. Ported and tuned scientific codes. Worked with HPC vendors and contractors.

EDUCATION

Ph.D. in Chemistry, *Jackson State University*, Jackson, MS, USA — 2008
M.S. in Chemistry with Honor (summa cum laude), *Dnepropetrovsk National University,* Ukraine — 2002

TECHNICAL SKILLS

Programming Languages: Python, R, PHP, Shell script
ML & Data Mining: Scikit Learn, pandas, Theano, caret, etc.
Molecular modeling: AMBER, NAMD, GROMACS, Sybyl, Schrodinger 2011/2012, MOE, Tinker, LAMMPS.
Docking: Autodock, Vina, Glide, Induced Fit, QPLD, Molegro.
Bioinformatics tools: Prime, Clustal, BLAST/PSI-BLAST, ICM-Homology etc.
Wavefunction based codes: Gaussian 03/09, NWChem, Qchem, ORCA, GAMESS, ACES III, AIM2000, etc.
Plane–waves/hybrid codes: CPMD, Quantum Espresso, CP2K, Materials Studio, VASP.
Visualization: VMD, Chimera, MGL Tools, ePMV, Molekel, Molden, Pymol, GaussView, and many more.

IT & HIGH PERFORMANCE COMPUTING

HPC: MPI, OpenMP/OpenACC, CUDA.
Math/Statistical analysis: MATLAB, Origin Pro, Mathcad, Mathematica, Grapher, R.
Libraries: MKL, BLAS, LAPACK, ACML, FFTW.
Platforms: Cray XT3…XE6, SGI Altix, Altix ICE, IBM BlueGene, hybrid GPU systems, GPGPU, Rocks Cluster etc.
Web development: Apache, nginx, varnish, PHP/MySQL, Content Management Systems, (X)HTML, CSS, XML.
Graphic Design/Animation: Adobe CS Suite – Photoshop, InDesign, After Effects, Premiere; Autodesk Maya, V-Ray.

AWARDS (selected)

ACS COMP Division Emerging Technology Award (jointly with A. Tropsha, D. Fourches and E. Muratov)	2014
ACS COMP Division GPU Computing award	2014
NSF Travel Award, Materials Computation Center, *University of Illinois at Urbana-Champaign*, IL	2006, 2010
US Department of Energy Scholarship, *Molecular Quantum Mechanics Conference*, Berkeley, CA	2010
IBM–Löwdin memorial Fellowship	2009
NBCR Summer Institute Scholarship, *University of California, San Diego, CA*	2008
Best Professional Oral Presentation, *70th Annual Meeting, Mississippi Academy of Sciences*	2006
Honor for Outstanding Academic Leadership, *Jackson State University*	2005

ORGANIZATION OF SCIENTIFIC EVENTS

Co-organizer Conference on Current Trend of Computational Chemistry (CCTCC), Jackson MS.	2008-present
Co-organizer Southern School on Computational Chemistry (SSCC), Jackson MS.	2008-present
Co-organizer/Instructor NSF Center for Workshops in the Chemical Sciences (SWCS) workshop on Molecular Modeling of Biomolecules, Jackson MS.	2007

SERVICE TO THE PROFESSION

Reviewer for: Scientific Reports, Journal of Chemical Information and Modeling, Environmental Science & Technology, RSC Advances, Journal of Chemical Physics, Journal of Physical Chemistry, Phys. Chem. Chem. Phys., Journal of Molecular Graphics & Modeling, Journal of Molecular Modeling, Journal of Physical Organic Chemistry, Materials Chemistry and Physics, Structural Chemistry, etc.

PROFESSIONAL AFFILIATIONS

American Chemical Society (ACS, 2004–)
Association for Computing Machinery (ACM, 2008–)
Special Interest Group on Computer Graphics (SIGGRAPH, 2009–)
Special Interest Group on High Performance Computing (SIGHPC, 2011–)
Royal Society of Chemistry (RSC, 2012–)
Mississippi Academy of Sciences (MAS, 2004–2007)

PUBLICATIONS

1. O. Isayev, D. Fourches, E.N. Muratov, C. Oses, K.M. Rasch, A. Tropsha, and S. Curtarolo. Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. *Chem. Mater.*, 2015, 27, 735-742. (Editor's Choice Article) (Press Coverage). [DOI]
2. L. K. Sviatenko, O. Isayev, L. Gorb, F. C. Hill, D. Leszczynska, J. Leszczynski. Are the reduction and oxidation properties of nitrocompounds dissolved in water different from those adsorbed on a silica surface*? J. Comp. Chem.* In Press, 2015 (Cover Article) [DOI]
3. O. Isayev, C.E. Crespo-Hernández, L. Gorb, F.C. Hill, J. Leszczynski. *In Silico* Structure-Function Analysis of *E. cloacae* Nitroreductase. *Proteins*, 2012, 80, 2728. [DOI]
4. A. Furmanchuk, O. Isayev, T. Dinadayalane, J. Leszczynski. Mechanical Properties of Silicon Nanowires (Review Article). *WIREs Comput. Mol. Sci.*, 2012, 2, 817. [DOI]

5. P.E. Campbell, O. Isayev, S.A. Ali, M.-B. Huang, W.W. Roth, M.D. Powell, J. Leszczynski, V.C. Bond. Validation of a Novel Secretory Modification Region (SMR) of HIV-1 Nef Using Cohort Sequence and Molecular Modeling**.** *J. Mol. Model.* 2012, **18**, 4603. [DOI]
6. J. Ford-Green, O. Isayev, L. Gorb, E. Perkins, J. Leszczynski. Evaluation of Nitramine Binding Free Energy to 3-D Models of the Transmembrane and S1S2 Domains in the Human N-Methyl-D-Aspartate Receptor. *J. Mol. Model.* 2012, 18, 1273-1284. [DOI]
7. A. Furmanchuk, O. Isayev, T. Dinadayalane, J. Leszczynski. Car-Parrinello Molecular Dynamics Simulations of Tensile Tests in Si <001> Nanowires. *J. Phys. Chem. C,* 2011, 115, 12283. [DOI]
8. D. Ghosh, O. Isayev, L. Slipchenko, A. Krylov The Effect of Solvation on Vertical Ionization Energy of Thymine: From Microhydration to Bulk. *J. Phys. Chem. A,* 2011, 115, 6028. [DOI]
9. L. Sviatenko, O. Isayev, L. Gorb, F. Hill, J. Leszczynski, Toward Robust Computational Electro-chemical Predicting the Environmental Fate of Organic Pollutants. *J. Comp. Chem.* 2011, 32, 2195. [DOI]
10. L. Kasyan, S. Pridma, V. Palchikov, L. Karat, A. Turov, O. Isayev. Reaction of bicyclo[2.2.1]-hept-5-ene-endo-2-ylmethylamine and nitrophenyl glycidyl ethers. *J. Phys. Org. Chem.* 2011, 24, 705. [DOI]
11. A. Furmanchuk, O. Isayev, O. Shishkin, L. Gorb, D. Hovorun, J. Leszczynski. Novel View on the Mechanism of Water-Assisted Proton Transfer in the DNA Bases: Bulk Water Hydration. *Phys. Chem. Chem. Phys.*, 2011, 13, 4311. [DOI]
12. A. Furmanchuk, O. Isayev, O. Shishkin, L. Gorb, J. Leszczynski Hydraion of Nucleic Acid Bases: a Car-Parrinello Molecular Dynamics Approach. *Phys. Chem. Chem. Phys.*, 2010, 12, 3363-3375. (Cover article). [DOI]
13. M. Uchimiya, L. Gorb, O. Isayev, M. Qasim, J. Leszczynski. One-electron standard reduction po-tentials of nitroaromatic and cyclic nitramine explosives. *Environ. Pollut.*, 2010, 158, 3048-53. [DOI]
14. A. Furmanchuk, O. Shishkin, O. Isayev, L. Gorb, J. Leszczynski. New Insight on Structural Properties of Hydrated Nucleic Acid Bases from ab initio Molecular Dynamics. *Phys. Chem. Chem. Phys.,* 2010, 12, 9945-54. [DOI]
15. 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. [DOI]
16. 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. [DOI]
17. 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.[DOI]
18. O. Isayev, L. Gorb, I. Zilberberg, J. Leszczynski. Electronic Structure and Bonding of $\{Fe(PhNO_2)\}^6$ complexes: A Density Functional Theory Study. *J. Phys. Chem. A,* 2007, 111, 3571. [DOI]
19. O. Isayev, L. Gorb, J. Leszczynski. Theoretical Calculations: Can Gibbs Free Energy for Inter-molecular Complexes Be Predicted Efficiently and Accurately? *J. Comp. Chem.* 2007, 28, 1598. [DOI]
20. O. Isayev, B. Rasulev, L. Gorb, J. Leszczynski. Structure-Toxicity Relationships of Nitroaromatic Compounds. *Molecular Diversity*, 2006, 10, 233. [DOI]
21. 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. [DOI]
22. 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. [DOI]
23. L.I. Kas'yan, A.K. Isaev, 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. [DOI]
24. O.V. Krishchik, I.N. Tarabara, A.O. Kas'yan, S.V. Shishkina, O.V. Shishkin, A.K. Isaev, L.I. Kas'yan. Reaction of Endic Anhydride with Hydrazines and Acylhydrazines. *Russian J. Org. Chem.,* 2004, 40, 1140. [DOI]
25. L.I. Kas'yan, E.A. Golodaeva, A.O. Kas'yan, A.K. Isaev, Amino Alcohols with Bicyclic Carbon Skeleton. Alternative Functionalization of Nucleophilic Reaction Centers. *Russian J. Org. Chem.,* 2003, 39, 1398. [DOI]
26. A.O. Kas'yan, A.K. Isaev, L.I. Kas'yan. New N-(Arylsulfonyl)-5-aminomethylbicyclo[2.2.1]-hept-2-enes. Synthesis, ^1H and ^{13}C NMR Spectra, and Chemical Reactions. *Russian J. Org. Chem.,* 2002, 38, 553. [DOI]

BOOK CHAPTERS

Chapter 6. Mechanisms and Kinetics of CL-20 Modes of Transformation via Alkali Hydrolysis and via Photolysis and Thermolysis Free Radical Reactions (with M. Qasim, Y. Kholod, S. Okovytyy, L. Gorb, V. Boddhu and J. Leszczynski). In *Energetic Materials: Thermophysical Properties, Predictions, and Experimental Measurements*, CRC Press, 2010.

INVITED, ORAL TALKS & SEMINARS

1. Structure-Function Analysis of Biopolymers, *School of Pharmacy, University of North Carolina at Chapel Hill*, December 2012.

2. Probing bio-nano interface structure from microsecond molecular dynamics on GPUs, *GPU Technology Conference*, San Jose, CA, May 2012.
3. Molecular Modeling at Frontiers of Environmental Science. *Department of Chemistry and Biochemistry, North Dakota State University,* March 2012.
4. Computational Chemistry: Toward Real-Life Petascale simulations. *HPC Advisory Council Stanford Workshop*, Stanford University, December 2011.
5. Toward real-life petascale applications: Experience at ERDC. *242th ACS National Meeting*, Denver,CO August 2011.
6. Toward Robust Computational Electrochemical Predicting the Environmental Fate of Organic Pollutants. *Department of Chemistry, University of Sothern California*, November 2010 (Seminar).
7. Stability of molecular dynamics on GPUs: Is your card better than mine? *240th ACS National Meeting*, Boston, MA, August 2010.
8. Hydration of biomolecules: first principles molecular dynamics simulations. *Department of Chemistry, Stanford University*, March 2010 (Martinez Group seminar).
9. Hydration of biomolecules: first principles molecular dynamics simulations. *Department of Chemistry, University of Sothern California*, March 2010 (Krylov Group seminar).
10. Reduction of nitrogen containing aromatic compounds: Computational chemistry perspective. *239th ACS National Meeting (Symposium in Honor of Donald L. Macalady)*, San Francisco, CA, March 2010.
11. Next-Generation Visualization Technologies: How close we are to the Science 2.0? *239th ACS National Meeting*, San Francisco, CA, March 2010.
12. Mechanism and Kinetics of Thermal Decomposition of CL-20. *3rd Symposium Methods and Applications of Computational Chemistry*, Odessa, Ukraine, July 2009.
13. Theoretical insight into the nitroreductase mechanism. *237th ACS National Meeting*, Salt Lake City, UT, March 2009.
14. Ab initio and hybrid QM/MM simulations on massively parallel supercomputers: Experience at ERDC. *237th ACS National Meeting*, Salt Lake City, UT, March 2009.
15. Modern web technologies and Science 2.0. *Department of Chemistry, Jackson State University,* Jackson, MS, February 2009.
16. Transformation of nitrocompounds by nitroreductase. *Department of Pharmacy, University of Mississippi*, Oxford MS, November, 2008.
17. Transformation of nitrocompounds by nitroreductase. *236th ACS National Meeting*, Philadelphia, PA, 2008.
18. Convergence of Liquid Water Properties to the Complete Plane Wave Basis Set Limit. *8th Southern School in Computational Chemistry and Materials Science*, Jackson MS, April 2008.
19. 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.
20. An ab initio Molecular Dynamics Study of the Thermal Decomposition of CL-20. *235th ACS National Meeting,* New Orleans, LA, 2008.
21. 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.
22. Toward Accuracy Free Energy Estimation from First Principles Simulations. *Université Henri Poincaré*, Nancy, France, 2006.
23. Structural Nonregidity of Nucleic Acids Bases from ab initio Molecular Dynamics Simulations, *Psi-K micro-workshop*, CECAM, Ecole Normale Supérieure de Lyon, France, 2006.
24. Car-Parrinello Molecular Dynamics Benchmark Performance on Altix 3700 High Performance Computing System. *70th Annual Meeting, Mississippi Academy of Sciences*, Vicksburg MS, 2006.
25. One-Electron Reduction of Nitrobenzene by Iron (II) Compounds. *Jackson State University*, Jackson MS, 2004.

POSTER PRESENTATIONS (selected from over 40)

1. What DFT can tell us about vertical ionization energy of thymine in water? *242th ACS National Meeting*, Denver, CO August 2011. (with D. Ghosh, C.E. Crespo-Hernández, A. Krylov).
2. Effective Fragment potential study of thymine in water: From microsolvation to bulk. Molecular Quantum Mechanics 2010, Berkeley, CA 2010 (with D. Ghosh, L. Slipchenko, A. Krylov).
3. Theoretical Study of Nitrogen Containing Energetic Compounds Reduction. *50th Sanibel Symposium*, St. Simons Island, GA 2010 (with L. Svatenko, L. Gorb, F. Hill and J. Leszczynski).
4. Simulations of Tensile Tests in Si <001> Nanowires. *19th Conference of Current Trends in Computational Chemistry,* Jackson, MS 2010. (with A. Furmanchuk, T. Dinadayalane, and J. Leszczynski).
5. Molecular Dynamics Simulation of Nitroreductase in Three States. *4th International Workshop and School TDDFT: Prospects and Applications*, Benasque, Spain, 2010.

6. Molecular Dynamics of Nitroreductase in Three States. *49th Sanibel Symposium*, St. Simons Island, GA 2009 (with L. Gorb, F. Hill and J. Leszczynski).
7. Toward Real-life Petascale Applications: Experience at JSU and ERDC. *Summer Program "Classical and Quantum Approaches in Molecular Modeling"*, Institute for Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN, 2008.
8. 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).
9. Toward Chemical Accuracy of Gibbs Free Energy Evaluation for Weakly Bound Systems. *5th Congress of the International Society for Theoretical Chemical Physics.* New Orleans, LA 2005 (with L. Gorb, and J. Leszczynski).
10. 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).