

## Olexandr Isayev

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## Education

Dnepropetrovsk National University, Ukraine	Chemistry	M.S. (summa cum laude)	2002
Jackson State University, Jackson MS	Chemistry	Ph.D.	2008
Case Western Reserve University, Cleveland, OH	Chemistry	Postdoc	2009-2012

## Appointments

2013–present **Research Scientist**, *UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill*

2012–2013 **Sr. Scientist**, *Badger Technical Services, LLC / US Army ERDC, San Antonio, TX*

2009–2012 **Postdoctoral Fellow**, *Department of Chemistry, Case Western Reserve University, Cleveland, OH*

2002–2008 **Graduate Research Assistant**, *Department of Chemistry and Biochemistry, Jackson State University, Jackson MS*

2006 **Visiting Research Fellow**, *Equipe de Chimie et Biochimie Théoriques, Université Henri Poincaré, Nancy, France*

2003–2008 **System Administrator**, *Computational Center for Molecular Structure and Interactions, Jackson State University, Jackson MS*

## Publications (selected from 30 peer-reviewed publications)

(i)

1. O. Isayev, D. Fourches, E.N. Muratov, C. Oses, K.M. Rasch, A. Tropsha, and S. Curtarolo. *Chem. Mater.*, 2015, 27, 735-742.
2. 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, 2728–2741.
3. Furmanchuk, O. Isayev, T. Dinadayalane, J. Leszczynski. Mechanical Properties of Silicon Nanowires (Review Article). *WIREs Comput. Mol. Sci.*, 2012, 2 817-828.
4. 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.
5. 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.
6. O. Isayev, B. Rasulev, L. Gorb, J. Leszczynski. Structure-Toxicity Relationships of Nitroaromatic Compounds, *Molecular Diversity*, 2006, 10, 233.

(ii)

7. 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.
8. L. Sviatenko, O. Isayev, L. Gorb, F. Hill, J. Leszczynski, Toward Robust Computational Electrochemical Predicting the Environmental Fate of Organic Pollutants. *J. Comp. Chem.* 2011, 32, 2195.
9. M. Uchimiya, L. Gorb, O. Isayev, M. Qasim, J. Leszczynski. One-electron standard reduction potentials of nitroaromatic and cyclic nitramine explosives. *Environ. Pollut.*, 2010, 158, 3048-53.

10. 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.
11. 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.

### **Synergistic Activities**

ACS COMP Division Emerging Technology Award (2014, jointly with A. Tropsha, D. Fourches and E. Muratov)

ACS COMP Division GPU Computing award (2014)

IBM-Löwdin memorial Fellowship (2009)

Member of the Organizing Committee of Conference on Current Trend of Computational Chemistry (2007 – present) and Southern School on Computational Chemistry (2004 – present).

Research mentoring and teaching NSF-CREST undergraduate summer school on computational chemistry, Department of Chemistry Jackson State University (2003–2007).

Co-organized and led workshop "Molecular modeling of biomolecules" [NSF Center for Workshops in the Chemical Sciences series], Jackson State University, 2007.

Reviewer for: Scientific Reports, Journal of Chemical Information and Modeling, Environmental Science & Technology, RSC Advances, Journal of Physical Chemistry, Physical Chemistry Chemical Physics, Journal of Chemical Physics, International Journal of Quantum Chemistry and others.

### **Collaborators**

Vincent C. Bond, William Roth, *Morehouse School of Medicine*; Stefano Curtarolo, *Duke University*; Leonid Gorb, Ed Perkins, Frances Hill, *US Army ERDC*; Svetlana Kilina, *North Dakota State University*; Anna I. Krylov, *University of Southern California*; Oleg Shishkin, *National Academy of Sciences of Ukraine*.

### **Graduate and Postdoctoral Advisors**

Prof. Jerzy Leszczynski, *Jackson State University* (graduate advisor)

Prof. Carlos Crespo-Hernandez, *Case Western Reserve University* (postdoc advisor)