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Education

2009–2012	Postdoctoral Fellow	Case Western Reserve University, Cleveland, OH
2008	Ph.D. in Theoretical Chemistry	Jackson State University, Jackson MS
2002	M.S. in Chemistry (*summa cum laude*)	Dnepropetrovsk National University, Ukraine

Professional Experience

2017–	Research Assistant Professor, *UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill*
2016	Sr. Fellow, *Institute for Pure & Applied Mathematics, University of California, Los Angeles*
2013–2016	Research Scientist, *UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill*
2012–2013	Sr. Scientist, *US Army Engineering Research & Development Center (Duty station: Vicksburg, MS)*

Selected Honors & Awards

2017, 2014	ACS Emerging Technology Award
2016	Eshelman Institute for Innovation Award
2015	Chemical Structure Association Trust Award
2014	NVIDIA GPU Computing award
2009	IBM–Löwdin memorial Fellowship

Peer-reviewed Publications *(* - Indicates corresponding author)*

1. S. A. Tawfik, **O. Isayev**, C. Stampfl, J. Shapter, D. A. Winkler, M. J. Ford. Efficient prediction of structural and electronic properties of hybrid 2D materials using complementary DFT and machine learning approaches. *Advanced Theory and Simulations*, 2019, 2: 1800128 [DOI]
2. M. Popova, **O. Isayev***, A. Tropsha. Deep Reinforcement Learning for *de-novo* Drug Design. *Science Adv. 2018* 4 (7), eaap7885. (**Highlighted by ACS C&EN**) [DOI]
3. K. T Butler, D. W Davies, H. Cartwright, **O. Isayev***, A. Walsh. Machine learning for molecular and materials science. *Nature*. 2018, 559, 547–555. [DOI]
4. J. S. Smith, A. E. Roitberg, **O. Isayev*.** Transforming Computational Drug Discovery with Machine Learning and AI. *ACS Med. Chem. Lett.* 2018. 9, 1065–1069. [DOI]

5. E. Gossett, C. Toher, C. Oses, **O. Isayev**, F. Legrain, F. Rose, E. Zurek, J. Carrete, N. Mingo, A. Tropsha, S. Curtarolo. AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. *Computational Materials Science,* 2018, 152, 134-145. [DOI]
6. J. S. Smith, B. Nebgen, N. Lubbers, **O. Isayev***, A. E. Roitberg. Less is more: Sampling chemical space with active learning *J. Chem. Phys.* 2018. 148, 241733. [DOI]
7. A. E Sifain, N. Lubbers, B. T Nebgen, J. S Smith, A. Lokhov, **O. Isayev**, A. E Roitberg, K. Barros, S. Tretiak. Discovering a Transferable Charge Assignment Model Using Machine Learning. *J. Phys. Chem. Lett.,* 2018, 9, 4495–4501. [DOI]
8. B. Nebgen, N. Lubbers, J. S Smith, A. E Sifain, A. Lokhov, **O. Isayev**, A. E Roitberg, K. Barros, S. Tretiak. Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. *J. Chem. Theory Comput.*, 2018, 14, 4687–4698. [DOI]
9. J. S. Smith, **O. Isayev***, A. E. Roitberg. ANI-1: An extensible neural network potential with DFT accuracy at force field computational cost. *Chem. Sci.,* 2017, 8, 3192-3203. [DOI]
   ***Highlighted by Chemistry World, Computational Chemistry Highlights, RSC Chemical Science Blog. Most downloaded articles of 2017: Inorganic and Physical Chemistry.*
10. **O. Isayev***, C. Oses, C. Toher, E. Gossett, S. Curtarolo, A. Tropsha. Universal Fragment Descriptors for Predicting Electronic Properties of Inorganic Crystals. *Nature Commun.* 2017, 8, 15679. [DOI]
    ***Highlighted by MRS Bulletin, American Ceramic Society, Materials Today, Science Daily, EurekAlert!*
11. J. S. Smith, **O. Isayev***, A. E. Roitberg. ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules. *Scientific Data,* 2017, 4, Article number: 170193. [DOI]
12. T. Moot, **O. Isayev**, R. W. Call, S. M. McCullough, M. Zemaitis, R. Lopez, J. F. Cahoon, A. Tropsha. Material Informatics Driven Design and Experimental Validation of Lead Titanate as an Aqueous Solar Photocathode. *Materials Discovery.* 2017, *6, 9-16.* [DOI]
13. S. J. Capuzzi, R. Politi, **O. Isayev**, S. Farag, A. Tropsha. QSAR modeling of Tox21 challenge stress response and nuclear receptor signaling toxicity assays, *Frontiers in Environmental Science*, 2016, 4, 3. [DOI]
14. **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**, **Highly Cited Paper**) [DOI]
    ***Highlighted by: MRS Bulletin, ACS C&EN, Computational Chemistry Highlights*
15. 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.* 2015, 36 1029-1036. (**Cover Article**) [DOI]
16. **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]
17. A. Furmanchuk, **O. Isayev**, T. Dinadayalane, J. Leszczynski. Mechanical Properties of Silicon Nanowires (**Review Article**). *WIREs Comput. Mol. Sci.*, 2012, 2, 817. [DOI]
18. 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]

19. 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]
20. 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]
21. 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]
22. 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. [DOI]
23. 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]
24. 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]
25. 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]
26. 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. [DOI]
27. 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]
28. **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]
29. **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]
30. **O. Isayev**, A. Furmanchuk, O. Shishkin, L. Gorb, J. Leszczynsski. Are Isolated Nucleic Acid Bases Really Planar? A Car-Parrinello Molecular Dynamics Study. *J. Phys. Chem. B,* 2007, 111, 3476. [DOI]
31. **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]
32. **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. [DOI]
33. **O. Isayev**, B. Rasulev, L. Gorb, J. Leszczynski. Structure-Toxicity Relationships of Nitroaromatic Compounds. *Molecular Diversity*, 2006, 10, 233. [DOI]
34. 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]
35. 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]

36. 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]
37. 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]
38. 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]
39. A.O. Kas'yan, **A.K. Isaev**, L.I. Kas'yan. New N-(Arylsulfonyl)-5-aminomethylbicyclo[2.2.1]-hept-2-enes. Synthesis, ^{1}H and ^{13}C NMR Spectra, and Chemical Reactions. *Russian J. Org. Chem.,* 2002, 38, 553. [DOI]

Preprints

1. J S Smith, BT Nebgen, R Zubatyuk, N Lubbers, C Devereux, K Barros. S. Tretiak, **O. Isayev***, A. Roitberg. Outsmarting quantum chemistry through transfer learning. 2018. *Preprint* ChemRxiv: https://chemrxiv.org/articles/Outsmarting_Quantum_Chemistry_Through_Transfer_Learning/6744440
2. R Zubatyuk, J S Smith, J. Leszczynski. **O. Isayev***. Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecule neural network. 2018. *Preprint* ChemRxiv: https://chemrxiv.org/articles/Accurate_and_Transferable_Multitask_Prediction_of_Chemical_Properties_with_an_Atoms-in-Molecule_Neural_Network/7151435

Older publications and Google Scholar Profile:
https://scholar.google.com/citations?user=7ICaR4EAAAAJ&hl=en

Patent Applications

O. Isayev, M. Popova, A. Tropsha. "Methods, systems and non-transitory computer readable media for automated design of molecules with desired properties using Artificial Intelligence". US Patent Application 62/535,069 (Filed in 2017)

Selected Seminar and Invited Presentations

1. Neural Networks Learning Quantum Chemistry: The Rise of the Machines. *254th ACS National Meeting,* Washington, DC, August, 2017.
2. Seminar: Accelerating computational chemistry with machine learning, *Hebrew University Jerusalem, Israel.* June 2017
3. Seminar: Accelerating computational chemistry with machine learning, *GSK.* May 2017
4. Cheminformatics-Inspired Materials Discovery Platform, *2017 MRS Spring Meeting.* April 2017.
5. Seminar: Predicting the electronic structure and properties of inorganic materials with machine learning. *Los Alamos National Lab*, Los Alamos NM. February 2017.

6. Seminar: KinomeNet: accurate prediction of protein kinase inhibitors with deep convolutional neural networks, *Joint Carnegie Mellon - University of Pittsburgh Computational Biology Program*. October 2016
7. Accelerating discovery of selective protein kinase inhibitors with deep learning. *252th ACS National Meeting*, Philadelphia, PA. August, 2016.
8. Predicting the electronic structure and properties of inorganic materials with machine learning. *252th ACS National Meeting*, Philadelphia, PA. August, 2016
9. Computational drug discovery with deep learning approaches. *Deep Learning in Healthcare Summit*, London UK, April 2016
10. Computational drug discovery with deep learning. *GPU Technology Conference 2016*, San Jose CA. April 2016.

Professional Activities

Crganized ACS COMP symposium "Revolutionizing Chemistry with AI" (August 2018).
Co-organized Telluride workshop on Machine Learning in Quantum Chemistry (2018)
Member of the Organizing Committee of Conference on Current Trends in Computational Chemistry (2007 – present) and Southern School on Computational Chemistry (2004 –2012).
Co-organized and led workshop "Molecular modeling of biomolecules" [NSF Center for Workshops in the Chemical Sciences series], Jackson State University, 2007.

Reviewer Grants: NSF (2015–), DoD SERDP (2016–), Natural Sciences and Engineering Research Council of Canada (2016–), Swiss National Science Foundation (2018 -).

Reviewer Publications: Nature, Nature Communications, JACS, Science Advances, Scientific Reports, Chemical Communications, 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, Journal of Molecular Modeling, Journal of Chemical Education and others.

Research Funding

NSF-CHE (PI) *CDS&E: Development and application of accurate, transferable and extensible deep neural network potentials for molecules and reactions.*
LANL-CINT Center for Integrated Nanotechnologies (PI) *Development state of the art computational methods with neural networks*
Eshelman Institute for Innovation (PI) *Accurate property prediction for drug polymorphs.*
Department of Defense (Co-I; PI: Heneghan) *Medical Learning Through Machine Learning (ML2).*
Office of Naval Research (Co-I; PI: Tropsha) *Materials Informatics Platform for Property Prediction.*

Students Mentored

Mariya Popova, Daniel Korn