Olexandr Isayev, Ph.D.

Department of Chemistry,
Mellon College of Science,
Carnegie Mellon University,
4400 Fifth Avenue, Pittsburgh, PA 15213

email: olexandr@cmu.edu
web: www.olexandrisayev.com
phone: 412 268-3140
fax: 412 268-1061

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

2020–	Assistant Professor, Department of Chemistry, *Carnegie Mellon University*
2017–2019	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
2015	Chemical Structure Association Trust Award
2014	NVIDIA GPU Computing award
2009	IBM–Löwdin memorial Fellowship

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

1. S.A. Tawfik, **O. Isayev**, M.J.S. Spencer, D.A. Winkler. Predicting Thermal Properties of Crystals Using Machine Learning. *Advanced Theory and Simulations*. 2020. In press. doi:10.1002/adts.201900208
2. R Zubatyuk, J S Smith, J. Leszczynski. **O. Isayev***. Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecules neural network. *Science Adv*. 2019 5 (8), aav6490. [DOI]
3. J S Smith, BT Nebgen, R Zubatyuk, N Lubbers, C Devereux, K Barros. S. Tretiak, **O. Isayev***, A. Roitberg. Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. *Nature Commun*. 2019, 10, 2903. [DOI]
4. 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]

5. S. Farag, R. M. Bleich, E. A. Shank, **O. Isayev**, A. A. Bowers, A. Tropsha, Inter-Modular Linkers play a crucial role in governing the biosynthesis of non-ribosomal peptides, *Bioinformatics*, 2019, 35, 3584–3591. [DOI]
6. 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]
7. 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]
8. 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]
9. 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]
10. 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]
11. 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]
12. 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]
13. 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.*
14. **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!*
15. 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]
16. 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]
17. C. Toher, C. Oses, D. Hicks, E. Gossett, F. Rose, P. Nath, D. Usanmaz, D. C. Ford, E. Perim, C. E. Calderon, J. J. Plata, Y. Lederer, M. Jahnátek, W. Setyawan, S. Wang, J. Xue, K. Rasch, R. V. Chepulskii, R. H. Taylor, G. Gomez, H. Shi, A. R. Supka, R. Al Rahal Al Orabi, P. Gopal, F. T. Cerasoli, L. Liyanage, H. Wang, I. Siloi, L. A. Agapito, C. Nyshadham, G. L. W Hart, J. Carrete, F. Legrain, N. Mingo, E. Zurek, O. Isayev, A. Tropsha, S. Sanvito, R. M. Hanson, I. Takeuchi, M. J. Mehl, A. N. Kolmogorov, K. Yang, P. DAmico, A . Calzolari, M. Costa, R. De Gennaro, M. Buongiorno Nardelli, M. Fornari, O. Levy, S. Curtarolo. The AFLOW Fleet for Materials Discovery *arXiv:1712.00422*

18. 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]
19. **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*
20. 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]

Preprints

1. C. Devereux, J. Smith, K. Davis, K. Barros, R. Zubatyuk, **O. Isayev***, A. Roitberg. Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. 2020. *Preprint* ChemRxiv: https://chemrxiv.org/articles/Extending_the_Applicability_of_the_ANI_Deep_Learning_Molecular_Potential_to_Sulfur_and_Halogens/11819268/1
2. A. Cichonska, B. Ravikumar, R. J Allaway, S. Park, F. Wan, **O. Isayev**, S. Li, M. Mason, A. Lamb, Z. Tanoli, M. Jeon, S. Kim, M. Popova, S. Capuzzi, J. Zeng, K. Dang, G. Koytiger, J. Kang, C. I. Wells, T. M. Willson, The IDG-DREAM Drug-Kinase Binding Prediction Challenge Consortium, T. I. Oprea, A. Schlessinger, D. H. Drewry, G. Stolovitzky, K. Wennerberg, J. Guinney, T. Aittokallio. Crowdsourced mapping extends the target space of kinase inhibitors. 2020, *Preprint* bioRxiv 2019.12.31.891812; doi: https://doi.org/10.1101/2019.12.31.891812
3. M. Fronzi, M. Abu Ghazaleh, **O. Isayev**, D. A.Winkler, J. Shapter, M. J. Ford. Impressive computational acceleration by using machine learning for 2-dimensional super-lubricant materials discovery. 2019. *Preprint*. arXiv:1911.11559. https://arxiv.org/abs/1911.11559
4. J. S. Smith, R. Zubatyuk, B. T. Nebgen, N. Lubbers, Kipton Barros, A. Roitberg, **O. Isayev***, S. Tretiak. 2019. *Preprint*. ChemRxiv: https://chemrxiv.org/articles/The_ANI-1ccx_and_ANI-1x_Data_Sets_Coupled-Cluster_and_Density_Functional_Theory_Properties_for_Molecules/10050737

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

Selected Seminar and Invited Presentations

GSK (2020), invited seminar at Purdue University (2019), invited seminar at University of Arkansas (2019), BASF Corporation (Ludwigshafen, Germany; 2019), 10th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP, Norway 2019), International Conference on Molecular Simulation (ICMS, Korea 2019), Workshop on Crystal Structure Prediction at the International Centre for Theoretical Physics (ICTP, Trieste Italy; 2019), Winter School in Theoretical Chemistry (University of Helsinki, Finland 2018), Thirty-second Annual Conference on Neural Information Processing Systems (NIPS, 2018), Löwdin symposium (Uppsala University, Sweden, 2018), PASC18 conference (Basel, Switzerland, 2018), CECAM workshop on Machine learning (Tel-Aviv, Israel 2018), Telluride workshop Machine Learning and Informatics for Chemistry and Materials (USA, 2018), GPU Technology Conference (GTC, 2018), NSF Institute for Pure and Applied Mathematics (IPAM, 2018), invited seminar at Los Alamos National Laboratory (2018), CMU-Georgia Tech conference on machine learning in science and engineering (Carnegie Mellon U, 2018), invited seminar at SISSA (International School for Advanced Studies, Italy 2018), Universal Display Corporation (2018), National Meeting of the American Chemical Society (2020, 2019, 2018, 2017), Pfizer (2018), invited seminar at Berkeley National Laboratory (2018), invited seminar at Michigan State University (2018), invited seminar at the University of California at Los Angeles (2017), Hebrew University of Jerusalem (2017) etc.

Professional Activities

Editorial board member: Journal of Chemical Information and Modeling (American Chemical Society, 2019), Machine Learning: Science and Technology (Institute of Physics, 2019)
Member of the executive committee of Computers in Chemistry division (COMP) of the American Chemical Society (ACS)
Co-organizing Telluride workshop series on Machine Learning in Quantum Chemistry (2020, 2018)
Co-organizer ACS COMP symposium “Revolutionizing Chemistry with AI” (August 2018).

Reviewer Grants: NSF (2018–), DoD SERDP (2016), Natural Sciences and Engineering Research Council of Canada (2016–), Swiss National Science Foundation (2018 -), Dutch Research Council (2019 -).

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.

Students Advised

Mariya Popova, Filipp Gusev

Postdoctoral Fellows

Roman Zubatyuk, Hatice Gokan