

Olexandr Isayev

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

Phone: (412) 268-1062; fax: (412) 268-1061

Email: olexandr@olexandrisayev.com; web: www.olexandrisayev.com

(a) Professional Preparation

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

(b) Appointments

2020 -	Assistant Professor , <i>Department of Chemistry, Carnegie Mellon University, Pittsburgh, PA</i>
2017–2019	Research Assistant Professor , <i>UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill</i>
2016	Sr. Fellow , <i>Institute of Pure and Applied Mathematics (IPAM), University of California, Los Angeles CA.</i>
2013–2017	Research Scientist , <i>UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill</i>
2012–2013	Sr. Scientist , <i>Badger Technical Services, LLC / US Army Engineer Research and Development Center (USACE-ERDC) (Duty station: Vicksburg, MS)</i>

(c) Products (total number of publications = 48, *- corresponding author)

(i)

1. 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]
2. 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.* 2018 4 (7), eaap7885. [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, **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. (**Highly Cited Paper; Highlighted by RSC Chemistry World**). [DOI] Code: https://github.com/isayev/ASE_ANI
5. **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]

(ii)

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**).
7. **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]

8. 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]
9. 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.
10. J. S. Smith, **O. Isayev***, A. E. Roitberg. ANI-1: A data set of 20M off-equilibrium DFT calculations for organic molecules. *Scientific Data*, 2017, 4, Article 170193 [DOI]
Code/Data: https://github.com/isayev/ANI1_dataset

(d) Synergistic Activities

- Editorial board member: Journal of Chemical Information and Modeling (American Chemical Society, 2019), Machine Learning: Science and Technology (Institute of Physics, 2019)
- ACS (American Chemical Society) COMP Division Emerging Technology Award (2017)
- **Grant Review:** NSF (2015 -), DoD SERDP (2016 -), Natural Sciences and Engineering Research Council of Canada (2016 -), Swiss National Science Foundation (2018 -).
- Organizer of American Chemical Society (ACS) symposium “Revolutionizing Chemistry with AI” (August 2018).
- Member of the executive committee of Computers in Chemistry division (COMP) of the American Chemical Society (ACS)