Olexandr Isayev
Division of Chemical Biology and Medicinal Chemistry, UNC Eshelman School of Pharmacy,
University of North Carolina at Chapel Hill, 301 Beard Hall, S Columbia St, Chapel Hill, NC 27599
Phone: 919 966-3459; fax: 919 966-0204
Email: olexandr@olexandrisayev.com; web: www.olexandrisayev.com

(a) Professional Preparation

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	2012

(b) Appointments

2017– **Research Assistant Professor**, *UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill*

2016 **Sr. Fellow**, *Institute of Pure and Applied Mathematics (IPAM), University of California, Los Angeles CA.*

2013–2017 **Research Scientist**, *UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill*

2012–2013 **Sr. Scientist**, *Badger Technical Services, LLC / US Army Engineer Research and Development Center (USACE-ERDC)* (Duty station: Vicksburg, MS)

(c) Products

(i)

1. 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]
2. 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]
3. 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
4. **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]
5. **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]

(ii)

6. 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]
7. M. Popova, **O. Isayev***, A. Tropsha. Deep Reinforcement Learning for *de-novo* Drug Design. Under review in *Science Adv. 2018* 4 (7), eaap7885. (**Highlighted by ACS C&EN**).
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 advisory board member for Journal of Chemical Information and Modeling (American Chemical Society, 2019)
- Eshelman Institute for Innovation Fellow (2016)
- 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 -)
- Member of the Organizing Committee of Conference on Current Trend of Computational Chemistry (2007 – present) and Southern School on Computational Chemistry (2004 – 2013).
- Research mentoring and teaching NSF-CREST undergraduate summer school on computational chemistry for underrepresented groups, Jackson State University (2003–2007).