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**(a) Professional Preparation**

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|---|---|---|---|
| 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. 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]
   Code: https://github.com/isayev/ASE_ANI
2. **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]
3. 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, Accepted. https://arxiv.org/abs/1708.04987
   Code/Data: https://github.com/isayev/ANI1_dataset
4. 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]
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. M. Popova, **O. Isayev***, A. Tropsha. Deep Reinforcement Learning for *de-novo* Drug Design. Under review in *Science Adv. 2017.*
7. **O. Isayev**, C.E. Crespo-Hern**á**ndez, L. Gorb, F.C. Hill, J. Leszczynski. *In Silico* Structure-Function Analysis of *E. cloacae* Nitroreductase. *Proteins*, 2012, 80, 2728. [DOI]
8. 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]
9. 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]

10. 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]

**(d) Synergistic Activities**

- Eshelman Institute for Innovation Fellow (2016)
- ACS (American Chemical Society) COMP Division Emerging Technology Award (2017)
- DoD SERDP grant reviewer (2015-)
- 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).