Olexandr Isayev

List of Publications by Year in Descending Order

92 papers	5,189 citations	29 h-index	71 g-index
124 ext. papers	7,129 ext. citations	8.9 avg, IF	6.51 L-index

#	Paper	IF	Citations
92	Prediction of protein p with representation learning.. *Chemical Science*, **2022**, 13, 2462-2474	9.4	3
91	The transformational role of GPU computing and deep learning in drug discovery. *Nature Machine Intelligence*, **2022**, 4, 211-221	22.5	6
90	Toward Chemical Accuracy in Predicting Enthalpies of Formation with General-Purpose Data-Driven Methods.. *Journal of Physical Chemistry Letters*, **2022**, 3479-3491	6.4	5
89	Machine-Learning-Guided Discovery of F MRI Agents Enabled by Automated Copolymer Synthesis. *Journal of the American Chemical Society*, **2021**, 143, 17677-17689	16.4	10
88	Development of Multimodal Machine Learning Potentials: Toward a Physics-Aware Artificial Intelligence. *Accounts of Chemical Research*, **2021**, 54, 1575-1585	24.3	30
87	Best practices in machine learning for chemistry. *Nature Chemistry*, **2021**, 13, 505-508	17.6	61
86	Crowdsourced mapping of unexplored target space of kinase inhibitors. *Nature Communications*, **2021**, 12, 3307	17.4	8
85	Machine learned H□kel theory: Interfacing physics and deep neural networks. *Journal of Chemical Physics*, **2021**, 154, 244108	3.9	12
84	OpenChem: A Deep Learning Toolkit for Computational Chemistry and Drug Design. *Journal of Chemical Information and Modeling*, **2021**, 61, 7-13	6.1	13
83	Teaching a neural network to attach and detach electrons from molecules. *Nature Communications*, **2021**, 12, 4870	17.4	14
82	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
81	Artificial intelligence-enhanced quantum chemical method with broad applicability. *Nature Communications*, **2021**, 12, 7022	17.4	11
80	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. *Scientific Data*, **2020**, 7, 134	8.2	47
79	TorchANI: A Free and Open Source PyTorch-Based Deep Learning Implementation of the ANI Neural Network Potentials. *Journal of Chemical Information and Modeling*, **2020**, 60, 3408-3415	6.1	49
78	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. *Journal of Chemical Theory and Computation*, **2020**, 16, 4192-4202	6.4	45
77	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
76	The AFLOW Fleet for Materials Discovery **2020**, 1785-1812		1

75	Predicting Thermal Properties of Crystals Using Machine Learning. *Advanced Theory and Simulations* , **2020**, 3, 1900208	3.5	14
74	DRACON: disconnected graph neural network for atom mapping in chemical reactions. *Physical Chemistry Chemical Physics*, **2020**, 22, 26478-26486	3.6	4
73	High Throughput Screening of Millions of van der Waals Heterostructures for Superlubricant Applications. *Advanced Theory and Simulations*, **2020**, 3, 2000029	3.5	4
72	The Inorganic Crystal Structure Database (ICSD): A Tool for Materials Sciences **2019**, 41-54		2
71	From Topological Descriptors to Expert Systems: A Route to Predictable Materials **2019**, 107-147		2
70	Machine Learning Interatomic Potentials for Global Optimization and Molecular Dynamics Simulation **2019**, 253-288		2
69	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. *Nature Communications*, **2019**, 10, 2674	17.4	119
68	The AFLOW Fleet for Materials Discovery **2019**, 1-28		
67	Quantitative Structure-Price Relationship (QS$R) Modeling and the Development of Economically Feasible Drug Discovery Projects. *Journal of Chemical Information and Modeling*, **2019**, 59, 1306-1313	6.1	3
66	Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecules neural network. *Science Advances*, **2019**, 5, eaav6490	14.3	82
65	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. *Nature Communications*, **2019**, 10, 2903	17.4	213
64	Modeling Materials Quantum Properties with Machine Learning **2019**, 171-179		1
63	Crystallography Open Database: History, Development, and Perspectives **2019**, 1-39		1
62	Pauling File: Toward a Holistic View **2019**, 55-106		5
61	Cognitive Chemistry: The Marriage of Machine Learning and Chemistry to Accelerate Materials Discovery **2019**, 223-251		
60	Automated Computation of Materials Properties **2019**, 181-222		1
59	A High-Throughput Computational Study Driven by the AiiDA Materials Informatics Framework and the PAULING FILE as Reference Database **2019**, 149-170		1
58	Inter-Modular Linkers play a crucial role in governing the biosynthesis of non-ribosomal peptides. *Bioinformatics*, **2019**, 35, 3584-3591	7.2	5

57	Adsorption of nitrogen-containing compounds on hydroxylated quartz surfaces.. *RSC Advances*, **2019**, 9, 36066-36074	3.7	
56	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	3.5	34
55	Materials discovery by chemical analogy: role of oxidation states in structure prediction. *Faraday Discussions*, **2018**, 211, 553-568	3.6	14
54	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. *Journal of Chemical Theory and Computation*, **2018**, 14, 4687-4698	6.4	65
53	Discovering a Transferable Charge Assignment Model Using Machine Learning. *Journal of Physical Chemistry Letters*, **2018**, 9, 4495-4501	6.4	65
52	Machine learning for molecular and materials science. *Nature*, **2018**, 559, 547-555	50.4	1282
51	Deep reinforcement learning for de novo drug design. *Science Advances*, **2018**, 4, eaap7885	14.3	401
50	The AFLOW Fleet for Materials Discovery **2018**, 1-28		9
49	Less is more: Sampling chemical space with active learning. *Journal of Chemical Physics*, **2018**, 148, 241733	3.9	249
48	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. *Computational Materials Science*, **2018**, 152, 134-145	3.2	51
47	ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost. *Chemical Science*, **2017**, 8, 3192-3203	9.4	705
46	ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules. *Scientific Data*, **2017**, 4, 170193	8.2	114
45	Universal fragment descriptors for predicting properties of inorganic crystals. *Nature Communications*, **2017**, 8, 15679	17.4	289
44	Atlas Regeneration, Inc. *Regenerative Medicine*, **2016**, 11, 141-3	2.5	
43	QSAR Modeling of Tox21 Challenge Stress Response and Nuclear Receptor Signaling Toxicity Assays. *Frontiers in Environmental Science*, **2016**, 4,	4.8	42
42	Material informatics driven design and experimental validation of lead titanate as an aqueous solar photocathode. *Materials Discovery*, **2016**, 6, 9-16		21
41	Are the reduction and oxidation properties of nitrocompounds dissolved in water different from those produced when adsorbed on a silica surface? A DFT M05-2X computational study. *Journal of Computational Chemistry*, **2015**, 36, 1029-35	3.5	10
40	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. *Chemistry of Materials*, **2015**, 27, 735-743	9.6	172

39	Computational modeling of bacteriophage self-assembly during formation of hierarchical structures. *Materials Research Society Symposia Proceedings*, **2015**, 1722, 7		
38	Validation of a novel secretion modification region (SMR) of HIV-1 Nef using cohort sequence analysis and molecular modeling. *Journal of Molecular Modeling*, **2012**, 18, 4603-13	2	8
37	In silico structure-function analysis of E. cloacae nitroreductase. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2728-41	4.2	10
36	Mechanical properties of silicon nanowires. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 817-828	7.9	11
35	Evaluation of natural and nitramine binding energies to 3-D models of the S1S2 domains in the N-methyl-D-aspartate receptor. *Journal of Molecular Modeling*, **2012**, 18, 1273-84	2	
34	Effect of solvation on the vertical ionization energy of thymine: from microhydration to bulk. *Journal of Physical Chemistry A*, **2011**, 115, 6028-38	2.8	84
33	Novel view on the mechanism of water-assisted proton transfer in the DNA bases: bulk water hydration. *Physical Chemistry Chemical Physics*, **2011**, 13, 4311-7	3.6	54
32	Reaction of bicyclo[2.2.1]hept-5-ene-endo-2-ylmethylamine and nitrophenyl glycidyl ethers. *Journal of Physical Organic Chemistry*, **2011**, 24, 705-713	2.1	4
31	Toward robust computational electrochemical predicting the environmental fate of organic pollutants. *Journal of Computational Chemistry*, **2011**, 32, 2195-203	3.5	37
30	Car-Parrinello Molecular Dynamics Simulations of Tensile Tests on Si<001> Nanowires. *Journal of Physical Chemistry C*, **2011**, 115, 12283-12292	3.8	5
29	Hydration of nucleic acid bases: a Car-Parrinello molecular dynamics approach. *Physical Chemistry Chemical Physics*, **2010**, 12, 3363-75	3.6	23
28	New insight on structural properties of hydrated nucleic acid bases from ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2010**, 12, 9945-54	3.6	22
27	One-electron standard reduction potentials of nitroaromatic and cyclic nitramine explosives. *Environmental Pollution*, **2010**, 158, 3048-53	9.3	35
26	Ab initio molecular dynamics study on the initial chemical events in nitramines: thermal decomposition of CL-20. *Journal of Physical Chemistry B*, **2008**, 112, 11005-13	3.4	80
25	Efficient and accurate ab initio prediction of thermodynamic parameters for intermolecular complexes. *Chemical Physics Letters*, **2008**, 451, 147-152	2.5	7
24	Are isolated nucleic acid bases really planar? A Car-Parrinello molecular dynamics study. *Journal of Physical Chemistry B*, **2007**, 111, 3476-80	3.4	23
23	Electronic structure and bonding of {Fe(PhNO2)}6 complexes: a density functional theory study. *Journal of Physical Chemistry A*, **2007**, 111, 3571-6	2.8	4
22	Theoretical calculations: can Gibbs free energy for intermolecular complexes be predicted efficiently and accurately?. *Journal of Computational Chemistry*, **2007**, 28, 1598-1609	3.5	28

21	Carboxamides and amines having two and three adamantane fragments. *Russian Journal of Organic Chemistry*, **2007**, 43, 1642-1650	0.7	2
20	Structure-toxicity relationships of nitroaromatic compounds. *Molecular Diversity*, **2006**, 10, 233-45	3.1	75
19	Synthesis and Reactivity of Amines Containing Several Cage-like Fragments. *Russian Journal of Organic Chemistry*, **2005**, 41, 678-688	0.7	3
18	Acylation of Aminopyridines and Related Compounds with Endic Anhydride. *Russian Journal of Organic Chemistry*, **2005**, 41, 1530-1538	0.7	12
17	Reaction of Endic Anhydride with Hydrazines and Acylhydrazines. *Russian Journal of Organic Chemistry*, **2004**, 40, 1140-1145	0.7	3
16	Amides containing two norbornene fragments. Synthesis and chemical transformations. *Russian Journal of Organic Chemistry*, **2004**, 40, 1415-1426	0.7	4
15	Modeling the Gas-Phase Reduction of Nitrobenzene to Nitrosobenzene by Iron Monoxide: A Density Functional Theory Study. *Journal of Physical Chemistry A*, **2004**, 108, 4878-4886	2.8	11
14	Amino Alcohols with Bicyclic Carbon Skeleton. Alternative Functionalization of Nucleophilic Reaction Centers. *Russian Journal of Organic Chemistry*, **2003**, 39, 1398-1405	0.7	3
13	New N-(Arylsulfonyl)-5-aminomethylbicyclo[2.2.1]hept-2-enes. Synthesis, 1H and 13C NMR Spectra, and Chemical Reactions. *Russian Journal of Organic Chemistry*, **2002**, 38, 553-563	0.7	3
12	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens		2
11	Teaching a Neural Network to Attach and Detach Electrons from Molecules		7
10	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning		3
9	Crowdsourced mapping extends the target space of kinase inhibitors		3
8	Towards chemical accuracy for alchemical free energy calculations with hybrid physics-based machine learning / molecular mechanics potentials		15
7	Teaching a Neural Network to Attach and Detach Electrons from Molecules		2
6	Teaching a Neural Network to Attach and Detach Electrons from Molecules		2
5	Learning molecular potentials with neural networks. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,e1564	7.9	2
4	A Bag of Tricks for Automated De Novo Design of Molecules with the Desired Properties: Application to EGFR Inhibitor Discovery		3

List of Publications

3	A Bag of Tricks for Automated De Novo Design of Molecules with the Desired Properties: Application to EGFR Inhibitor Discovery		2
2	Active Learning in Bayesian Neural Networks for Bandgap Predictions of Novel Van der Waals Heterostructures. *Advanced Intelligent Systems*,2100080	6	1
1	Roadmap on Machine Learning in Electronic Structure. *Electronic Structure*,	2.6	7