## Yury Lysogorskiy

List of Publications by Year in descending order

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840776 752698 21 406 11 20 citations h-index g-index papers 21 21 21 430 docs citations times ranked citing authors all docs

#	Article	lF	CITATIONS
1	Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon. Npj Computational Materials, 2021, 7, .	8.7	76
2	pyiron: An integrated development environment for computational materials science. Computational Materials Science, 2019, 163, 24-36.	3.0	64
3	Crowd-sourcing materials-science challenges with the NOMAD 2018 Kaggle competition. Npj Computational Materials, 2019, 5, .	8.7	39
4	Crystallography companion agent for high-throughput materials discovery. Nature Computational Science, 2021, 1, 290-297.	8.0	38
5	Predicting structure zone diagrams for thin film synthesis by generative machine learning. Communications Materials, 2020, $1$ , .	6.9	27
6	Optimized interatomic potential for study of structure and phase transitions in Si-Au and Si-Al systems. Computational Materials Science, 2020, 184, 109891.	3.0	26
7	Efficient parametrization of the atomic cluster expansion. Physical Review Materials, 2022, 6, .	2.4	23
8	BOPfox program for tight-binding and analytic bond-order potential calculations. Computer Physics Communications, 2019, 235, 221-233.	<b>7.</b> 5	21
9	Angular-dependent interatomic potential for large-scale atomistic simulation of iron: Development and comprehensive comparison with existing interatomic models. Physical Review Materials, 2021, 5, .	2.4	18
10	Transferability of interatomic potentials for molybdenum and silicon. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 025007.	2.0	17
11	Oxygen vacancies and hydrogen doping in LaAlO3/SrTiO3 heterostructures: electronic properties and impact on surface and interface reconstruction. Journal of Physics Condensed Matter, 2019, 31, 295601.	1.8	14
12	Structural Transitions in a Quasi-1D Wigner Solid on Liquid Helium. Journal of Low Temperature Physics, 2016, 182, 28-37.	1.4	8
13	Design of refractory compositionally complex alloys with optimal mechanical properties. Physical Review Materials, 2021, 5, .	2.4	7
14	Quantum fluids in nanoporous mediaâ€"Effects of the confinement and fractal geometry. Science Bulletin, 2011, 56, 3617-3622.	1.7	6
15	Automated free-energy calculation from atomistic simulations. Physical Review Materials, 2021, 5, .	2.4	6
16	Reconciling Experimental and Theoretical Data in the Structural Analysis of Ti–Ta Shape-Memory Alloys. Shape Memory and Superelasticity, 2019, 5, 6-15.	2.2	5
17	Mössbauer spectroscopy evidence of intrinsic nonâ€stoichiometry in iron telluride single crystals. Annalen Der Physik, 2017, 529, 1600241.	2.4	3
18	Vibrational properties and lattice specific heat of KFeS2. AIP Conference Proceedings, 2018, , .	0.4	3

#	Article	IF	CITATIONS
19	Phase transitions in titanium with an analytic bond-order potential. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 085008.	2.0	3
20	Adsorption of Helium Atoms on Two-Dimensional Substrates. Journal of Low Temperature Physics, 2016, 185, 392-398.	1.4	2
21	Vibrational properties and lattice specific heat of RbFeS2. AIP Conference Proceedings, 2018, , .	0.4	0