Konstantin Gubaev

List of Publications by Year in descending order

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1040056 1474206 9 689 9 9 citations h-index g-index papers 9 9 9 710 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Accelerating high-throughput searches for new alloys with active learning of interatomic potentials. Computational Materials Science, 2019, 156, 148-156.	3.0	218
2	The MLIP package: moment tensor potentials with MPI and active learning. Machine Learning: Science and Technology, 2021, 2, 025002.	5.0	181
3	Machine learning of molecular properties: Locality and active learning. Journal of Chemical Physics, 2018, 148, 241727.	3.0	116
4	Machine-learned interatomic potentials for alloys and alloy phase diagrams. Npj Computational Materials, 2021, 7, .	8.7	75
5	Frontiers in atomistic simulations of high entropy alloys. Journal of Applied Physics, 2020, 128, .	2.5	40
6	Elinvar effect in \hat{I}^2 -Ti simulated by on-the-fly trained moment tensor potential. New Journal of Physics, 2020, 22, 113005.	2.9	20
7	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. Npj Computational Materials, 2021, 7, .	8.7	17
8	Active Learning and Uncertainty Estimation. Lecture Notes in Physics, 2020, , 309-329.	0.7	13
9	Finite-temperature interplay of structural stability, chemical complexity, and elastic properties of bcc multicomponent alloys from <i>ab initio</i> trained machine-learning potentials. Physical Review Materials, 2021, 5, .	2.4	9