

Anton S Bochkarev

List of Publications by Year in descending order

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Version: 2024-02-01

11
papers

222
citations

1163117
8
h-index

1281871
11
g-index

11
all docs

11
docs citations

11
times ranked

204
citing authors

#	ARTICLE	IF	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	Cu diffusion in single-crystal and polycrystalline TiN barrier layers: A high-resolution experimental study supported by first-principles calculations. Journal of Applied Physics, 2015, 118, .	2.5	36
3	Efficient parametrization of the atomic cluster expansion. Physical Review Materials, 2022, 6, .	2.4	23
4	Point defects at the $\langle 01\bar{2} \rangle [100]$ grain boundary in TiN and the early stages of Cu diffusion: An ab initio study. Acta Materialia, 2018, 144, 496-504.	7.9	20
5	Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. Nanoscale, 2019, 11, 16007-16016.	5.6	17
6	<i>Ab initio</i> study of Cu impurity diffusion in bulk TiN. Physical Review B, 2016, 94, .	3.2	14
7	Anharmonic thermodynamics of vacancies using a neural network potential. Physical Review Materials, 2019, 3, .	2.4	14
8	Modeling of Diffusion and Incorporation of Interstitial Oxygen Ions at the TiN/SiO ₂ Interface. ACS Applied Materials & Interfaces, 2019, 11, 36232-36243.	8.0	9
9	Free energy of (Co _x Mn _{1-x}) ₃ O ₄ mixed phases from machine-learning-enhanced ab initio calculations. Physical Review Materials, 2021, 5, .	2.4	5
10	A single-volume approach for vacancy formation thermodynamics calculations. Europhysics Letters, 2016, 116, 16001.	2.0	4
11	Modeling the high-temperature phase coexistence region of mixed transition metal oxides from <i>ab initio</i> calculations. Physical Review Research, 2021, 3, .	3.6	4