Anton S Bochkarev

List of Publications by Year
in descending order

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	Efficient parametrization of the atomic cluster expansion. Physical Review Materials, 2022, 6, .	2.4	23
2	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
3	Free energy of (CoxMn1â^'x)3O4 mixed phases from machine-learning-enhanced ab initio calculations. Physical Review Materials, 2021, 5, .	2.4	5
4	Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon. Npj Computational Materials, 2021, 7, .	8.7	76
5	Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. Nanoscale, 2019, 11, 16007-16016.	5.6	17
6	Modeling of Diffusion and Incorporation of Interstitial Oxygen Ions at the TiN/SiO₂ Interface. ACS Applied Materials & Interfaces, 2019, 11, 36232-36243.	8.0	9
7	Anharmonic thermodynamics of vacancies using a neural network potential. Physical Review Materials, 2019, 3, .	2.4	14
8	Point defects at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mtext>Î£</mml:mtext><mml:mn>5</mml:mn></mml:mrow></mml:math>(012)[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
9	A single-volume approach for vacancy formation thermodynamics calculations. Europhysics Letters, 2016, 116, 16001.	2.0	4
10	<i>Ab initio</i>study of Cu impurity diffusion in bulk TiN. Physical Review B, 2016, 94, .	3.2	14
11	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