Dallas R Trinkle

List of Publications by Year
in descending order

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76 papers	4,586 citations	186254 28 h-index	98792 67 g-index
80 all docs	80 docs citations	80 times ranked	5227 citing authors

#	Article	IF	Citations
1	Solutes that reduce yield strength anisotropies in magnesium from first principles. Physical Review Materials, 2022, 6, .	2.4	1
2	First-principles core energies of isolated basal and prism screw dislocations in magnesium. Materials Research Letters, 2022, 10, 360-368.	8.7	4
3	Accelerated molecular dynamics simulations of dislocation climb in nickel. Physical Review Materials, 2021, 5, .	2.4	1
4	Exploring the necessary complexity of interatomic potentials. Computational Materials Science, 2021, 200, 110752.	3.0	8
5	Stress-dependent dislocation core structures leading to non-Schmid behavior. Materials Research Letters, 2021, 9, 134-140.	8.7	9
6	Designing Optimal Perovskite Structure for High Ionic Conduction. Advanced Materials, 2020, 32, e1905178.	21.0	30
7	Uncertainty quantification of solute transport coefficients. , 2020, , 93-118.		1
8	Split-vacancy defect complexes of oxygen in hcp and fcc cobalt. Physical Review Materials, 2020, 4, .	2.4	1
9	Impact of solutes on the lattice parameters and elastic stiffness coefficients of hcp Fe from first-principles calculations. Computational Materials Science, 2019, 164, 116-126.	3.0	7
10	First-principles calculations of solute transport in zirconium: Vacancy-mediated diffusion with metastable states and interstitial diffusion. Physical Review Materials, 2019, 3, .	2.4	12
11	Dislocation core structures in Ni-based superalloys computed using a density functional theory based flexible boundary condition approach. Physical Review Materials, 2019, 3, .	2.4	11
12	Ab initio magnesium-solute transport database using exact diffusion theory. Acta Materialia, 2018, 150, 339-350.	7.9	35
13	Variational Principle for Mass Transport. Physical Review Letters, 2018, 121, 235901.	7.8	12
14	Effect of solutes on the lattice parameters and elastic stiffness coefficients of body-centered tetragonal Fe. Computational Materials Science, 2018, 152, 308-323.	3.0	15
15	First-principles prediction of oxygen diffusivity near the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>10</mml:mn><mml:mover> twin boundary in titanium. Acta Materialia, 2018, 156, 11-19.	7.9	23
16	Modeling the long-term evolution of dilute solid solutions in the presence of vacancy fluxes. Physical Review Materials, 2018, 2, .	2.4	6
17	Geometries of edge and mixed dislocations in bcc Fe from first-principles calculations. Physical Review Materials, 2018, 2, .	2.4	18
18	Data files for ab initio calculations of the lattice parameter and elastic stiffness coefficients of bcc Fe with solutes. Data in Brief, 2017, 10, 147-150.	1.0	4

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19	Exact Model of Vacancy-Mediated Solute Transport in Magnesium. Physical Review Letters, 2017, 118, 105901.	7.8	26
20	Solute-induced solid-solution softening and hardening in bcc tungsten. Acta Materialia, 2017, 141, 304-316.	7.9	88
21	Mesoscale modeling of vacancy-mediated Si segregation near an edge dislocation in Ni under irradiation. Physical Review B, 2017, 95, .	3.2	7
22	Design principles for radiation-resistant solid solutions. Physical Review B, 2017, 95, .	3.2	15
23	Automatic numerical evaluation of vacancy-mediated transport for arbitrary crystals: Onsager coefficients in the dilute limit using a Green function approach. Philosophical Magazine, 2017, 97, 2514-2563.	1.6	38
24	First principles calculations of beryllium stability in zirconium surfaces. Acta Materialia, 2017, 122, 359-368.	7.9	9
25	Ab initio calculations of the lattice parameter and elastic stiffness coefficients of bcc Fe with solutes. Computational Materials Science, 2017, 126, 503-513.	3.0	36
26	Mechanical properties and phase stability of monoborides using density functional theory calculations. Physical Review Materials, 2017, 1, .	2.4	4
27	Effect of charge on point defect size misfits from ab initio: Aliovalently doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Computational Materials Science, 2016, 119, 41-45.	3.0	5
28	Computation of the lattice Green function for a dislocation. Physical Review E, 2016, 94, 023308.	2.1	16
29	A modified embedded atom method potential for interstitial oxygen in titanium. Computational Materials Science, 2016, 124, 204-210.	3.0	14
30	Diffusivity and derivatives for interstitial solutes: activation energy, volume, and elastodiffusion tensors. Philosophical Magazine, 2016, 96, 2714-2735.	1.6	34
31	Ab initiomodeling of quasielastic neutron scattering of hydrogen pipe diffusion in palladium. Physical Review B, 2016, 94, .	3.2	5
32	Light-element diffusion in Mg using first-principles calculations: Anisotropy and elastodiffusion. Physical Review B, 2016, 94, .	3.2	21
33	Oxygen diffusion in hcp metals from first principles. Physical Review B, 2016, 94, .	3.2	16
34	Kinetic Monte Carlo investigation of tetragonal strain on Onsager matrices. Physical Review E, 2016, 93, 053305.	2.1	1
35	Importance of coordination number and bond length in titanium revealed by electronic structure investigations. Physica Status Solidi (B): Basic Research, 2015, 252, 1907-1924.	1.5	27
36	Thermal transport across high-pressure semiconductor-metal transition in Si and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mrow><mml:mn>0.991</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Ge</mml:mi><mml:mrow><mml:mn>0.009</mml:mn></mml:mrow></mml:msub></mml:math>. Physical Review B, 2015, 91, .	3.2	28

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37	Energetics of Rutile TiO₂ Vicinal Surfaces with âŸ¨001âŸ© Steps from the Energy Density Method. Journal of Physical Chemistry C, 2015, 119, 18203-18209.	3.1	8
38	A study of stress relaxation in AZ31 using high-energy X-ray diffraction. Acta Materialia, 2015, 101, 71-79.	7.9	11
39	Database optimization for empirical interatomic potential models. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 065011.	2.0	5
40	Calculation of strain effects on vacancy-mediated diffusion of impurities in fcc structures: General approach and application toNi1â^'xSix. Physical Review B, 2014, 90, .	3.2	13
41	Diffusion of Si impurities in Ni under stress: A first-principles study. Physical Review B, 2014, 90, .	3.2	26
42	Direct Measurement of Hydrogen Dislocation Pipe Diffusion in Deformed Polycrystalline Pd Using Quasielastic Neutron Scattering. Physical Review Letters, 2014, 113, 025504.	7.8	26
43	Quantitative modeling of solute drag by vacancies in face-centered-cubic alloys. Physical Review B, 2014, 89, .	3.2	31
44	Interaction of oxygen interstitials with lattice faults in Ti. Acta Materialia, 2014, 76, 82-86.	7.9	45
45	First-principles study of interfacial boundaries in Niâ€“Ni3Al. Acta Materialia, 2014, 75, 60-70.	7.9	42
46	Hydrogen trapping at dislocation cores at room temperature in deformed Pd. Journal of Alloys and Compounds, 2013, 577, 189-191.	5.5	5
47	Stress-induced anisotropic diffusion in alloys: Complex Si solute flow near a dislocation core in Ni. Physical Review B, 2013, 88, .	3.2	47
48	Solute effect on oxygen diffusion in Î±-titanium. Journal of Applied Physics, 2013, 113, .	2.5	15
49	Solute drag by vacancies in body-centered cubic alloys. Physical Review B, 2013, 88, .	3.2	40
50	Direct calculation of the lattice Green function with arbitrary interactions for general crystals. Physical Review E, 2012, 85, 066706.	2.1	13
51	Ab initiobased empirical potential used to study the mechanical properties of molybdenum. Physical Review B, 2012, 85, .	3.2	71
52	Core structure of a screw dislocation in Ti from density functional theory and classical potentials. Acta Materialia, 2012, 60, 1287-1292.	7.9	81
53	Prediction of thermal cross-slip stress in magnesium alloys from a geometric interaction model. Acta Materialia, 2012, 60, 2350-2358.	7.9	103
54	Direct Diffusion through Interpenetrating Networks: Oxygen in Titanium. Physical Review Letters, 2011, 107, 045504.	7.8	102

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55	Au/TiO₂(110) Interfacial Reconstruction Stability from ab Initio. Journal of Physical Chemistry C, 2011, 115, 17799-17805.	3.1	16
56	Energy density in density functional theory: Application to crystalline defects and surfaces. Physical Review B, 2011, 83, .	3.2	58
57	Prediction of thermal cross-slip stress in magnesium alloys from direct first-principles data. Acta Materialia, 2011, 59, 5652-5660.	7.9	99
58	Nanoscale hydride formation at dislocations in palladium:Ab initiotheory and inelastic neutron scattering measurements. Physical Review B, 2011, 83, .	3.2	8
59	Thermal conductivity of compressed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O to 22 GPa: A test of the Leibfried-SchlÃ¶mann equation. Physical Review B, 2011, 83, .	3.2	68
60	Accurate and efficient algorithm for Bader charge integration. Journal of Chemical Physics, 2011, 134, 064111.	3.0	1,393
61	Predicting Mg Strength from First-Principles: Solid-Solution Strengthening, Softening, and Cross-Slip. , 2011, , 13-15.		0
62	Atomistic study of edge and screw ã€ˆc+aã€‰ dislocations in magnesium. Acta Materialia, 2010, 58, 4332-4343.	7.9	117
63	Applying for computational time on NSFâ€™s TeraGridâ€”the worldâ€™s largest cyberinfrastructure supporting open research. Jom, 2010, 62, 17-18.	1.9	0
64	Misfit-dislocation-mediated heteroepitaxial island diffusion. Surface Science, 2010, 604, L67-L70.	1.9	7
65	First-principles data for solid-solution strengthening of magnesium: From geometry and chemistry to properties. Acta Materialia, 2010, 58, 5704-5713.	7.9	325
66	Ab initio simulations of molten Ni alloys. Journal of Applied Physics, 2010, 107, .	2.5	33
67	First-principles calculation of H vibrational excitations at a dislocation core of Pd. Physical Review B, 2010, 82, .	3.2	13
68	Island shape controls magic-size effect for heteroepitaxial diffusion. Journal of Applied Physics, 2010, 108, 023521.	2.5	11
69	Cu/Ag EAM potential optimized for heteroepitaxial diffusion from ab initio data. Computational Materials Science, 2009, 47, 577-583.	3.0	54
70	Ab-initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys. , 2008, , .		3
71	Mechanism of a prototypical synthetic membrane-active antimicrobial: Efficient hole-punching via interaction with negative intrinsic curvature lipids. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20595-20600.	7.1	107
72	Contribution to size effect of yield strength from the stochastics of dislocation source lengths in finite samples. Scripta Materialia, 2007, 56, 313-316.	5.2	475

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73	Ab-Initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys. , 2006, , .		0
74	Impurities block the Î± to Ï‰ martensitic transformation in titanium. Nature Materials, 2005, 4, 129-133.	27.5	207
75	The Chemistry of Deformation: How Solutes Soften Pure Metals. Science, 2005, 310, 1665-1667.	12.6	206
76	Shock-induced Î±â€“Ï‰ transition in titanium. Journal of Applied Physics, 2001, 90, 2221-2226.	2.5	110