Karsten Albe

List of Publications by Year
in descending order

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209 papers	12,586 citations	22132 59 h-index	27389 106 g-index
216 all docs	216 docs citations	216 times ranked	12481 citing authors

#	Article	IF	Citations
1	Extracting dislocations and non-dislocation crystal defects from atomistic simulation data. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 085001.	0.8	815
2	Analytical potential for atomistic simulations of silicon, carbon, and silicon carbide. Physical Review B, 2005, 71, .	1.1	485
3	First-principles study of intrinsic point defects in ZnO: Role of band structure, volume relaxation, and finite-size effects. Physical Review B, 2006, 73, .	1.1	463
4	Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals. Acta Materialia, 2008, 56, 1126-1135.	3.8	455
5	The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals. Scripta Materialia, 2006, 54, 1163-1168.	2.6	380
6	Fundamental degradation mechanisms of layered oxide Li-ion battery cathode materials: Methodology, insights and novel approaches. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2015, 192, 3-25.	1.7	357
7	display= "inline" ><mml:mi>n</mml:mi></mml:math>-Type Behavior in Transparent Conducting Oxides: A Comparative Hybrid-Functional Study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	2.9	295
8	Caloric Effects in Ferroic Materials: New Concepts for Cooling. Advanced Engineering Materials, 2012, 14, 10-19.	1.6	278
9	Mechanisms of aging and fatigue in ferroelectrics. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2015, 192, 52-82.	1.7	278
10	Analytical interatomic potential for modeling nonequilibrium processes in the Wâ€“Câ€“H system. Journal of Applied Physics, 2005, 98, 123520.	1.1	244
11	Modelling of compound semiconductors: analytical bond-order potential for gallium, nitrogen and gallium nitride. Journal of Physics Condensed Matter, 2003, 15, 5649-5662.	0.7	222
12	Diffusion of zinc vacancies and interstitials in zinc oxide. Applied Physics Letters, 2006, 88, 201918.	1.5	202
13	Sizeâ€Dependent Lattice Expansion in Nanoparticles: Reality or Anomaly?. ChemPhysChem, 2012, 13, 2443-2454.	1.0	186
14	Band structure of indium oxide: Indirect versus direct band gap. Physical Review B, 2007, 75, .	1.1	180
15	Enhancing the plasticity of metallic glasses: Shear band formation, nanocomposites and nanoglasses investigated by molecular dynamics simulations. Mechanics of Materials, 2013, 67, 94-103.	1.7	171
16	First-principles study of the structure and stability of oxygen defects in zinc oxide. Physical Review B, 2005, 72, .	1.1	165
17	Modeling of compound semiconductors: Analytical bond-order potential for Ga, As, and GaAs. Physical Review B, 2002, 66, .	1.1	146
18	Modeling the metal-semiconductor interaction: Analytical bond-order potential for platinum-carbon. Physical Review B, 2002, 65, .	1.1	144

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19	Intrinsic point defects in CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and CuGaSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>as seen via screened-exchange hybrid density functional theory. Physical Review B, 2013, 87, .	1.1	141
20	Molecular-dynamics simulations of steady-state growth of ion-deposited tetrahedral amorphous carbon films. Journal of Applied Physics, 2000, 88, 1129-1135.	1.1	139
21	Dislocation detection algorithm for atomistic simulations. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 025016.	0.8	139
22	First-principles study of migration mechanisms and diffusion of oxygen in zinc oxide. Physical Review B, 2006, 73, .	1.1	133
23	Theoretical study of boron nitride modifications at hydrostatic pressures. Physical Review B, 1997, 55, 6203-6210.	1.1	131
24	Thermodynamics of mono- and di-vacancies in barium titanate. Journal of Applied Physics, 2007, 102, .	1.1	129
25	Deformation behavior of bulk and nanostructured metallic glasses studied via molecular dynamics simulations. Physical Review B, 2011, 83, .	1.1	128
26	Modelling of boron nitride: Atomic scale simulations on thin film growth. Computational Materials Science, 1998, 10, 111-115.	1.4	125
27	Analytic bond-order potential for bcc and fcc ironâ€”comparison with established embedded-atom method potentials. Journal of Physics Condensed Matter, 2007, 19, 326220.	0.7	124
28	Gallium gradients in Cu(In,Ga)Se₂thin-film solar cells. Progress in Photovoltaics: Research and Applications, 2015, 23, 717-733.	4.4	122
29	Nanotwinned fcc metals: Strengthening versus softening mechanisms. Physical Review B, 2010, 82, .	1.1	120
30	Lattice Monte Carlo simulations of FePt nanoparticles: Influence of size, composition, and surface segregation on order-disorder phenomena. Physical Review B, 2005, 72, .	1.1	119
31	Defect-Dipole Formation in Copper-Doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Ferroelectrics. Physical Review Letters, 2008, 100, 095504.	2.9	118
32	Anomalous compliance and early yielding of nanoporous gold. Acta Materialia, 2015, 93, 144-155.	3.8	116
33	Reaching theoretical strengths in nanocrystalline Cu by grain boundary doping. Scripta Materialia, 2011, 65, 660-663.	2.6	115
34	Local Structural Investigations, Defect Formation, and Ionic Conductivity of the Lithium Ionic Conductor Li₄P₂S₆. Chemistry of Materials, 2016, 28, 8764-8773.	3.2	111
35	Structure, stability and mechanical properties of internal interfaces in Cu64Zr36 nanoglasses studied by MD simulations. Acta Materialia, 2011, 59, 6588-6593.	3.8	107
36	Extended Tersoff potential for boron nitride: Energetics and elastic properties of pristine and defective <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>h</mml:mi></mml:math> -BN. Physical Review B, 2017, 96, .	1.1	97

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37	Association of oxygen vacancies with impurity metal ions in lead titanate. Physical Review B, 2007, 76, .	1.1	94
38	Mechanisms of Radiation-Induced Viscous Flow: Role of Point Defects. Physical Review Letters, 2003, 90, 055505.	2.9	91
39	Computer simulation and boron nitride. Radiation Effects and Defects in Solids, 1997, 141, 85-97.	0.4	84
40	Chemical order and local structure of the lead-free relaxor ferroelectric. Journal of Solid State Chemistry, 2011, 184, 2041-2046.	1.4	84
41	From nanoglasses to bulk massive glasses. Applied Physics Letters, 2009, 94, .	1.5	82
42	Reaction and Space Charge Layer Formation at the LiCoO₂â€“LiPON Interface: Insights on Defect Formation and Ion Energy Level Alignment by a Combined Surface Scienceâ€“Simulation Approach. Chemistry of Materials, 2017, 29, 7675-7685.	3.2	81
43	Atomistic origin of microstrain broadening in diffraction data of nanocrystalline solids. Acta Materialia, 2009, 57, 1648-1654.	3.8	79
44	Thermodynamics and kinetics of the copper vacancy in CuInSe2, CuGaSe2, CuInS2, and CuGaS2 from screened-exchange hybrid density functional theory. Journal of Applied Physics, 2010, 108, .	1.1	79
45	Thermodynamic stability, stoichiometry, and electronic structure of bcc-In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>surfaces. Physical Review B, 2011, 84, .	1.1	77
46	Formation and switching of defect dipoles in acceptor-doped lead titanate: A kinetic model based on first-principles calculations. Physical Review B, 2013, 88, .	1.1	75
47	Reconciling Local Structure Disorder and the Relaxor State in (Bi1/2Na1/2)TiO3-BaTiO3. Scientific Reports, 2016, 6, 31739.	1.6	73
48	Highly Porous Silicon Embedded in a Ceramic Matrix: A Stable High-Capacity Electrode for Li-Ion Batteries. ACS Nano, 2017, 11, 11409-11416.	7.3	73
49	Rapid Crystallization and Kinetic Freezing of Site-Disorder in the Lithium Superionic Argyrodite Li₆PS₅Br. Chemistry of Materials, 2019, 31, 10178-10185.	3.2	72
50	Geometry, electronic structure and thermodynamic stability of intrinsic point defects in indium oxide. Journal of Physics Condensed Matter, 2009, 21, 455801.	0.7	71
51	Analytic bond-order potential for atomistic simulations of zinc oxide. Journal of Physics Condensed Matter, 2006, 18, 6585-6605.	0.7	68
52	Atomistic mechanism of shock-induced void collapse in nanoporous metals. Physical Review B, 2005, 72, .	1.1	67
53	Thermodynamics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>L</mml:mi><mml:msub><mml:mn>1</mml:mn><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math>in FePt nanoparticles studied by Monte Carlo simulations based on an analytic bond-order potential. Physical Review B, 2007, 76, .	1.1	67
54	Competing deformation mechanisms in nanocrystalline metals and alloys: Coupled motion versus grain boundary sliding. Acta Materialia, 2012, 60, 6076-6085.	3.8	67

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55	Molecular dynamics study of defect formation in GaN cascades. Nuclear Instruments & Methods in Physics Research B, 2003, 202, 93-99.	0.6	66
56	Grain boundary structure and mobility in high-entropy alloys: A comparative molecular dynamics study on a Î£11 symmetrical tilt grain boundary in face-centered cubic CuNiCoFe. Acta Materialia, 2020, 186, 11-19.	3.8	66
57	Ionic conductivity of acceptor doped sodium bismuth titanate: influence of dopants, phase transitions and defect associates. Journal of Materials Chemistry C, 2017, 5, 8958-8965.	2.7	65
58	Modeling the electrical conductivity in BaTiO3 on the basis of first-principles calculations. Journal of Applied Physics, 2008, 104, .	1.1	61
59	Local segregation versus irradiation effects in high-entropy alloys: Steady-state conditions in a driven system. Journal of Applied Physics, 2017, 122, .	1.1	61
60	Limits for n-type doping in In2O3 and SnO2: A theoretical approach by first-principles calculations using hybrid-functional methodology. Journal of Applied Physics, 2010, 108, .	1.1	57
61	Engineering the Siteâ€Disorder and Lithium Distribution in the Lithium Superionic Argyrodite Li₆PS₅Br. Advanced Energy Materials, 2021, 11, 2003369.	10.2	57
62	Dislocation-toughened ceramics. Materials Horizons, 2021, 8, 1528-1537.	6.4	56
63	Density-functional-theory calculations of electronic band structure of single-crystal and single-layerWS2. Physical Review B, 2002, 66, .	1.1	55
64	Simulation of grain growth in nanocrystalline nickel induced by ion irradiation. Nuclear Instruments & Methods in Physics Research B, 2003, 202, 230-235.	0.6	54
65	Ab initiomodeling of diffusion in indium oxide. Physical Review B, 2010, 81, .	1.1	54
66	Influence of orbital contributions to the valence band alignment of Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>, Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	53
67	Low Temperature Heat Capacity of a Severely Deformed Metallic Glass. Physical Review Letters, 2014, 112, 135501.	2.9	52
68	Finite-size effects in the phonon density of states of nanostructured germanium: A comparative study of nanoparticles, nanocrystals, nanoglasses, and bulk phases. Physical Review B, 2011, 83, .	1.1	49
69	Interfacial instability of amorphous LiPON against lithium: A combined Density Functional Theory and spectroscopic study. Journal of Power Sources, 2017, 354, 124-133.	4.0	49
70	Microstructure formation of metallic nanoglasses: Insights from molecular dynamics simulations. Acta Materialia, 2018, 145, 322-330.	3.8	48
71	Grain size dependence of the bulk modulus of nanocrystalline nickel. Scripta Materialia, 2006, 55, 473-476.	2.6	47
72	Plastic deformation of nanocrystalline Pdâ€“Au alloys: On the interplay of grain boundary solute segregation, fault energies and grain size. Acta Materialia, 2011, 59, 2957-2968.	3.8	47

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73	Chemical and topological order in shear bands of Cu64Zr36 and Cu36Zr64 glasses. Journal of Applied Physics, 2012, 111, .	1.1	47
74	Compositional and electrical properties of line and planar defects in Cu(In,Ga)Se₂ thin films for solar cells â€“ a review. Physica Status Solidi - Rapid Research Letters, 2016, 10, 363-375.	1.2	47
75	Interfaces and interphases in nanoglasses: Surface segregation effects and their implications on structural properties. Acta Materialia, 2016, 113, 284-292.	3.8	47
76	Stacking-Fault Nucleation on Ir(111). Physical Review Letters, 2003, 91, 056103.	2.9	45
77	First-principles calculations on solid nitrogen: A comparative study of high-pressure phases. Physical Review B, 2008, 77, .	1.1	45
78	Influence of solutes on the competition between mesoscopic grain boundary sliding and coupled grain boundary motion. Scripta Materialia, 2012, 66, 315-317.	2.6	45
79	Influence of phase transitions and defect associates on the oxygen migration in the ion conductor Na_{1/2}Bi_{1/2}TiO₃. Journal of Materials Chemistry A, 2017, 5, 4368-4375.	5.2	45
80	Influence of grain size and composition, topology and excess free volume on the deformation behavior of Cuâ€“Zr nanoglasses. Beilstein Journal of Nanotechnology, 2015, 6, 537-545.	1.5	44
81	Contact epitaxy by deposition of Cu, Ag, Au, Pt, and Ni nanoclusters on (100) surfaces: Size limits and mechanisms. Physical Review B, 2007, 75, .	1.1	43
82	Formation of parallel (111) twin boundaries in silicon growth from the melt explained by molecular dynamics simulations. Journal of Crystal Growth, 2010, 312, 1411-1415.	0.7	42
83	Influence of Crystalline Nanoprecipitates on Shear-Band Propagation in Cu-Zr-Based Metallic Glasses. Physical Review Applied, 2016, 5, .	1.5	42
84	Structure and Properties of Nanoglasses. Advanced Engineering Materials, 2018, 20, 1800404.	1.6	42
85	Formation entropies of intrinsic point defects in cubic In2O3 from first-principles density functional theory calculations. Physical Chemistry Chemical Physics, 2009, 11, 3226.	1.3	41
86	Structural origins of the boson peak in metals: From high-entropy alloys to metallic glasses. Physical Review B, 2016, 94, .	1.1	41
87	Positive and negative electrocaloric effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><i>in the presence of defect dipoles. Physical Review B, 2016, 94, .	1.1	41
88	Concentration of thermal vacancies in metallic nanoparticles. Acta Materialia, 2007, 55, 3237-3244.	3.8	39
89	Origins of the Inverse Electrocaloric Effect. Energy Technology, 2018, 6, 1491-1511.	1.8	39
90	From metallic glasses to nanocrystals: Molecular dynamics simulations on the crossover from glass-like to grain-boundary-mediated deformation behaviour. Acta Materialia, 2018, 156, 205-214.	3.8	38

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91	Metallic glass nanolaminates with shape memory alloys. Acta Materialia, 2018, 159, 344-351.	3.8	38
92	Orientation dependent ionization potential of In₂O₃: a natural source for inhomogeneous barrier formation at electrode interfaces in organic electronics. Journal of Physics Condensed Matter, 2011, 23, 334203.	0.7	36
93	A machine-learned interatomic potential for silica and its relation to empirical models. Npj Computational Materials, 2022, 8, .	3.5	36
94	Thermal annealing of shear bands in deformed metallic glasses: Recovery mechanisms in Cu64Zr36 studied by molecular dynamics simulations. Acta Materialia, 2011, 59, 7082-7094.	3.8	34
95	Size-dependent phase diagrams of metallic alloys: A Monte Carlo simulation study on orderâ€“disorder transitions in Ptâ€“Rh nanoparticles. Beilstein Journal of Nanotechnology, 2012, 3, 1-11.	1.5	33
96	First-principles calculations on structure and properties of amorphous Li5P4O8N3 (LiPON). Journal of Power Sources, 2016, 331, 382-390.	4.0	33
97	Pressure-induced phase transitions and structure of chemically ordered nanoregions in the lead-free relaxor ferroelectric Na<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>.	1.1	32
98	Insights into Degradation of Si Anodes from First-Principle Calculations. Journal of Physical Chemistry C, 2013, 117, 18796-18803.	1.5	32
99	Atomistic understanding of the LiNiO₂â€“NiO₂ phase diagram from experimentally guided lattice models. Journal of Materials Chemistry A, 2021, 9, 14928-14940.	5.2	31
100	Structural stability of multiply twinned FePt nanoparticles. Acta Materialia, 2007, 55, 6617-6626.	3.8	30
101	Disordered reconstructions of the reduced SnO2-(110) surface. Surface Science, 2011, 605, 714-722.	0.8	30
102	Origins of strength and plasticity in the precious metal based high-entropy alloy AuCuNiPdPt. Acta Materialia, 2020, 185, 400-411.	3.8	30
103	Controlled softening of Cu64Zr36 metallic glass by ion irradiation. Applied Physics Letters, 2013, 102, .	1.5	28
104	Experimental and theoretical study of tracer diffusion in a series of (CoCrFeMn)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif"><mml:msub><mml:mrow /><mml:mrow><mml:mn>100</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Ni alloys. Acta Materialia, 2020, 194, 236-248.	3.8	28
105	Deformation-induced grain growth and twinning in nanocrystalline palladium thin films. Beilstein Journal of Nanotechnology, 2013, 4, 554-566.	1.5	27
106	State transition and electrocaloric effect of BaZrxTi1â^'xO3: Simulation and experiment. Journal of Applied Physics, 2017, 121, .	1.1	27
107	Influence of microstructural features on the plastic deformation behavior of metallic nanoglasses. Acta Materialia, 2019, 168, 393-400.	3.8	27
108	Lattice-based Monte Carlo simulations of the electrocaloric effect in ferroelectrics and relaxor ferroelectrics. Physical Review B, 2015, 91, .	1.1	26

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109	Nanocluster rotation on Pt surfaces: Twist boundaries. Physical Review B, 2001, 64, .	1.1	25
110	The role of thermostats in modeling vapor phase condensation of silicon nanoparticles. Applied Surface Science, 2004, 226, 12-18.	3.1	25
111	Island shapes, island densities, and stacking-fault formation onIr(111): Kinetic Monte Carlo simulations and experiments. Physical Review B, 2005, 71, .	1.1	25
112	Role of copper interstitials in CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: First-principles calculations. Physical Review B, 2011, 84, .	1.1	25
113	Enhanced electrocaloric cooling in ferroelectric single crystals by electric field reversal. Physical Review B, 2016, 94, .	1.1	25
114	On the origin of the anomalous compliance of dealloying-derived nanoporous gold. Scripta Materialia, 2017, 130, 74-77.	2.6	25
115	And Yet It Moves: LiNiO₂, a Dynamic Jahnâ€“Teller System. Chemistry of Materials, 2020, 32, 10096-10103.	3.2	25
116	Study of electrical fatigue by defect engineering in organic light-emitting diodes. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2015, 192, 26-51.	1.7	24
117	Reinforcement of nanoglasses by interface strengthening. Scripta Materialia, 2017, 141, 115-119.	2.6	24
118	Reactivity of Isocyanate-Functionalized Lignins: A Key Factor for the Preparation of Lignin-Based Polyurethanes. Frontiers in Chemistry, 2019, 7, 562.	1.8	24
119	Influence of topological structure and chemical segregation on the thermal and mechanical properties of Pdâ€“Si nanoglasses. Acta Materialia, 2020, 193, 252-260.	3.8	24
120	From multiply twinned to fcc nanoparticles via irradiation-induced transient amorphization. Europhysics Letters, 2009, 85, 26001.	0.7	23
121	Kinetic lattice Monte-Carlo simulations on the ordering kinetics of free and supported FePt L1₀-nanoparticles. Beilstein Journal of Nanotechnology, 2011, 2, 40-46.	1.5	23
122	Diffusion mechanism in the superionic conductor Li4PS4I studied by first-principlesÂcalculations. Solid State Ionics, 2018, 319, 83-91.	1.3	23
123	High-Pressure Synthesis of Novel Boron Oxynitride B6N4O3 with Sphalerite Type Structure. Chemistry of Materials, 2015, 27, 5907-5914.	3.2	22
124	Intrinsic point defects in Î²-In2S3 studied by means of hybrid density-functional theory. Journal of Applied Physics, 2018, 123, .	1.1	22
125	Structure and stability of non-molecular nitrogen at ambient pressure. Europhysics Letters, 2004, 65, 400-406.	0.7	20
126	Octahedral tilt transitions in the relaxor ferroelectric Na1/2Bi1/2TiO3. Journal of Solid State Chemistry, 2015, 227, 117-122.	1.4	20

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127	Interface-controlled creep in metallic glass composites. Acta Materialia, 2017, 141, 251-260.	3.8	20
128	The influence of anisotropic surface stresses and bulk stresses on defect thermodynamics in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiCoO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml Acta Materialia, 2018, 159, 225-240.	3.8	19
129	Cohesive strength of zirconia/molybdenum interfaces and grain boundaries in molybdenum: A comparative study. Acta Materialia, 2017, 135, 150-157.	3.8	19
130	Self-limited oxygen exchange kinetics at SnO2 surfaces. Physical Chemistry Chemical Physics, 2011, 13, 3223.	1.3	18
131	Comparative study of A-site order in the lead-free bismuth titanates M1/2Bi1/2TiO3 (M=Li, Na, K, Rb, Cs,) Tj ETQq1 1 0.784314 rgBT /Ov	1.4	18
132	Effect of Ti content and nitrogen on the high-temperature oxidation behavior of (Mo,Ti)5Si3. Intermetallics, 2017, 90, 103-112.	1.8	18
133	Energy level alignment of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cu</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml absorber compounds with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mro.	0.9	18
134	Breakdown of Varvenne scaling in (AuNiPdPt)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Cu high-entropy alloys. Scripta Materialia, 2020, 181, 15-18.	2.6	17
135	A-site occupancy in the lead-free (Bi1/2Na1/2TiO3)0.94â€“(BaTiO3)0.06 piezoceramic: Combining first-principles study and TEM. Journal of Applied Physics, 2010, 107, .	1.1	16
136	Effect of solute segregation on thermal creep in dilute nanocyrstalline Cu alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2012, 546, 307-313.	2.6	16
137	On the origin of anisotropic lithiation of silicon. Journal of Power Sources, 2015, 293, 221-227.	4.0	15
138	Atomistic modelling of zirconium and silicon segregation at twist and tilt grain boundaries in molybdenum. Journal of Materials Science, 2016, 51, 1873-1881.	1.7	15
139	Simulations of the inert gas condensation processes. International Journal of Materials Research, 2003, 94, 1098-1105.	0.8	15
140	Ion beam smoothening of metal surfaces. Journal of Applied Physics, 2003, 94, 4432-4439.	1.1	14
141	Structural modification of a multiply twinned nanoparticle by ion irradiation: A molecular dynamics study. Journal of Applied Physics, 2007, 102, 124304.	1.1	14
142	Damage production in nanoparticles under light ion irradiation. Physical Review B, 2009, 80, .	1.1	14
143	Diffusion of yttrium in bcc-iron studied by kinetic Monte Carlo simulations. Journal of Nuclear Materials, 2017, 494, 157-164.	1.3	14
144	Influence of Cu and Na incorporation on the thermodynamic stability and electronic properties of Î²-In₂S₃. Journal of Materials Chemistry C, 2018, 6, 7226-7231.	2.7	14

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145	Molecular-dynamics simulations of energetic C60 impacts on (2Ã—1)-(100) silicon. Journal of Applied Physics, 2000, 88, 49-54.	1.1	13
146	Line stress of step edges at crystal surfaces. Surface Science, 2011, 605, 947-957.	0.8	13
147	Molecular Dynamics Simulations of Gas Phase Condensation of Silicon Carbide Nanoparticles. Advanced Engineering Materials, 2005, 7, 937-945.	1.6	12
148	Effect of Ti addition on the thermal expansion anisotropy of Mo5Si3. Acta Materialia, 2017, 132, 25-34.	3.8	12
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