Karsten Albe

List of Publications by Citations

206 papers	10,128 citations	53 h-index	95 g-index
216 ext. papers	11,318 ext. citations	4.9 avg, IF	6.67 L-index

#	Paper	IF	Citations
206	Extracting dislocations and non-dislocation crystal defects from atomistic simulation data. *Modelling and Simulation in Materials Science and Engineering*, **2010**, 18, 085001	2	546
205	First-principles study of intrinsic point defects in ZnO: Role of band structure, volume relaxation, and finite-size effects. *Physical Review B*, **2006**, 73,	3.3	425
204	Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals. *Acta Materialia*, **2008**, 56, 1126-1135	8.4	381
203	Analytical potential for atomistic simulations of silicon, carbon, and silicon carbide. *Physical Review B*, **2005**, 71,	3.3	346
202	The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals. *Scripta Materialia*, **2006**, 54, 1163-1168	5.6	313
201	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	3.1	287
200	Intrinsic n-type behavior in transparent conducting oxides: a comparative hybrid-functional study of In2O3, SnO2, and ZnO. *Physical Review Letters*, **2009**, 103, 245501	7.4	274
199	Caloric Effects in Ferroic Materials: New Concepts for Cooling. *Advanced Engineering Materials*, **2012**, 14, 10-19	3.5	242
198	Analytical interatomic potential for modeling nonequilibrium processes in the W□H system. *Journal of Applied Physics*, **2005**, 98, 123520	2.5	213
197	Mechanisms of aging and fatigue in ferroelectrics. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2015**, 192, 52-82	3.1	205
196	Diffusion of zinc vacancies and interstitials in zinc oxide. *Applied Physics Letters*, **2006**, 88, 201918	3.4	187
195	Modelling of compound semiconductors: analytical bond-order potential for gallium, nitrogen and gallium nitride. *Journal of Physics Condensed Matter*, **2003**, 15, 5649-5662	1.8	174
194	Band structure of indium oxide: Indirect versus direct band gap. *Physical Review B*, **2007**, 75,	3.3	169
193	Size-dependent lattice expansion in nanoparticles: reality or anomaly?. *ChemPhysChem*, **2012**, 13, 2443-54	3.2	152
192	First-principles study of the structure and stability of oxygen defects in zinc oxide. *Physical Review B*, **2005**, 72,	3.3	145
191	Molecular-dynamics simulations of steady-state growth of ion-deposited tetrahedral amorphous carbon films. *Journal of Applied Physics*, **2000**, 88, 1129-1135	2.5	134
190	Enhancing the plasticity of metallic glasses: Shear band formation, nanocomposites and nanoglasses investigated by molecular dynamics simulations. *Mechanics of Materials*, **2013**, 67, 94-103	3.3	132

189	Modeling the metal-semiconductor interaction: Analytical bond-order potential for platinum-carbon. *Physical Review B*, **2002**, 65,	3.3	130
188	Intrinsic point defects in CuInSe2 and CuGaSe2 as seen via screened-exchange hybrid density functional theory. *Physical Review B*, **2013**, 87,	3.3	120
187	First-principles study of migration mechanisms and diffusion of oxygen in zinc oxide. *Physical Review B*, **2006**, 73,	3.3	119
186	Modeling of compound semiconductors: Analytical bond-order potential for Ga, As, and GaAs. *Physical Review B*, **2002**, 66,	3.3	119
185	Theoretical study of boron nitride modifications at hydrostatic pressures. *Physical Review B*, **1997**, 55, 6203-6210	3.3	116
184	Modelling of boron nitride: Atomic scale simulations on thin film growth. *Computational Materials Science*, **1998**, 10, 111-115	3.2	116
183	Thermodynamics of mono- and di-vacancies in barium titanate. *Journal of Applied Physics*, **2007**, 102, 084111	2.5	116
182	Lattice Monte Carlo simulations of FePt nanoparticles: Influence of size, composition, and surface segregation on order-disorder phenomena. *Physical Review B*, **2005**, 72,	3.3	113
181	Deformation behavior of bulk and nanostructured metallic glasses studied via molecular dynamics simulations. *Physical Review B*, **2011**, 83,	3.3	108
180	Nanotwinned fcc metals: Strengthening versus softening mechanisms. *Physical Review B*, **2010**, 82,	3.3	108
179	Defect-Dipole Formation in Copper-Doped PbTiO3 Ferroelectrics. *Physical Review Letters*, **2008**, 100, 095504	7.4	108
178	Analytic bond-order potential for bcc and fcc iron□comparison with established embedded-atom method potentials. *Journal of Physics Condensed Matter*, **2007**, 19, 326220	1.8	108
177	Anomalous compliance and early yielding of nanoporous gold. *Acta Materialia*, **2015**, 93, 144-155	8.4	106
176	Dislocation detection algorithm for atomistic simulations. *Modelling and Simulation in Materials Science and Engineering*, **2010**, 18, 025016	2	105
175	Gallium gradients in Cu(In,Ga)Se2 thin-film solar cells. *Progress in Photovoltaics: Research and Applications*, **2015**, 23, 717-733	6.8	97
174	Reaching theoretical strengths in nanocrystalline Cu by grain boundary doping. *Scripta Materialia*, **2011**, 65, 660-663	5.6	91
173	Structure, stability and mechanical properties of internal interfaces in Cu64Zr36 nanoglasses studied by MD simulations. *Acta Materialia*, **2011**, 59, 6588-6593	8.4	86
172	Association of oxygen vacancies with impurity metal ions in lead titanate. *Physical Review B*, **2007**, 76,	3.3	86

171	Mechanisms of radiation-induced viscous flow: role of point defects. *Physical Review Letters*, **2003**, 90, 055505	7.4	81
170	Local Structural Investigations, Defect Formation, and Ionic Conductivity of the Lithium Ionic Conductor Li4P2S6. *Chemistry of Materials*, **2016**, 28, 8764-8773	9.6	74
169	From nanoglasses to bulk massive glasses. *Applied Physics Letters*, **2009**, 94, 191911	3.4	74
168	Computer simulation and boron nitride. *Radiation Effects and Defects in Solids*, **1997**, 141, 85-97	0.9	73
167	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, 023509	2.5	70
166	Chemical order and local structure of the lead-free relaxor ferroelectric. *Journal of Solid State Chemistry*, **2011**, 184, 2041-2046	3.3	69
165	Atomistic origin of microstrain broadening in diffraction data of nanocrystalline solids. *Acta Materialia*, **2009**, 57, 1648-1654	8.4	68
164	Geometry, electronic structure and thermodynamic stability of intrinsic point defects in indium oxide. *Journal of Physics Condensed Matter*, **2009**, 21, 455801	1.8	65
163	Thermodynamic stability, stoichiometry, and electronic structure of bcc-In2O3 surfaces. *Physical Review B*, **2011**, 84,	3.3	62
162	Thermodynamics of L10 ordering in FePt nanoparticles studied by Monte Carlo simulations based on an analytic bond-order potential. *Physical Review B*, **2007**, 76,	3.3	62
161	Reconciling Local Structure Disorder and the Relaxor State in (Bi1/2Na1/2)TiO3-BaTiO3. *Scientific Reports*, **2016**, 6, 31739	4.9	61
160	Extended Tersoff potential for boron nitride: Energetics and elastic properties of pristine and defective h-BN. *Physical Review B*, **2017**, 96,	3.3	60
159	Formation and switching of defect dipoles in acceptor-doped lead titanate: A kinetic model based on first-principles calculations. *Physical Review B*, **2013**, 88,	3.3	59
158	Reaction and Space Charge Layer Formation at the LiCoO2□LiPON Interface: Insights on Defect Formation and Ion Energy Level Alignment by a Combined Surface Science–Simulation Approach. *Chemistry of Materials*, **2017**, 29, 7675-7685	9.6	57
157	Competing deformation mechanisms in nanocrystalline metals and alloys: Coupled motion versus grain boundary sliding. *Acta Materialia*, **2012**, 60, 6076-6085	8.4	57
156	Analytic bond-order potential for atomistic simulations of zinc oxide. *Journal of Physics Condensed Matter*, **2006**, 18, 6585-6605	1.8	57
155	Highly Porous Silicon Embedded in a Ceramic Matrix: A Stable High-Capacity Electrode for Li-Ion Batteries. *ACS Nano*, **2017**, 11, 11409-11416	16.7	56
154	Molecular dynamics study of defect formation in GaN cascades. *Nuclear Instruments & Methods in Physics Research B*, **2003**, 202, 93-99	1.2	53

153	Atomistic mechanism of shock-induced void collapse in nanoporous metals. *Physical Review B*, **2005**, 72,	3.3	53
152	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, 053511	2.5	52
151	Simulation of grain growth in nanocrystalline nickel induced by ion irradiation. *Nuclear Instruments & Methods in Physics Research B*, **2003**, 202, 230-235	1.2	52
150	Ab initio modeling of diffusion in indium oxide. *Physical Review B*, **2010**, 81,	3.3	51
149	Modeling the electrical conductivity in BaTiO3 on the basis of first-principles calculations. *Journal of Applied Physics*, **2008**, 104, 044315	2.5	51
148	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	7.1	46
147	Density-functional-theory calculations of electronic band structure of single-crystal and single-layer WS2. *Physical Review B*, **2002**, 66,	3.3	46
146	Influence of orbital contributions to the valence band alignment of Bi2O3, Fe2O3, BiFeO3, and Bi0.5Na0.5TiO3. *Physical Review B*, **2013**, 88,	3.3	44
145	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,	3.3	44
144	Stacking-fault nucleation on Ir(111). *Physical Review Letters*, **2003**, 91, 056103	7.4	44
143	Grain size dependence of the bulk modulus of nanocrystalline nickel. *Scripta Materialia*, **2006**, 55, 473-476	5.6	43
142	Influence of solutes on the competition between mesoscopic grain boundary sliding and coupled grain boundary motion. *Scripta Materialia*, **2012**, 66, 315-317	5.6	42
141	Compositional and electrical properties of line and planar defects in Cu(In,Ga)Se2 thin films for solar cells – a review. *Physica Status Solidi - Rapid Research Letters*, **2016**, 10, 363-375	2.5	42
140	Contact epitaxy by deposition of Cu, Ag, Au, Pt, and Ni nanoclusters on (100) surfaces: Size limits and mechanisms. *Physical Review B*, **2007**, 75,	3.3	41
139	Chemical and topological order in shear bands of Cu64Zr36 and Cu36Zr64 glasses. *Journal of Applied Physics*, **2012**, 111, 103527	2.5	39
138	Plastic deformation of nanocrystalline Pd–Au alloys: On the interplay of grain boundary solute segregation, fault energies and grain size. *Acta Materialia*, **2011**, 59, 2957-2968	8.4	39
137	Positive and negative electrocaloric effect in BaTiO3 in the presence of defect dipoles. *Physical Review B*, **2016**, 94,	3.3	39
136	Influence of phase transitions and defect associates on the oxygen migration in the ion conductor Na1/2Bi1/2TiO3. *Journal of Materials Chemistry A*, **2017**, 5, 4368-4375	13	38

135	Influence of Crystalline Nanoprecipitates on Shear-Band Propagation in Cu-Zr-Based Metallic Glasses. *Physical Review Applied*, **2016**, 5,	4.3	38
134	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	1.6	38
133	Rapid Crystallization and Kinetic Freezing of Site-Disorder in the Lithium Superionic Argyrodite Li6PS5Br. *Chemistry of Materials*, **2019**, 31, 10178-10185	9.6	38
132	Interfacial instability of amorphous LiPON against lithium: A combined Density Functional Theory and spectroscopic study. *Journal of Power Sources*, **2017**, 354, 124-133	8.9	37
131	Low temperature heat capacity of a severely deformed metallic glass. *Physical Review Letters*, **2014**, 112, 135501	7.4	37
130	Influence of grain size and composition, topology and excess free volume on the deformation behavior of Cu-Zr nanoglasses. *Beilstein Journal of Nanotechnology*, **2015**, 6, 537-545	3	37
129	Formation entropies of intrinsic point defects in cubic In(2)O(3) from first-principles density functional theory calculations. *Physical Chemistry Chemical Physics*, **2009**, 11, 3226-32	3.6	37
128	Local segregation versus irradiation effects in high-entropy alloys: Steady-state conditions in a driven system. *Journal of Applied Physics*, **2017**, 122, 105106	2.5	36
127	Concentration of thermal vacancies in metallic nanoparticles. *Acta Materialia*, **2007**, 55, 3237-3244	8.4	35
126	Interfaces and interphases in nanoglasses: Surface segregation effects and their implications on structural properties. *Acta Materialia*, **2016**, 113, 284-292	8.4	35
125	Microstructure formation of metallic nanoglasses: Insights from molecular dynamics simulations. *Acta Materialia*, **2018**, 145, 322-330	8.4	31
124	First-principles calculations on solid nitrogen: A comparative study of high-pressure phases. *Physical Review B*, **2008**, 77,	3.3	31
123	Structural origins of the boson peak in metals: From high-entropy alloys to metallic glasses. *Physical Review B*, **2016**, 94,	3.3	31
122	Size-dependent phase diagrams of metallic alloys: A Monte Carlo simulation study on order-disorder transitions in Pt-Rh nanoparticles. *Beilstein Journal of Nanotechnology*, **2012**, 3, 1-11	3	30
121	Structural stability of multiply twinned FePt nanoparticles. *Acta Materialia*, **2007**, 55, 6617-6626	8.4	30
120	Origins of the Inverse Electrocaloric Effect. *Energy Technology*, **2018**, 6, 1491-1511	3.5	29
119	Metallic glass nanolaminates with shape memory alloys. *Acta Materialia*, **2018**, 159, 344-351	8.4	29
118	Thermal annealing of shear bands in deformed metallic glasses: Recovery mechanisms in Cu64Zr36 studied by molecular dynamics simulations. *Acta Materialia*, **2011**, 59, 7082-7094	8.4	29

117	Structure and Properties of Nanoglasses. *Advanced Engineering Materials*, **2018**, 20, 1800404	3.5	29
116	Insights into Degradation of Si Anodes from First-Principle Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 18796-18803	3.8	28
115	Pressure-induced phase transitions and structure of chemically ordered nanoregions in the lead-free relaxor ferroelectric Na1/2Bi1/2TiO3. *Physical Review B*, **2012**, 86,	3.3	28
114	First-principles calculations on structure and properties of amorphous Li5P4O8N3 (LiPON). *Journal of Power Sources*, **2016**, 331, 382-390	8.9	28
113	Deformation-induced grain growth and twinning in nanocrystalline palladium thin films. *Beilstein Journal of Nanotechnology*, **2013**, 4, 554-66	3	27
112	Disordered reconstructions of the reduced SnO2-(110) surface. *Surface Science*, **2011**, 605, 714-722	1.8	27
111	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	1.8	27
110	State transition and electrocaloric effect of BaZrxTi1−xO3: Simulation and experiment. *Journal of Applied Physics*, **2017**, 121, 024103	2.5	25
109	Island shapes, island densities, and stacking-fault formation on Ir(111): Kinetic Monte Carlo simulations and experiments. *Physical Review B*, **2005**, 71,	3.3	25
108	Nanocluster rotation on Pt surfaces: Twist boundaries. *Physical Review B*, **2001**, 64,	3.3	25
107	Grain boundary structure and mobility in high-entropy alloys: A comparative molecular dynamics study on a Σ11 symmetrical tilt grain boundary in face-centered cubic CuNiCoFe. *Acta Materialia*, **2020**, 186, 11-19	8.4	25
106	Role of copper interstitials in CuInSe2: First-principles calculations. *Physical Review B*, **2011**, 84,	3.3	24
105	The role of thermostats in modeling vapor phase condensation of silicon nanoparticles. *Applied Surface Science*, **2004**, 226, 12-18	6.7	24
104	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	3.1	23
103	Controlled softening of Cu64Zr36 metallic glass by ion irradiation. *Applied Physics Letters*, **2013**, 102, 181910	3.4	23
102	From multiply twinned to fcc nanoparticles via irradiation-induced transient amorphization. *Europhysics Letters*, **2009**, 85, 26001	1.6	23
101	Kinetic lattice Monte-Carlo simulations on the ordering kinetics of free and supported FePt L1(0)-nanoparticles. *Beilstein Journal of Nanotechnology*, **2011**, 2, 40-6	3	22
100	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	8.4	22

99	Engineering the Site-Disorder and Lithium Distribution in the Lithium Superionic Argyrodite Li6PS5Br. *Advanced Energy Materials*, **2021**, 11, 2003369	21.8	21
98	Enhanced electrocaloric cooling in ferroelectric single crystals by electric field reversal. *Physical Review B*, **2016**, 94,	3.3	20
97	Lattice-based Monte Carlo simulations of the electrocaloric effect in ferroelectrics and relaxor ferroelectrics. *Physical Review B*, **2015**, 91,	3.3	19
96	On the origin of the anomalous compliance of dealloying-derived nanoporous gold. *Scripta Materialia*, **2017**, 130, 74-77	5.6	19
95	Intrinsic point defects in In2S3 studied by means of hybrid density-functional theory. *Journal of Applied Physics*, **2018**, 123, 103103	2.5	17
94	Structure and stability of non-molecular nitrogen at ambient pressure. *Europhysics Letters*, **2004**, 65, 400-406	1.6	17
93	Diffusion mechanism in the superionic conductor Li4PS4I studied by first-principles calculations. *Solid State Ionics*, **2018**, 319, 83-91	3.3	16
92	Octahedral tilt transitions in the relaxor ferroelectric Na1/2Bi1/2TiO3. *Journal of Solid State Chemistry*, **2015**, 227, 117-122	3.3	15
91	High-Pressure Synthesis of Novel Boron Oxynitride B6N4O3 with Sphalerite Type Structure. *Chemistry of Materials*, **2015**, 27, 5907-5914	9.6	15
90	The influence of anisotropic surface stresses and bulk stresses on defect thermodynamics in LiCoO2 nanoparticles. *Acta Materialia*, **2018**, 159, 225-240	8.4	15
89	Interface-controlled creep in metallic glass composites. *Acta Materialia*, **2017**, 141, 251-260	8.4	15
88	Effect of Ti content and nitrogen on the high-temperature oxidation behavior of (Mo,Ti) 5 Si 3. *Intermetallics*, **2017**, 90, 103-112	3.5	15
87	Reinforcement of nanoglasses by interface strengthening. *Scripta Materialia*, **2017**, 141, 115-119	5.6	15
86	Self-limited oxygen exchange kinetics at SnO2 surfaces. *Physical Chemistry Chemical Physics*, **2011**, 13, 3223-6	3.6	15
85	Simulations of the inert gas condensation processes. *International Journal of Materials Research*, **2003**, 94, 1098-1105		15
84	Influence of microstructural features on the plastic deformation behavior of metallic nanoglasses. *Acta Materialia*, **2019**, 168, 393-400	8.4	15
83	Reactivity of Isocyanate-Functionalized Lignins: A Key Factor for the Preparation of Lignin-Based Polyurethanes. *Frontiers in Chemistry*, **2019**, 7, 562	5	14
82	Influence of topological structure and chemical segregation on the thermal and mechanical properties of PdBi nanoglasses. *Acta Materialia*, **2020**, 193, 252-260	8.4	14

81	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	5.3	14
80	A-site occupancy in the lead-free (Bi1/2Na1/2TiO3)0.94(BaTiO3)0.06 piezoceramic: Combining first-principles study and TEM. *Journal of Applied Physics*, **2010**, 107, 114113	2.5	14
79	Structural modification of a multiply twinned nanoparticle by ion irradiation: A molecular dynamics study. *Journal of Applied Physics*, **2007**, 102, 124304	2.5	14
78	Experimental and theoretical study of tracer diffusion in a series of (CoCrFeMn)100−xNi alloys. *Acta Materialia*, **2020**, 194, 236-248	8.4	14
77	On the origin of anisotropic lithiation of silicon. *Journal of Power Sources*, **2015**, 293, 221-227	8.9	13
76	Comparative study of A-site order in the lead-free bismuth titanates M1/2Bi1/2TiO3 (M=Li, Na, K, Rb, Cs, Ag, Tl) from first-principles. *Journal of Solid State Chemistry*, **2014**, 213, 138-144	3.3	13
75	Line stress of step edges at crystal surfaces. *Surface Science*, **2011**, 605, 947-957	1.8	13
74	Molecular-dynamics simulations of energetic C60 impacts on (2×1)-(100) silicon. *Journal of Applied Physics*, **2000**, 88, 49-54	2.5	13
73	Cohesive strength of zirconia/molybdenum interfaces and grain boundaries in molybdenum: A comparative study. *Acta Materialia*, **2017**, 135, 150-157	8.4	13
72	Diffusion of yttrium in bcc-iron studied by kinetic Monte Carlo simulations. *Journal of Nuclear Materials*, **2017**, 494, 157-164	3.3	12
71	Ion beam smoothening of metal surfaces. *Journal of Applied Physics*, **2003**, 94, 4432-4439	2.5	12
70	Molecular Dynamics Simulations of Gas Phase Condensation of Silicon Carbide Nanoparticles. *Advanced Engineering Materials*, **2005**, 7, 937-945	3.5	12
69	Origins of strength and plasticity in the precious metal based high-entropy alloy AuCuNiPdPt. *Acta Materialia*, **2020**, 185, 400-411	8.4	12
68	Dislocation-toughened ceramics. *Materials Horizons*, **2021**, 8, 1528-1537	14.4	12
67	Plasticity of Cu nanoparticles: Dislocation-dendrite-induced strain hardening and a limit for displacive plasticity. *Beilstein Journal of Nanotechnology*, **2013**, 4, 173-9	3	11
66	Goston et al. Reply:. *Physical Review Letters*, **2011**, 106,	7.4	11
65	Energy level alignment of Cu(In,Ga)(S,Se)2 absorber compounds with In2S3, NaIn5S8, and CuIn5S8 Cd-free buffer materials. *Physical Review Materials*, **2019**, 3,	3.2	11
64	Atomistic modelling of zirconium and silicon segregation at twist and tilt grain boundaries in molybdenum. *Journal of Materials Science*, **2016**, 51, 1873-1881	4.3	10

63	Influence of Cu and Na incorporation on the thermodynamic stability and electronic properties of In2S3. *Journal of Materials Chemistry C*, **2018**, 6, 7226-7231	7.1	10
62	Theoretical prediction of morphotropic compositions in Na1/2Bi1/2TiO3-based solid solutions from transition pressures. *Physical Review B*, **2014**, 89,	3.3	10
61	Damage production in nanoparticles under light ion irradiation. *Physical Review B*, **2009**, 80,	3.3	10
60	Impact of Polarization Dynamics and Charged Defects on the Electrocaloric Response of Ferroelectric Pb(Zr,Ti)O3 Ceramics. *Energy Technology*, **2018**, 6, 1519-1525	3.5	10
59	Structure and stability of alpha- and beta-Ti2Se. Electron diffraction versus density-functional theory calculations. *Acta Crystallographica Section A: Foundations and Advances*, **2003**, 59, 18-21		9
58	Atomistic understanding of the LiNiO2NiO2 phase diagram from experimentally guided lattice models. *Journal of Materials Chemistry A*, **2021**, 9, 14928-14940	13	9
57	Effect of Ti addition on the thermal expansion anisotropy of Mo5Si3. *Acta Materialia*, **2017**, 132, 25-34	8.4	8
56	Solubility of zirconium and silicon in molybdenum studied by first-principles calculations. *Scripta Materialia*, **2015**, 97, 1-4	5.6	8
55	Effect of ion irradiation on structural properties of Cu64Zr36 metallic glass. *Nuclear Instruments & Methods in Physics Research B*, **2014**, 341, 22-26	1.2	8
54	Point defect segregation and its role in the detrimental nature of Frank partials in Cu(In,Ga)Se2 thin-film absorbers. *Physical Review B*, **2017**, 95,	3.3	8
53	Solid-state amorphization of Cu nanolayers embedded in a Cu64Zr36 glass. *Physical Review B*, **2015**, 91,	3.3	8
52	On the hierarchy of deformation processes in nanocrystalline alloys: Grain boundary mediated plasticity vs. dislocation slip. *Journal of Applied Physics*, **2013**, 114, 143501	2.5	8
51	Optimized electrocaloric effect by field reversal: Analytical model. *Applied Physics Letters*, **2016**, 109, 202906	3.4	8
50	Anisotropic solidquid interface kinetics in silicon: an atomistically informed phase-field model. *Modelling and Simulation in Materials Science and Engineering*, **2017**, 25, 065015	2	7
49	New insights on the nature of impurity levels in V-doped In2S3: why is it impossible to obtain a metallic intermediate band?. *Journal of Materials Chemistry A*, **2019**, 7, 7745-7751	13	7
48	Dopants and dopantvacancy complexes in tetragonal lead titanate: A systematic first principles study. *Computational Materials Science*, **2015**, 103, 224-230	3.2	7
47	Defect thermodynamics and interfacial instability of crystalline Li4P2S6. *Solid State Ionics*, **2018**, 319, 53-60	3.3	7
46	Phase transformations in the relaxor Na1/2Bi1/2TiO3 studied by means of density functional theory calculations. *Journal of the American Ceramic Society*, **2018**, 101, 472-482	3.8	7

45	Relaxation of dynamically disordered tetragonal platelets in the relaxor ferroelectric 0.964Na1/2Bi1/2TiO3□.036BaTiO3. *Physical Review B*, **2017**, 96,	3.3	7
44	Phase equilibria and ordering in solid Pt□Rh calculated by means of a refined bond-order simulation mixing model. *Acta Materialia*, **2009**, 57, 4140-4147	8.4	7
43	On the origin of inhomogeneous stress and strain distributions in single-crystalline metallic nanoparticles. *International Journal of Materials Research*, **2011**, 102, 1-5	0.5	7
42	Dynamic charge-transfer bond-order potential for gallium nitride. *Philosophical Magazine*, **2009**, 89, 3477-3497	1.8	7
41	Low energy cluster deposition of nanoalloys. *Journal of Applied Physics*, **2009**, 106, 063516	2.5	7
40	Molecular-dynamics study of the density scaling of inert gas condensation. *Journal of Chemical Physics*, **2005**, 123, 154314	3.9	7
39	Tailoring the Electrocaloric Effect by Internal Bias Fields and Field Protocols. *Physical Review Applied*, **2018**, 10,	4.3	7
38	Breakdown of Varvenne scaling in (AuNiPdPt)1□Cu high-entropy alloys. *Scripta Materialia*, **2020**, 181, 15-18	5.6	6
37	Si- and Sn-containing SiOCN-based nanocomposites as anode materials for lithium ion batteries: synthesis, thermodynamic characterization and modeling. *International Journal of Materials Research*, **2017**, 108, 920-932	0.5	6
36	Atomic and electronic structure of perfect dislocations in the solar absorber materials CuInSe2 and CuGaSe2 studied by first-principles calculations. *Physical Review B*, **2017**, 95,	3.3	5
35	Radiation stability of nanocrystalline single-phase multicomponent alloys. *Journal of Materials Research*, **2019**, 34, 854-866	2.5	5
34	Elastostatic loading of metallic glass-crystal nanocomposites: Relationship of creep rate and interface energy. *Physical Review Materials*, **2019**, 3,	3.2	5
33	And Yet It Moves: LiNiO2, a Dynamic Jahn□Teller System. *Chemistry of Materials*, **2020**, 32, 10096-10103	9.6	5
32	The fate of aluminium in (Na,Bi)TiO3-based ionic conductors. *Journal of Materials Chemistry A*, **2020**, 8, 18188-18197	13	5
31	Role of oxygen and chlorine impurities in □h2S3: A first-principles study. *Physical Review B*, **2018**, 98,	3.3	5
30	Modelling of dislocation-solute interaction in ODS steels: Analytic bond-order potential for the iron-yttrium system. *Journal of Nuclear Materials*, **2018**, 509, 102-113	3.3	4
29	Structure, Electronic Structure and Defect Formation Energies of LixCo1-yNiyO2 as a Function of x (0. *Zeitschrift Fur Physikalische Chemie*, **2009**, 223, 1327-1340	3.1	4
28	Influence of elastic strain on the thermodynamics and kinetics of lithium vacancy in bulk LiCoO2. *Physical Review Materials*, **2018**, 2,	3.2	4

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