Fumiyasu Oba

List of Publications by Year
in descending order

187	14,430	36203 51	19690 117
papers	citations	h-index	g-index

192	192	192	14803
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles calculations of the ferroelastic transition between rutile-type and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaCl</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>-type <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> at high pressures. Physical Review B, 2008, 78, .	1.1	4,498
2	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. Physical Review B, 2008, 77, .	1.1	655
3	Band structure diagram paths based on crystallography. Computational Materials Science, 2017, 128, 140-184.	1.4	457
4	Energetics of native defects in ZnO. Journal of Applied Physics, 2001, 90, 824-828.	1.1	360
5	Electrostatics-based finite-size corrections for first-principles point defect calculations. Physical Review B, 2014, 89, .	1.1	320
6	Effect of MnO₂ Crystal Structure on Aerobic Oxidation of 5-Hydroxymethylfurfural to 2,5-Furandicarboxylic Acid. Journal of the American Chemical Society, 2019, 141, 890-900.	6.6	299
7	Point defects in ZnO: an approach from first principles. Science and Technology of Advanced Materials, 2011, 12, 034302.	2.8	279
8	First-principles calculations of native defects in tin monoxide. Physical Review B, 2006, 74, .	1.1	276
9	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. Physical Review B, 2014, 90, .	1.1	271
10	Structures and energetics of Ga₂O₃polymorphs. Journal of Physics Condensed Matter, 2007, 19, 346211.	0.7	253
11	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. Physical Review B, 2006, 73, .	1.1	218
12	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. Physical Review B, 2008, 78, .	1.1	210
13	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. Nature Communications, 2016, 7, 11962.	5.8	208
14	Lattice dynamics of the tin sulphides SnS₂, SnS and Sn₂S₃: vibrational spectra and thermal transport. Physical Chemistry Chemical Physics, 2017, 19, 12452-12465.	1.3	187
15	Ionization Potentials of Solids: The Importance of Vertex Corrections. Physical Review Letters, 2014, 112, 096401.	2.9	184
16	Carbon supersaturation due to paraequilibrium carburization: Stainless steels with greatly improved mechanical properties. Acta Materialia, 2006, 54, 1597-1606.	3.8	161
17	Intercalation and Pushâ€Out Process with Spinelâ€toâ€Rocksalt Transition on Mg Insertion into Spinel Oxides in Magnesium Batteries. Advanced Science, 2015, 2, 1500072.	5.6	153
18	Structure and Stability of a Homologous Series of Tin Oxides. Physical Review Letters, 2008, 100, 045702.	2.9	146

#	Article	IF	Citations
19	Electronic Structure and Defect Physics of Tin Sulfides: SnS,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Sn</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>, Sn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" mathvariant="normal">S</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>Sn</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi></mml:msub></mml:mrow></mml:math>. Physical Review Applied, 2016,	1.3	138
20	Shape Control in Epitaxial Electrodeposition:â€‰ Cu2O Nanocubes on InP(001). Chemistry of Materials, 2003, 15, 4882-4885.	3.2	115
21	Role of Ti Antisitelike Defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 103, 185502.	2.9	109
22	Design and exploration of semiconductors from first principles: A review of recent advances. Applied Physics Express, 2018, 11, 060101.	1.1	109
23	Antiferromagnetic superexchange via<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>states of titanium in EuTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>as seen from hybrid Hartree-Fock density functional calculations. Physical Review B, 2011, 83, .	1.1	104
24	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. Materials Transactions, 2002, 43, 1426-1429.	0.4	101
25	Core-hole effects on theoretical electron-energy-loss near-edge structure and near-edge x-ray absorption fine structure of MgO. Physical Review B, 2000, 61, 2180-2187.	1.1	98
26	Pressure-induced phase transition in ZnO andZnOâ^'MgOpseudobinary system: A first-principles lattice dynamics study. Physical Review B, 2005, 72, .	1.1	98
27	Room temperature ferromagnetism in Mn-doped Î³-Ga2O3 with spinel structure. Applied Physics Letters, 2006, 89, 181903.	1.5	97
28	Structure, energy and solute segregation behaviour of [110] symmetric tilt grain boundaries in yttria-stabilized cubic zirconia. Philosophical Magazine, 2004, 84, 2381-2415.	0.7	96
29	Antiâ€ferrodistortiveâ€Like Oxygenâ€Octahedron Rotation Induced by the Oxygen Vacancy in Cubic SrTiO₃. Advanced Materials, 2013, 25, 86-90.	11.1	94
30	Prediction of ground-state structures and order-disorder phase transitions in II-III spinel oxides: A combined cluster-expansion method and first-principles study. Physical Review B, 2006, 73, .	1.1	91
31	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. Physical Review B, 2017, 96, .	1.1	85
32	First-principles study of self-trapped holes and acceptor impurities in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> polymorphs. Physical Review Materials, 2019, 3, .	0.9	80
33	Epitaxial Electrodeposition of High-Aspect-Ratio Cu2O(110) Nanostructures on InP(111). Chemistry of Materials, 2005, 17, 725-729.	3.2	74
34	Chemical and Lattice Stability of the Tin Sulfides. Journal of Physical Chemistry C, 2017, 121, 6446-6454.	1.5	73
35	Toward â€œrocking-chair typeâ€•Mgâ€“Li dual-salt batteries. Journal of Materials Chemistry A, 2015, 3, 10188-10194.	5.2	72
36	of 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><m	1.1	70

#	Article	IF	Citations
37	Atomic structures of supersaturated ZnOâ€“Al2O3 solid solutions. Journal of Applied Physics, 2008, 103, 014309.	1.1	68
38	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. Physical Review B, 2006, 74, .	1.1	67
39	Transition pathway of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>crystals under high pressures. Physical Review B, 2008, 77, .	1.1	65
40	Hardness of cubic silicon nitride. Journal of Materials Research, 2002, 17, 731-733.	1.2	64
41	Epitaxial Growth of Cuprous Oxide Electrodeposited onto Semiconductor and Metal Substrates. Journal of the American Ceramic Society, 2005, 88, 253-270.	1.9	63
42	Atomic structure of [0001]-tilt grain boundaries in ZnO:â€‚â€‰A high-resolution TEM study of fiber-textured thin films. Physical Review B, 2004, 70, .	1.1	61
43	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. Physical Review B, 2010, 81, .	1.1	61
44	Electronic and structural properties of the oxygen vacancy in BaTiO3. Applied Physics Letters, 2011, 98, .	1.5	61
45	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. Physical Review B, 2017, 95, .	1.1	59
46	Fast Diffusion of Multivalent Ions Facilitated by Concerted Interactions in Dualâ€Ion Battery Systems. Advanced Energy Materials, 2018, 8, 1801475.	10.2	59
47	Zinc-based spinel cathode materials for magnesium rechargeable batteries: toward the reversible spinelâ€“rocksalt transition. Journal of Materials Chemistry A, 2019, 7, 12225-12235.	5.2	59
48	First-principles study of native defects and lanthanum impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>NaTaO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 78, .	1.1	58
49	Native point defects and carbon clusters in 4H-SiC: A hybrid functional study. Journal of Applied Physics, 2019, 125, .	1.1	55
50	Crystal and Electronic Structure and Magnetic Properties of Divalent Europium Perovskite Oxides EuMO₃ (M = Ti, Zr, and Hf): Experimental and First-Principles Approaches. Inorganic Chemistry, 2012, 51, 4560-4567.	1.9	54
51	²⁷Al NMR Chemical Shifts in Oxide Crystals: A First-Principles Study. Journal of Physical Chemistry C, 2009, 113, 3869-3873.	1.5	53
52	Ab initiostudy of symmetric tilt boundaries in ZnO. Physical Review B, 2001, 63, .	1.1	52
53	Firstâ€Principles Calculations of Anion Vacancies in Oxides and Nitrides. Journal of the American Ceramic Society, 2002, 85, 68-74.	1.9	51
54	Metastable cubic tin sulfide: A novel phonon-stable chiral semiconductor. APL Materials, 2017, 5, 036101.	2.2	51

#	Article	IF	Citations
55	Band offsets of 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>/CdS and 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>/ZnS (110) interfaces: A hybrid density functional theory study. Physical Review B, 2013, 88, .	1.1	50
56	Heterogeneously Catalyzed Aerobic Oxidation of Sulfides with a BaRuO₃ Nanoperovskite. ACS Applied Materials & Interfaces, 2018, 10, 23792-23801.	4.0	50
57	Epitaxial electrodeposition of Cu2O films onto InP(001). Applied Physics Letters, 2003, 83, 1944-1946.	1.5	49
58	Local environment of Mn dopant in ZnO by near-edge x-ray absorption fine structure analysis. Applied Physics Letters, 2005, 86, 121902.	1.5	49
59	First-principles study of point defects in chalcopyrite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnSnP</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2014, 90, .	1.1	49
60	First-principles study of cation disordering inMgAl2O4spinel with cluster expansion and Monte Carlo simulation. Physical Review B, 2006, 73, .	1.1	47
61	Native defects in oxide semiconductors: a density functional approach. Journal of Physics Condensed Matter, 2010, 22, 384211.	0.7	47
62	Microstructure of Mn-doped Î³-Ga2O3 epitaxial film on sapphire (0001) with room temperature ferromagnetism. Journal of Applied Physics, 2007, 101, 063526.	1.1	46
63	Epitaxial growth of Mn-doped Î³-Ga₂O₃ on spinel substrate. Journal of Materials Research, 2011, 26, 578-583.	1.2	46
64	Defect chemistry of a BaZrO3 Î£3 (111) grain boundary by first principles calculations and spaceâ€“charge theory. Physical Chemistry Chemical Physics, 2012, 14, 12339.	1.3	46
65	Screening procedure for structurally and electronically matched contact layers for high-performance solar cells: hybrid perovskites. Journal of Materials Chemistry C, 2016, 4, 1149-1158.	2.7	45
66	General Rule for Displacive Phase Transitions in Perovskite Compounds Revisited by First Principles Calculations. Physical Review Letters, 2005, 94, 035502.	2.9	43
67	Coexistence of Mn2+and Mn3+in ferromagnetic GaMnN. Journal of Physics Condensed Matter, 2006, 18, 4615-4621.	0.7	43
68	Atomic Structure of Luminescent Centers in High-Efficiency Ce-doped w-AlN Single Crystal. Scientific Reports, 2014, 4, 3778.	1.6	43
69	Categorization of surface polarity from a crystallographic approach. Computational Materials Science, 2016, 113, 221-230.	1.4	43
70	Grain boundary dependency of nonlinear currentâ€“voltage characteristics in Pr and Co Doped ZnO Bicrystals. Journal of Applied Physics, 2004, 95, 1258-1264.	1.1	41
71	Strong Spinâ€“Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. Advanced Functional Materials, 2013, 23, 1864-1872.	7.8	41
72	Geometry and electronic structure of [0001]/(<ovl>1</ovl><ovl>2</ovl>30) Î£ = 7 symmetric tilt boundary in ZnO. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2000, 80, 1567-1581.	0.8	40

#	Article	IF	Citations
73	Atomic structure and solute segregation of a Î£ = 3, [110]/{111} grain boundary in an yttria-stabilized cubic zirconia bicrystal. Philosophical Magazine Letters, 2002, 82, 393-400.	0.5	40
74	Functional Complex Point-Defect Structure in a Huge-Size-Mismatch System. Physical Review Letters, 2013, 110, 065504.	2.9	40
75	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP₂, CdSnP₂, and Zn_{1-x}Cd_xSnP₂Alloys. Applied Physics Express, 2013, 6, 061201.	1.1	39
76	Electron-energy-loss near edge structures of six-fold-coordinated Zn in MgO. Ultramicroscopy, 2001, 86, 363-370.	0.8	38
77	Classification of spinel structures based on first-principles cluster expansion analysis. Physical Review B, 2010, 81, .	1.1	38
78	Effects of crystal structure on Co-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:mn> absorption near-edge structure and electron-energy-loss near-edge structure of trivalent cobalt oxides. Physical Review B, 2008, 77, .	1.1	37
79	First-principles-based phase diagram of the cubic BNC ternary system. Physical Review B, 2008, 77, .	1.1	36
80	Identification of native defects around grain boundary in Pr-doped ZnO bicrystal using electron energy loss spectroscopy and first-principles calculations. Applied Physics Letters, 2004, 84, 5311-5313.	1.5	35
81	Energetics and electronic structure of native point defects in Î±-Ga₂O₃. Applied Physics Express, 2019, 12, 091001.	1.1	35
82	Electrically Benign Defect Behavior in Zinc Tin Nitride Revealed from First Principles. Physical Review Applied, 2018, 10, .	1.5	34
83	Currentâ€Voltage Characteristics across (0001) Twist Boundaries in Zinc Oxide Bicrystals. Journal of the American Ceramic Society, 2002, 85, 2142-2144.	1.9	33
84	Point Defects and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math> -Type Doping in ScN from First Principles. Physical Review Applied, 2018, 9, .	1.5	33
85	Effective Doping in Cubic Si₃N₄ and Ge₃N₄: A Firstâ€Principles Study. Journal of the American Ceramic Society, 2002, 85, 97-100.	1.9	32
86	Atomic and electronic structure of [0001]/($$ar{1}ar{2}30$$) Î£7 symmetric tilt grain boundary in ZnO bicrystal with linear current-voltage characteristic. Journal of Materials Science, 2005, 40, 3059-3066.	1.7	32
87	First-principles calculations of the phase diagrams and band gaps in CuInSe2-CuGaSe2and CuInSe2-CuAlSe2pseudobinary systems. Physical Review B, 2012, 85, .	1.1	32
88	Finite-size corrections for defect-involving vertical transitions in supercell calculations. Physical Review B, 2020, 101, .	1.1	32
89	Band alignment at surfaces and heterointerfaces of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Al</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:mrow></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:mrow></mml:math>,<mml:math. Physical Review Materials, 2019, 3, .	0.9	32
90	Arrangement of multiple structural units in a [0001]Î£49tilt grain boundary in ZnO. Physical Review B, 2005, 72, .	1.1	31

#	Article	IF	Citations
91	Ordering and segregation of aCu75Pt25(111)surface: A first-principles cluster expansion study. Physical Review B, 2007, 76, .	1.1	31
92	Highâ€Mobility pâ€Type and nâ€Type Copper Nitride Semiconductors by Direct Nitriding Synthesis and In Silico Doping Design. Advanced Materials, 2018, 30, e1801968.	11.1	30
93	Theoretical Prediction of Postâ€Spinel Phases of Silicon Nitride. Journal of the American Ceramic Society, 2002, 85, 7-10.	1.9	29
94	Grain-boundary faceting at a = 3, [110]/{112} grain boundary in a cubic zirconia bicrystal. Philosophical Magazine, 2003, 83, 2221-2246.	0.7	28
95	Carrier-Induced Band-Gap Variation and Point Defects in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Zn</mml:mi></mml:mrow><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> from First Principles. Physical Review Applied, 2017, 8, .	4.6	28
96	Machine learning models for predicting the dielectric constants of oxides based on high-throughput first-principles calculations. Physical Review Materials, 2020, 4, .	0.9	27
97	Cluster calculation of oxygenK-edge electron-energy-loss near-edge structure of NiO. Physical Review B, 1998, 58, 9693-9696.	1.1	26
98	First-Principles Calculations of Migration Energy of Lithium Ions in Halides and Chalcogenides. Journal of Physical Chemistry B, 2006, 110, 8258-8262.	1.2	26
99	Hybrid density functional study of oxygen vacancies in KTaO3and NaTaO3. Physical Review B, 2011, 83, .	1.1	26
100	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb₂O₆. Journal of Physical Chemistry C, 2016, 120, 9604-9611.	1.5	25
101	Insights into oxygen vacancies from high-throughput first-principles calculations. Physical Review Materials, 2021, 5, .	0.9	25
102	First-principles study of valence band offsets at ZnSnP2/CdS, ZnSnP2/ZnS, and related chalcopyrite/zincblende heterointerfaces. Journal of Applied Physics, 2013, 114, .	1.1	24
103	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	24
104	Energetics and electronic structure of point defects associated with oxygen excess at a tilt boundary of ZnO. Journal of Materials Research, 2000, 15, 2167-2175.	1.2	23
105	Complex Structural Behavior of BiMn₇O₁₂ Quadruple Perovskite. Inorganic Chemistry, 2017, 56, 12272-12281.	1.9	23
106	Direct Observation of Magnetization Reversal by Electric Field at Room Temperature in Co-Substituted Bismuth Ferrite Thin Film. Nano Letters, 2019, 19, 1767-1773.	4.5	23
107	Effect of Oxidation on Chemical Bonding around 3dTransition-Metal Impurities in ZnO. Japanese Journal of Applied Physics, 1999, 38, 3569-3575.	0.8	22
108	n- and p-type dopants for cubic silicon nitride. Applied Physics Letters, 2001, 78, 1577-1579.	1.5	22

#	Article	IF	Citations
109	Currentâ€“Voltage Characteristics of Cobaltâ€Doped Inversion Boundaries in Zinc Oxide Bicrystals. Journal of the American Ceramic Society, 2003, 86, 1616-1618.	1.9	22
110	Discovery of a Novel Sn(II)â€Based Oxide Î²â€SnMoO₄ for Daylightâ€Driven Photocatalysis. Advanced Science, 2017, 4, 1600246.	5.6	22
111	Theoretical exploration of mixed-anion antiperovskite semiconductors <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mn>3</mml:mn></mml: width="4pt"		

#	Article	IF	Citations
127	Stabilization of small polarons 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><mml:mi>δ</mml:mi></mml:math> by local distortions. Physical Review Materials, 2019, 3, .	0.9	16
128	Non-linear currentâ€“voltage characteristics related to native defects in SrTiO3 and ZnO bicrystals. Science and Technology of Advanced Materials, 2003, 4, 605-611.	2.8	12
129	Atomistic structure and energetics of interface between Mn-doped Î³-Ga2O3 and MgAl2O4. Journal of Materials Science, 2011, 46, 4169-4175.	1.7	12
130	Coexisting Mechanisms for the Ferroelectric Phase Transition in Li₂SrNb₂O₇. Chemistry of Materials, 2021, 33, 1257-1264.	3.2	12
131	SrZn₂N₂ as a Solar Absorber: Theoretical Defect Chemistry and Synthesis by Metal Alloy Nitridation. Chemistry of Materials, 2021, 33, 2864-2870.	3.2	12
132	Valence Band Structure of ZnO (1010) Surface by Cluster Calculation. , 1999, 4, 69-80.		11
133	Phonon scattering limited mobility in the representative cubic perovskite semiconductors <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrGeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaSnO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>, and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>	1.1	11
134	Current-Voltage Characteristics Across Small Angle Symmetric Tilt Boundaries in Nb-Doped SrTiO₃ Bicrystals. Materials Transactions, 2002, 43, 1537-1541.	0.4	10
135	Interfacial structures of Y123 and Nd123 films formed on MgO(001) substrates by liquid phase epitaxy. Journal of Materials Research, 2004, 19, 2674-2682.	1.2	10
136	Local environment of silicon in cubic boron nitride. Journal of Applied Physics, 2013, 114, 233502.	1.1	10
137	Strain-engineered Peierls instability in layered perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> from first principles. Physical Review Materials, 2018, 2, .	0.9	10
138	One-dimensionally extended oxygen vacancy states in perovskite oxides. Physical Review B, 2019, 99, .	1.1	8
139	Surface reconstruction and band alignment of nonmetallic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>	0.9	8
140	Antiferroelectricity and robust dielectric response owing to competing polar and antipolar instabilities in tetragonal tungsten bronze <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">K</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mi>R</mml:mi></mml:mrow><mml:mi>Nb</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>15</mml:mn></mml:msub></mml:math> (R :) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.9	8
141	The Role of Co Ions on the Appearance of Non-Linear I-V Characteristics of ZnO-Based Ceramics. Key Engineering Materials, 1999, 157-158, 249-256.	0.4	7
142	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. Journal of Materials Chemistry, 2010, 20, 10335.	6.7	7
143	Perovskite-Type InCoO3 with Low-Spin Co3+: Effect of Inâ€“O Covalency on Structural Stabilization in Comparison with Rare-Earth Series. Inorganic Chemistry, 2017, 56, 11113-11122.	1.9	7
144	Spin-Glass Magnetic Properties of A-Site Columnar-Ordered Quadruple Perovskites Y2MnGa(Mn4â€“xGax)O12 with 0 â‰¤ x â‰¤ 3. Inorganic Chemistry, 2019, 58, 14830-14841.	1.9	7

#	Article	IF	Citations
145	Achieving non-degenerate Zn3N2 thin films by near room temperature sputtering deposition. Applied Physics Letters, 2019, 115, .	1.5	7
146	Theoretical Prediction and Thin-Film Growth of the Defect-Tolerant Nitride Semiconductor YZn₃N₃. Chemistry of Materials, 2021, 33, 8205-8211.	3.2	7
147	Point defects in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>p</mml:mi></mml:mrow></mml:math> -type transparent conductive <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cu</mml:mi><mml:mi>M</mml:mi></mml:mrow><mm		

#	Article	IF	Citations
163	Epitaxial Growth and Characterization of Rocksalt ZnO Thin Films with Low-Level NiO Alloying. Japanese Journal of Applied Physics, 2011, 50, 075503.	0.8	3
164	Ground-state search in multicomponent magnetic systems. Physical Review B, 2012, 85, .	1.1	3
165	Ligancy-Driven Controlling of Covalency and Metallicity in a Ruthenium Two-Dimensional System. Chemistry of Materials, 2016, 28, 5784-5790.	3.2	3
166	Unraveling crystal symmetry and strain effects on electronic band structures of SiC polytypes. AIP Advances, 2020, 10, 105014.	0.6	3
167	Phase variation of ferroelectric <mml:math		

#	Article	IF	Citations
181	First Principles Calculations of Advanced Nitrides, Oxides and Alloys. Key Engineering Materials, 2008, 403, 73-76.	0.4	0
182	First Principles Thermodynamics Calculations of Atomic Scale Modifications. Materia Japan, 2009, 48, 299-302.	0.1	0
183	Prediction of Fundamental Properties of Semiconductors and Materials Exploration Using First-Principles Calculations. Materia Japan, 2017, 56, 554-559.	0.1	0
184	Atomic Structure of Tilt Grain Boundaries in ZnO. Materia Japan, 2004, 43, 985-985.	0.1	0
185	Structure Units of <I>Σ</I>9 Zirconia Grain Boundary. Materia Japan, 2006, 45, 842-842.	0.1	0
186	Complex Point Defect Structure in Cubic Boron Nitride. Materia Japan, 2016, 55, 609-609.	0.1	0
187	Grain-Boundary Atomic Structures in Zirconia Ceramics. Ceramic Engineering and Science Proceedings, 0, , 171-181.	0.1	0