Fumiyasu Oba

List of Publications by Year in Descending Order

183 papers	11,387 citations	47 h-index	104 g-index
192 ext. papers	12,931 ext. citations	4.2 avg, IF	6.58 L-index

#	Paper	IF	Citations
183	Recommendation of interstitial hydrogen positions in metal oxides. *Computational Materials Science*, **2022**, 203, 111068	3.2	0
182	Insights into oxygen vacancies from high-throughput first-principles calculations. *Physical Review Materials*, **2021**, 5,	3.2	2
181	Point defects in p-type transparent conductive CuMO2 (M=Al, Ga, In) from first principles. *Physical Review Materials*, **2021**, 5,	3.2	2
180	SrZn2N2 as a Solar Absorber: Theoretical Defect Chemistry and Synthesis by Metal Alloy Nitridation. *Chemistry of Materials*, **2021**, 33, 2864-2870	9.6	4
179	Coexisting Mechanisms for the Ferroelectric Phase Transition in Li2SrNb2O7. *Chemistry of Materials*, **2021**, 33, 1257-1264	9.6	3
178	Phonon scattering limited mobility in the representative cubic perovskite semiconductors SrGeO3, BaSnO3, and SrTiO3. *Physical Review B*, **2020**, 101,	3.3	4
177	Finite-size corrections for defect-involving vertical transitions in supercell calculations. *Physical Review B*, **2020**, 101,	3.3	16
176	Theoretical exploration of mixed-anion antiperovskite semiconductors M3XN(M=Mg,Ca,Sr,Ba;X=P,As,Sb,Bi). *Physical Review Materials*, **2020**, 4,	3.2	8
175	Surface reconstruction and band alignment of nonmetallic A(II)B(IV)O3 perovskites. *Physical Review Materials*, **2020**, 4,	3.2	5
174	Machine learning models for predicting the dielectric constants of oxides based on high-throughput first-principles calculations. *Physical Review Materials*, **2020**, 4,	3.2	6
173	Antiferroelectricity and robust dielectric response owing to competing polar and antipolar instabilities in tetragonal tungsten bronze K2RNb5O15 (R: rare-earth). *Physical Review Materials*, **2020**, 4,	3.2	2
172	Phase Transition from Weak Ferroelectricity to Incipient Ferroelectricity in Li2Sr(Nb1−xTax)2O7. *Chemistry of Materials*, **2020**, 32, 744-750	9.6	9
171	Unraveling crystal symmetry and strain effects on electronic band structures of SiC polytypes. *AIP Advances*, **2020**, 10, 105014	1.5	1
170	Data-Mining Element Charges in Inorganic Materials. *Journal of Physical Chemistry Letters*, **2020**, 11, 8264-8267	6.4	1
169	Achieving non-degenerate Zn3N2 thin films by near room temperature sputtering deposition. *Applied Physics Letters*, **2019**, 115, 092104	3.4	5
168	Theoretical prediction of strain-induced carrier effective mass modulation in 4H-SiC and GaN. *Applied Physics Letters*, **2019**, 115, 112102	3.4	7
167	Direct Observation of Magnetization Reversal by Electric Field at Room Temperature in Co-Substituted Bismuth Ferrite Thin Film. *Nano Letters*, **2019**, 19, 1767-1773	11.5	15

166	Native point defects and carbon clusters in 4H-SiC: A hybrid functional study. *Journal of Applied Physics*, **2019**, 125, 125701	2.5	27
165	Zinc-based spinel cathode materials for magnesium rechargeable batteries: toward the reversible spinel□ocksalt transition. *Journal of Materials Chemistry A*, **2019**, 7, 12225-12235	13	36
164	One-dimensionally extended oxygen vacancy states in perovskite oxides. *Physical Review B*, **2019**, 99,	3.3	4
163	Energetics and electronic structure of native point defects in □Ga2O3. *Applied Physics Express*, **2019**, 12, 091001	2.4	12
162	Spin-Glass Magnetic Properties of A-Site Columnar-Ordered Quadruple Perovskites YMnGa(MnGa)O with 0 □B. *Inorganic Chemistry*, **2019**, 58, 14830-14841	5.1	2
161	First-principles study of self-trapped holes and acceptor impurities in Ga2O3 polymorphs. *Physical Review Materials*, **2019**, 3,	3.2	50
160	Band alignment at surfaces and heterointerfaces of Al2O3, Ga2O3, In2O3, and related group-III oxide polymorphs: A first-principles study. *Physical Review Materials*, **2019**, 3,	3.2	18
159	Stabilization of small polarons in BaTiO3 by local distortions. *Physical Review Materials*, **2019**, 3,	3.2	6
158	Effect of MnO Crystal Structure on Aerobic Oxidation of 5-Hydroxymethylfurfural to 2,5-Furandicarboxylic Acid. *Journal of the American Chemical Society*, **2019**, 141, 890-900	16.4	174
157	Point Defects and p-Type Doping in ScN from First Principles. *Physical Review Applied*, **2018**, 9,	4.3	24
156	Heterogeneously Catalyzed Aerobic Oxidation of Sulfides with a BaRuO Nanoperovskite. *ACS Applied Materials & Interfaces*, **2018**, 10, 23792-23801	9.5	29
155	Fast Diffusion of Multivalent Ions Facilitated by Concerted Interactions in Dual-Ion Battery Systems. *Advanced Energy Materials*, **2018**, 8, 1801475	21.8	36
154	Design and exploration of semiconductors from first principles: A review of recent advances. *Applied Physics Express*, **2018**, 11, 060101	2.4	70
153	High-Mobility p-Type and n-Type Copper Nitride Semiconductors by Direct Nitriding Synthesis and In Silico Doping Design. *Advanced Materials*, **2018**, 30, e1801968	24	19
152	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. *Physical Review Materials*, **2018**, 2,	3.2	16
151	Strain-engineered Peierls instability in layered perovskite La3Ni2O7 from first principles. *Physical Review Materials*, **2018**, 2,	3.2	5
150	Polar metallic behavior of strained antiperovskites ACNi3(A=Mg,Zn,and Cd) from first principles. *Physical Review Materials*, **2018**, 2,	3.2	10
149	Electrically Benign Defect Behavior in Zinc Tin Nitride Revealed from First Principles. *Physical Review Applied*, **2018**, 10,	4.3	21

148	Unusual magnetic structure of the high-pressure synthesized perovskites ACrO3 (A=Sc, In, Tl). *Physical Review B*, **2017**, 95,	3.3	11
147	Chemical and Lattice Stability of the Tin Sulfides. *Journal of Physical Chemistry C*, **2017**, 121, 6446-6454	3.8	52
146	DFT investigation into the underperformance of sulfide materials in photovoltaic applications. *Journal of Materials Chemistry A*, **2017**, 5, 9132-9140	13	16
145	Lattice dynamics of the tin sulphides SnS, SnS and SnS: vibrational spectra and thermal transport. *Physical Chemistry Chemical Physics*, **2017**, 19, 12452-12465	3.6	108
144	Metastable cubic tin sulfide: A novel phonon-stable chiral semiconductor. *APL Materials*, **2017**, 5, 036101	5.7	36
143	Theory of ionization potentials of nonmetallic solids. *Physical Review B*, **2017**, 95,	3.3	15
142	Band structure diagram paths based on crystallography. *Computational Materials Science*, **2017**, 128, 140-184	3.2	247
141	Complex Structural Behavior of BiMnO Quadruple Perovskite. *Inorganic Chemistry*, **2017**, 56, 12272-12281	5.1	16
140	Prediction of Fundamental Properties of Semiconductors and Materials Exploration Using First-Principles Calculations. *Materia Japan*, **2017**, 56, 554-559	0.1	
139	Perovskite-Type InCoO with Low-Spin Co: Effect of In-O Covalency on Structural Stabilization in Comparison with Rare-Earth Series. *Inorganic Chemistry*, **2017**, 56, 11113-11122	5.1	4
138	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. *Physical Review B*, **2017**, 96,	3.3	58
137	Carrier-Induced Band-Gap Variation and Point Defects in Zn3N2 from First Principles. *Physical Review Applied*, **2017**, 8,	4.3	25
136	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. *Physical Review B*, **2017**, 95,	3.3	45
135	Discovery of a Novel Sn(II)-Based Oxide SnMoO for Daylight-Driven Photocatalysis. *Advanced Science*, **2017**, 4, 1600246	13.6	18
134	Electronic Structure and Defect Physics of Tin Sulfides: SnS, Sn2S3, and SnS2. *Physical Review Applied*, **2016**, 6,	4.3	111
133	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. *Nature Communications*, **2016**, 7, 11962	17.4	133
132	Categorization of surface polarity from a crystallographic approach. *Computational Materials Science*, **2016**, 113, 221-230	3.2	31
131	LiNbO3-Type Oxide (Tl(1-x)Sc(x))ScO3: High-Pressure Synthesis, Crystal Structure, and Electronic Properties. *Inorganic Chemistry*, **2016**, 55, 1940-5	5.1	5

130	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	7.1	38
129	Complex Point Defect Structure in Cubic Boron Nitride. *Materia Japan*, **2016**, 55, 609-609	0.1	
128	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb2O6. *Journal of Physical Chemistry C*, **2016**, 120, 9604-9611	3.8	19
127	Ligancy-Driven Controlling of Covalency and Metallicity in a Ruthenium Two-Dimensional System. *Chemistry of Materials*, **2016**, 28, 5784-5790	9.6	3
126	Toward locking-chair type Mg Li dual-salt batteries. *Journal of Materials Chemistry A*, **2015**, 3, 10188-10194	8	64
125	Intercalation and Push-Out Process with Spinel-to-Rocksalt Transition on Mg Insertion into Spinel Oxides in Magnesium Batteries. *Advanced Science*, **2015**, 2, 1500072	13.6	117
124	Epitaxial growth of tin(II) niobate with a pyrochlore structure. *Journal of Crystal Growth*, **2015**, 416, 126-129	1.8	4
123	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. *Physical Review B*, **2014**, 90,	3.3	203
122	Ionization potentials of solids: the importance of vertex corrections. *Physical Review Letters*, **2014**, 112, 096401	7.4	148
121	First-principles study of point defects in chalcopyrite ZnSnP2. *Physical Review B*, **2014**, 90,	3.3	39
120	Atomic structure of luminescent centers in high-efficiency Ce-doped w-AlN single crystal. *Scientific Reports*, **2014**, 4, 3778	4.9	34
119	Electrostatics-based finite-size corrections for first-principles point defect calculations. *Physical Review B*, **2014**, 89,	3.3	239
118	Strong Spin-Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. *Advanced Functional Materials*, **2013**, 23, 1864-1872	15.6	28
117	First-principles study of valence band offsets at ZnSnP2/CdS, ZnSnP2/ZnS, and related chalcopyrite/zincblende heterointerfaces. *Journal of Applied Physics*, **2013**, 114, 043718	2.5	18
116	Functional complex point-defect structure in a huge-size-mismatch system. *Physical Review Letters*, **2013**, 110, 065504	7.4	33
115	Anti-ferrodistortive-like oxygen-octahedron rotation induced by the oxygen vacancy in cubic SrTiO3. *Advanced Materials*, **2013**, 25, 86-90	24	76
114	Valence band offsets at zinc-blende heterointerfaces with misfit dislocations: A first-principles study. *Physical Review B*, **2013**, 88,	3.3	10
113	Band offsets of CuInSe2/CdS and CuInSe2/ZnS (110) interfaces: A hybrid density functional theory study. *Physical Review B*, **2013**, 88,	3.3	38

112	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP2, CdSnP2, and Zn1-xCdxSnP2Alloys. *Applied Physics Express*, **2013**, 6, 061201	2.4	31
111	Local environment of silicon in cubic boron nitride. *Journal of Applied Physics*, **2013**, 114, 233502	2.5	10
110	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, 4560-7	5.1	38
109	Ionization potentials of (112) and (112□) facet surfaces of CuInSe2 and CuGaSe2. *Physical Review B*, **2012**, 86,	3.3	59
108	Defect chemistry of a BaZrO3 Σ3 (111) grain boundary by first principles calculations and space-charge theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 12339-46	3.6	44
107	Ground-state search in multicomponent magnetic systems. *Physical Review B*, **2012**, 85,	3.3	3
106	First-principles calculations of the phase diagrams and band gaps in CuInSe2-CuGaSe2 and CuInSe2-CuAlSe2 pseudobinary systems. *Physical Review B*, **2012**, 85,	3.3	31
105	Site preference of cation vacancies in Mn-doped Ga2O3 with defective spinel structure. *Applied Physics Letters*, **2012**, 101, 241906	3.4	8
104	Point defects in ZnO: an approach from first principles. *Science and Technology of Advanced Materials*, **2011**, 12, 034302	7.1	234
103	Hybrid density functional study of oxygen vacancies in KTaO3 and NaTaO3. *Physical Review B*, **2011**, 83,	3.3	23
102	Atomistic structure and energetics of interface between Mn-doped □Ga2O3 and MgAl2O4. *Journal of Materials Science*, **2011**, 46, 4169-4175	4.3	9
101	Antiferromagnetic superexchange via 3d states of titanium in EuTiO3 as seen from hybrid Hartree-Fock density functional calculations. *Physical Review B*, **2011**, 83,	3.3	86
100	Electronic and structural properties of the oxygen vacancy in BaTiO3. *Applied Physics Letters*, **2011**, 98, 172901	3.4	49
99	Epitaxial Growth and Characterization of Rocksalt ZnO Thin Films with Low-Level NiO Alloying. *Japanese Journal of Applied Physics*, **2011**, 50, 075503	1.4	3
98	Epitaxial growth of Mn-doped □Ga2O3 on spinel substrate. *Journal of Materials Research*, **2011**, 26, 578-583	2.5	35
97	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. *Physical Review B*, **2010**, 81,	3.3	53
96	Phase relationships and structures of inorganic crystals by a combination of the cluster expansion method and first principles calculations. *Journal of Physics Condensed Matter*, **2010**, 22, 384207	1.8	1
95	Classification of spinel structures based on first-principles cluster expansion analysis. *Physical Review B*, **2010**, 81,	3.3	27

94	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. *Journal of Materials Chemistry*, **2010**, 20, 10335		7
93	Native defects in oxide semiconductors: a density functional approach. *Journal of Physics Condensed Matter*, **2010**, 22, 384211	1.8	41
92	Non-Fermi-Liquid Behavior on an Iron-Based Itinerant Electron Magnet Fe3Mo3N. *Journal of the Physical Society of Japan*, **2010**, 79, 043701	1.5	17
91	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. *Physical Review B*, **2009**, 80,	3.3	4
90	First-principles study of defect-induced potentials in Ca2CuO2Cl2. *Physical Review B*, **2009**, 80,	3.3	5
89	Role of Ti antisitelike defects in SrTiO3. *Physical Review Letters*, **2009**, 103, 185502	7.4	90
88	27Al NMR Chemical Shifts in Oxide Crystals: A First-Principles Study. *Journal of Physical Chemistry C*, **2009**, 113, 3869-3873	3.8	44
87	First Principles Thermodynamics Calculations of Atomic Scale Modifications. *Materia Japan*, **2009**, 48, 299-302	0.1	
86	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. *Physical Review B*, **2008**, 77,	3.3	613
85	First-principles study of native defects and lanthanum impurities in NaTaO3. *Physical Review B*, **2008**, 78,	3.3	52
84	Structure and stability of a homologous series of tin oxides. *Physical Review Letters*, **2008**, 100, 045702	7.4	129
83	First-principles calculations of the ferroelastic transition between rutile-type and CaCl2-type SiO2 at high pressures. *Physical Review B*, **2008**, 78,	3.3	3593
82	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. *Physical Review B*, **2008**, 78,	3.3	160
81	First principles calculations for modern ceramic science and engineering. *Journal of Physics Condensed Matter*, **2008**, 20, 064215	1.8	4
80	First Principles Calculations of Advanced Nitrides, Oxides and Alloys. *Key Engineering Materials*, **2008**, 403, 73-76	0.4	
79	Effects of crystal structure on Co-L2,3 x-ray absorption near-edge structure and electron-energy-loss near-edge structure of trivalent cobalt oxides. *Physical Review B*, **2008**, 77,	3.3	34
78	Transition pathway of CO2 crystals under high pressures. *Physical Review B*, **2008**, 77,	3.3	54
77	First-principles-based phase diagram of the cubic BNC ternary system. *Physical Review B*, **2008**, 77,	3.3	33

76	First Principles Calculation of CO and H2 Adsorption on Strained Pt Surface. *Materials Transactions*, **2008**, 49, 2484-2490	1.3	4
75	Atomic structures of supersaturated ZnOAl2O3 solid solutions. *Journal of Applied Physics*, **2008**, 103, 014309	2.5	64
74	First-principles investigation of R2O3(ZnO)3 (R=Al, Ga, and In) in homologous series of compounds. *Journal of Solid State Chemistry*, **2008**, 181, 137-142	3.3	10
73	Structures and energetics of Ga2O3polymorphs. *Journal of Physics Condensed Matter*, **2007**, 19, 346211	1.8	182
72	First-principles study of defect equilibria in lithium zinc nitride. *Journal of Physics Condensed Matter*, **2007**, 19, 046201	1.8	6
71	Microstructure of Mn-doped Ga2O3 epitaxial film on sapphire (0001) with room temperature ferromagnetism. *Journal of Applied Physics*, **2007**, 101, 063526	2.5	36
70	Awaking of ferromagnetism in GaMnN through control of Mn valence. *Applied Physics Letters*, **2007**, 90, 012504	3.4	14
69	Ordering and segregation of a Cu75Pt25(111) surface: A first-principles cluster expansion study. *Physical Review B*, **2007**, 76,	3.3	28
68	Atomic-Scale Processes of Grain-Boundary Faceting in a Zirconia Bicrystal. *Materials Science Forum*, **2007**, 558-559, 955-958	0.4	
67	First-principles study of cation disordering in MgAl2O4 spinel with cluster expansion and Monte Carlo simulation. *Physical Review B*, **2006**, 73,	3.3	42
66	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,	3.3	72
65	Coexistence of Mn2+and Mn3+in ferromagnetic GaMnN. *Journal of Physics Condensed Matter*, **2006**, 18, 4615-4621	1.8	39
64	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. *Physical Review B*, **2006**, 74,	3.3	65
63	First-principles calculations of native defects in tin monoxide. *Physical Review B*, **2006**, 74,	3.3	240
62	First-principles calculations of migration energy of lithium ions in halides and chalcogenides. *Journal of Physical Chemistry B*, **2006**, 110, 8258-62	3.4	22
61	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. *Physical Review B*, **2006**, 73,	3.3	181
60	Carbon supersaturation due to paraequilibrium carburization: Stainless steels with greatly improved mechanical properties. *Acta Materialia*, **2006**, 54, 1597-1606	8.4	139
59	Room temperature ferromagnetism in Mn-doped Ga2O3 with spinel structure. *Applied Physics Letters*, **2006**, 89, 181903	3.4	84

58	Structure Units of Σ9 Zirconia Grain Boundary. *Materia Japan*, **2006**, 45, 842-842	0.1	
57	Pressure-induced phase transition in ZnO and ZnO□MgO pseudobinary system: A first-principles lattice dynamics study. *Physical Review B*, **2005**, 72,	3.3	91
56	Epitaxial Electrodeposition of High-Aspect-Ratio Cu2O(110) Nanostructures on InP(111). *Chemistry of Materials*, **2005**, 17, 725-729	9.6	68
55	Structure of Oxide Interfaces Viewed at An Atomistic and Electronic Level. *Materia Japan*, **2005**, 44, 687-690	0.1	
54	Epitaxial Growth of Cuprous Oxide Electrodeposited onto Semiconductor and Metal Substrates. *Journal of the American Ceramic Society*, **2005**, 88, 253-270	3.8	57
53	Atomic and electronic structure of [0001]/((bar{1}bar{2}30)) □ symmetric tilt grain boundary in ZnO bicrystal with linear current-voltage characteristic. *Journal of Materials Science*, **2005**, 40, 3059-3066	4.3	28
52	Effect of boundary plane on the atomic structure of [0001] □7 tilt grain boundaries in ZnO. *Journal of Materials Science*, **2005**, 40, 3067-3074	4.3	12
51	Grain Boundary Dependence of Dopant Segregation and Electrical Property in ZnO. *Materia Japan*, **2005**, 44, 965-965	0.1	
50	Current-Voltage Characteristic and Grain Boundary Structure in Undoped and Pr and Co Doped ZnO Bicrystals. *Materials Science Forum*, **2005**, 475-479, 3867-3870	0.4	1
49	Identification of Mg Vacancy in MgO by Positron Lifetime Measurements and First-Principles Calculations. *Defect and Diffusion Forum*, **2005**, 242-244, 1-8	0.7	1
48	Local environment of Mn dopant in ZnO by near-edge x-ray absorption fine structure analysis. *Applied Physics Letters*, **2005**, 86, 121902	3.4	47
47	General rule for displacive phase transitions in perovskite compounds revisited by first principles calculations. *Physical Review Letters*, **2005**, 94, 035502	7.4	36
46	Arrangement of multiple structural units in a [0001] □9 tilt grain boundary in ZnO. *Physical Review B*, **2005**, 72,	3.3	26
45	Grain boundary dependency of nonlinear current□voltage characteristics in Pr and Co Doped ZnO Bicrystals. *Journal of Applied Physics*, **2004**, 95, 1258-1264	2.5	37
44	Interfacial structures of Y123 and Nd123 films formed on MgO(001) substrates by liquid phase epitaxy. *Journal of Materials Research*, **2004**, 19, 2674-2682	2.5	9
43	Theoretical Prediction of Post-Spinel Phases of Silicon Nitride. *Journal of the American Ceramic Society*, **2004**, 85, 7-10	3.8	23
42	First-Principles Calculations of Anion Vacancies in Oxides and Nitrides. *Journal of the American Ceramic Society*, **2004**, 85, 68-74	3.8	47
41	Effective Doping in Cubic Si3N4 and Ge3N4: A First-Principles Study. *Journal of the American Ceramic Society*, **2004**, 85, 97-100	3.8	31

40	Effectiveness of BaZrO3 buffer layer in SmBa2Cu3Oy epitaxial growth on MgO substrate: A first-principles study. *Journal of Applied Physics*, **2004**, 95, 2309-2318	2.5	5
39	Structure, energy and solute segregation behaviour of [110] symmetric tilt grain boundaries in yttria-stabilized cubic zirconia. *Philosophical Magazine*, **2004**, 84, 2381-2415	1.6	86
38	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	3.4	32
37	Atomic structure of [0001]-tilt grain boundaries in ZnO: A high-resolution TEM study of fiber-textured thin films. *Physical Review B*, **2004**, 70,	3.3	56
36	Atomic Structure of Tilt Grain Boundaries in ZnO. *Materia Japan*, **2004**, 43, 985-985	0.1	
35	Grain-boundary faceting at a = 3, [110]/{112} grain boundary in a cubic zirconia bicrystal. *Philosophical Magazine*, **2003**, 83, 2221-2246	1.6	26
34	Al-doped ZnO ceramics fabricated by mechanical alloying and high-pressure sintering technique. *Journal of Materials Science Letters*, **2003**, 22, 1201-1204		4
33	Non-linear current–voltage characteristics related to native defects in SrTiO3 and ZnO bicrystals. *Science and Technology of Advanced Materials*, **2003**, 4, 605-611	7.1	11
32	First principles calculations of the formation energy of Cr/Al vacancies in spinel-type MgCr2O4 and MgAl2O4. *International Journal of Quantum Chemistry*, **2003**, 91, 208-210	2.1	3
31	Current–Voltage Characteristics of Cobalt-Doped Inversion Boundaries in Zinc Oxide Bicrystals. *Journal of the American Ceramic Society*, **2003**, 86, 1616-1618	3.8	18
30	Improvement of superconducting properties of SmBa2Cu3Oy films on MgO substrate by using BaZrO3 buffer layer. *Physica C: Superconductivity and Its Applications*, **2003**, 392-396, 835-840	1.3	14
29	Epitaxial electrodeposition of Cu2O films onto InP(001). *Applied Physics Letters*, **2003**, 83, 1944-1946	3.4	43
28	Shape Control in Epitaxial Electrodeposition: Cu2O Nanocubes on InP(001). *Chemistry of Materials*, **2003**, 15, 4882-4885	9.6	105
27	Electronic states associated with bond disorder at ZnO grain boundaries. *Advances in Quantum Chemistry*, **2003**, 42, 175-186	1.4	
26	First-Principles Calculations of Silicon Nitrides and SiAlONs. *Key Engineering Materials*, **2003**, 247, 149-154	0.4	
25	Mechanism for Improvement of In-Plane Alignment of SmBa2Cu3Oy Films by BaZrO3 Buffer Layer on MgO Substrate. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2003**, 67, 295-301	0.4	5
24	Current-Voltage Characteristics across (0001) Twist Boundaries in Zinc Oxide Bicrystals. *Journal of the American Ceramic Society*, **2002**, 85, 2142-2144	3.8	31
23	Formation energy of Cr/Al vacancies in spinel MgCr2O4 and MgAl2O4 by first-principles calculations. *Physical Review B*, **2002**, 65,	3.3	19

22	Atomic structure and solute segregation of a Σ 3, [110]/{111} grain boundary in an yttria-stabilized cubic zirconia bicrystal. *Philosophical Magazine Letters*, **2002**, 82, 393-400	1	39
21	Hardness of cubic silicon nitride. *Journal of Materials Research*, **2002**, 17, 731-733	2.5	52
20	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. *Materials Transactions*, **2002**, 43, 1426-1429	1.3	91
19	First-Principles Calculations of Co Impurities and Native Defects in ZnO. *Materials Transactions*, **2002**, 43, 1439-1443	1.3	18
18	Current-Voltage Characteristics Across Small Angle Symmetric Tilt Boundaries in Nb-Doped SrTiO3 Bicrystals. *Materials Transactions*, **2002**, 43, 1537-1541	1.3	9
17	Electron-energy-loss near edge structures of six-fold-coordinated Zn in MgO. *Ultramicroscopy*, **2001**, 86, 363-70	3.1	33
16	n- and p-type dopants for cubic silicon nitride. *Applied Physics Letters*, **2001**, 78, 1577-1579	3.4	20
15	Ab initio study of symmetric tilt boundaries in ZnO. *Physical Review B*, **2001**, 63,	3.3	46
14	Energetics of native defects in ZnO. *Journal of Applied Physics*, **2001**, 90, 824-828	2.5	330
13	Atomic and Electronic Structure of Symmetric Tilt Boundaries in ZnO. *Materials Research Society Symposia Proceedings*, **2000**, 654, 121		1
12	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	2.5	19
11	Geometry and electronic structure of [0001]/(1 230) Σ 7 symmetric tilt boundary in ZnO. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **2000**, 80, 1567-1581		36
10	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	3.3	89
9	Electronic Structure and Chemical Bondings of MgCr2-xO4. *Japanese Journal of Applied Physics*, **2000**, 39, 513-516	1.4	6
8	Effect of Oxidation on Chemical Bonding around 3dTransition-Metal Impurities in ZnO. *Japanese Journal of Applied Physics*, **1999**, 38, 3569-3575	1.4	19
7	Theoretical calculation of oxygen K electron-energy-loss near-edge structures of Si-doped MgO. *Journal of Physics Condensed Matter*, **1999**, 11, 5661-5670	1.8	4
6	Valence Band Structure of ZnO (1010) Surface by Cluster Calculation **1999**, 4, 69-80		11
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