

Fumiyasu Oba

List of Publications by Year in descending order

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187
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192
all docs

192
docs citations

192
times ranked

14803
citing authors

#	ARTICLE	IF	CITATIONS
1	Recommendation of interstitial hydrogen positions in metal oxides. Computational Materials Science, 2022, 203, 111068.	1.4	2
2	Adaptive sampling methods via machine learning for materials screening. Science and Technology of Advanced Materials Methods, 2022, 2, 55-66.	0.4	2
3	Phase variation of ferroelectric $\langle mml:math$		

#	ARTICLE	IF	CITATIONS
19	Energetics and electronic structure of native point defects in Ga_2O_3 . Applied Physics Express, 2019, 12, 091001.	1.1	35
20	Spin-Glass Magnetic Properties of A-Site Columnar-Ordered Quadruple Perovskites $\text{Y}_2\text{MnGa}(\text{Mn}_{4-x}\text{Ga}_x)\text{O}_{12}$ with $0 \leq x \leq 3$. Inorganic Chemistry, 2019, 58, 14830-14841.	1.9	7
21	Achieving non-degenerate Zn_3N_2 thin films by near room temperature sputtering deposition. Applied Physics Letters, 2019, 115, .	1.5	7
22	Theoretical prediction of strain-induced carrier effective mass modulation in 4H-SiC and GaN. Applied Physics Letters, 2019, 115, .	1.5	13
23	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
24	Native point defects and carbon clusters in 4H-SiC: A hybrid functional study. Journal of Applied Physics, 2019, 125, .	1.1	55
25	Zinc-based spinel cathode materials for magnesium rechargeable batteries: toward the reversible spinel \rightarrow rocksalt transition. Journal of Materials Chemistry A, 2019, 7, 12225-12235.	5.2	59
26	One-dimensionally extended oxygen vacancy states in perovskite oxides. Physical Review B, 2019, 99, .	1.1	8
27	Effect of MnO_2 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
28	First-principles study of self-trapped holes and acceptor impurities in Ga_2O_3 . Physical Review Materials, 2019, 3, 044001.	0.9	80
29	Polymorphs of Al_2O_3 and Ga_2O_3 . Physical Review Materials, 2019, 3, 044002.	0.9	32
30	Stabilization of small polarons in BaTiO_3 by local distortions. Physical Review Materials, 2019, 3, .	0.9	13
31	Point Defects and p -Type Doping in ScN from First Principles. Physical Review Applied, 2018, 9, .	1.5	33
32	Electrically Benign Defect Behavior in Zinc Tin Nitride Revealed from First Principles. Physical Review Applied, 2018, 10, .	1.5	34
33	Heterogeneously Catalyzed Aerobic Oxidation of Sulfides with a BaRuO_3 Nanoperovskite. ACS Applied Materials & Interfaces, 2018, 10, 23792-23801.	4.0	50
34	Fast Diffusion of Multivalent Ions Facilitated by Concerted Interactions in Dual-Ion Battery Systems. Advanced Energy Materials, 2018, 8, 1801475.	10.2	59
35	Design and exploration of semiconductors from first principles: A review of recent advances. Applied Physics Express, 2018, 11, 060101.	1.1	109
36	High-Mobility n -Type and p -Type Copper Nitride Semiconductors by Direct Nitriding Synthesis and In Silico Doping Design. Advanced Materials, 2018, 30, e1801968.	11.1	30

#	ARTICLE	IF	CITATIONS
37	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. <i>Physical Review Materials</i> , 2018, 2, .	0.9	24
38	Strain-engineered Peierls instability in layered perovskite $\text{La}_{0.3}\text{Mn}_{0.7}\text{O}_3$ from first principles. <i>Physical Review Materials</i> , 2018, 2, .	0.9	10
39	Polar metallic behavior of strained antiperovskites ACNi_3 (A=Mg,Zn,and Cd) from first principles. <i>Physical Review Materials</i> , 2018, 2, .	0.9	14
40	Unusual magnetic structure of the high-pressure synthesized perovskites $\text{CrO}_{1-x}\text{Ti}_x$	0.9	11
41	Chemical and Lattice Stability of the Tin Sulfides. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6446-6454.	1.5	73
42	DFT investigation into the underperformance of sulfide materials in photovoltaic applications. <i>Journal of Materials Chemistry A</i> , 2017, 5, 9132-9140.	5.2	19
43	Lattice dynamics of the tin sulphides SnS_2 , SnS and Sn_2S_3 : vibrational spectra and thermal transport. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12452-12465.	1.3	187
44	Metastable cubic tin sulfide: A novel phonon-stable chiral semiconductor. <i>APL Materials</i> , 2017, 5, 036101.	2.2	51
45	Theory of ionization potentials of nonmetallic solids. <i>Physical Review B</i> , 2017, 95, .	1.1	18
46	Band structure diagram paths based on crystallography. <i>Computational Materials Science</i> , 2017, 128, 140-184.	1.4	457
47	Complex Structural Behavior of $\text{BiMn}_7\text{O}_{12}$ Quadruple Perovskite. <i>Inorganic Chemistry</i> , 2017, 56, 12272-12281.	1.9	23
48	Perovskite-Type InCoO_3 with Low-Spin Co^{3+} : Effect of In-O Covalency on Structural Stabilization in Comparison with Rare-Earth Series. <i>Inorganic Chemistry</i> , 2017, 56, 11113-11122.	1.9	7
49	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. <i>Physical Review B</i> , 2017, 96, .	1.1	85
50	Carrier-Induced Band-Gap Variation and Point Defects in $\text{Zn}_3\text{Mn}_2\text{N}$ from First Principles. <i>Physical Review Applied</i> , 2017, 8, .	1.1	18
51	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. <i>Physical Review B</i> , 2017, 95, .	1.1	59
52	Discovery of a Novel Sn(II)-Based Oxide SnMoO_4 for Daylight-Driven Photocatalysis. <i>Advanced Science</i> , 2017, 4, 1600246.	5.6	22
53	Prediction of Fundamental Properties of Semiconductors and Materials Exploration Using First-Principles Calculations. <i>Materia Japan</i> , 2017, 56, 554-559.	0.1	0
54	Predictions of point defect, surface, and interface properties in semiconductors using first-principles calculations. <i>AIP Conference Proceedings</i> , 2016, , .	0.3	1

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55	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb_2O_6 . Journal of Physical Chemistry C, 2016, 120, 9604-9611.	1.5	25
56	Ligancy-Driven Controlling of Covalency and Metallicity in a Ruthenium Two-Dimensional System. Chemistry of Materials, 2016, 28, 5784-5790.	3.2	3
57	Electronic Structure and Defect Physics of Tin Sulfides: SnS_x . Physical Review Applied, 2016, 7, 041101.	1.5	138
58	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. Nature Communications, 2016, 7, 11962.	5.8	208
59	Categorization of surface polarity from a crystallographic approach. Computational Materials Science, 2016, 113, 221-230.	1.4	43
60	LiNbO_3 -Type Oxide $(\text{Ti}^x\text{Sc}^y)\text{ScO}_3$: High-Pressure Synthesis, Crystal Structure, and Electronic Properties. Inorganic Chemistry, 2016, 55, 1940-1945.	1.9	6
61	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
62	Complex Point Defect Structure in Cubic Boron Nitride. Materia Japan, 2016, 55, 609-609.	0.1	0
63	Intercalation and Push-Out Process with Spinel-Rocksalt Transition on Mg Insertion into Spinel Oxides in Magnesium Batteries. Advanced Science, 2015, 2, 1500072.	5.6	153
64	Epitaxial growth of tin(II) niobate with a pyrochlore structure. Journal of Crystal Growth, 2015, 416, 126-129.	0.7	5
65	Toward rocking-chair type Mg-Li dual-salt batteries. Journal of Materials Chemistry A, 2015, 3, 10188-10194.	5.2	72
66	Electrostatics-based finite-size corrections for first-principles point defect calculations. Physical Review B, 2014, 89, .	1.1	320
67	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. Physical Review B, 2014, 90, .	1.1	271
68	Ionization Potentials of Solids: The Importance of Vertex Corrections. Physical Review Letters, 2014, 112, 096401.	2.9	184
69	First-principles study of point defects in chalcopyrite ZnSnP_2 . Physical Review B, 2014, 90, .	1.1	19
70	Atomic Structure of Luminescent Centers in High-Efficiency Ce-doped w-AlN Single Crystal. Scientific Reports, 2014, 4, 3778.	1.6	43
71	Strong Spin-Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. Advanced Functional Materials, 2013, 23, 1864-1872.	7.8	41
72	First-principles study of valence band offsets at $\text{ZnSnP}_2/\text{CdS}$, $\text{ZnSnP}_2/\text{ZnS}$, and related chalcopyrite/zincblende heterointerfaces. Journal of Applied Physics, 2013, 114, .	1.1	24

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73	Functional Complex Point-Defect Structure in a Huge-Size-Mismatch System. <i>Physical Review Letters</i> , 2013, 110, 065504.	2.9	40
74	Anti-ferrodistortive-Like Oxygen Octahedron Rotation Induced by the Oxygen Vacancy in Cubic SrTiO ₃ . <i>Advanced Materials</i> , 2013, 25, 86-90.	11.1	94
75	Valence band offsets at zinc-blende heterointerfaces with misfit dislocations: A first-principles study. <i>Physical Review B</i> , 2013, 88, .	1.1	15
76	Band offsets of CuInSe ₂ /CdS and CuInSe ₂ /ZnS (110) interfaces: A hybrid density functional theory study. <i>Physical Review B</i> , 2013, 88, .	1.1	50
77	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP ₂ , CdSnP ₂ , and Zn _{1-x} Cd _x SnP ₂ Alloys. <i>Applied Physics Express</i> , 2013, 6, 061201.	1.1	39
78	Local environment of silicon in cubic boron nitride. <i>Journal of Applied Physics</i> , 2013, 114, 233502.	1.1	10
79	Site preference of cation vacancies in Mn-doped Ga ₂ O ₃ with defective spinel structure. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	14
80	Crystal and Electronic Structure and Magnetic Properties of Divalent Europium Perovskite Oxides Eu _M O ₃ (M = Ti, Zr, and Hf): Experimental and First-Principles Approaches. <i>Inorganic Chemistry</i> , 2012, 51, 4560-4567.	1.9	54
81	of CuInSe ₂ and CuGaSe ₂	1.1	70
82	Defect chemistry of a BaZrO ₃ (111) grain boundary by first principles calculations and space-charge theory. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12339.	1.3	46
83	Ground-state search in multicomponent magnetic systems. <i>Physical Review B</i> , 2012, 85, .	1.1	3
84	First-principles calculations of the phase diagrams and band gaps in CuInSe ₂ -CuGaSe ₂ and CuInSe ₂ -CuAlSe ₂ pseudobinary systems. <i>Physical Review B</i> , 2012, 85, .	1.1	32
85	Antiferromagnetic superexchange via d _{3d} states of titanium in EuTiO ₃ as seen from hybrid Hartree-Fock density functional calculations. <i>Physical Review B</i> , 2011, 83, .	1.1	104
86	Electronic and structural properties of the oxygen vacancy in BaTiO ₃ . <i>Applied Physics Letters</i> , 2011, 98, .	1.5	61
87	Point defects in ZnO: an approach from first principles. <i>Science and Technology of Advanced Materials</i> , 2011, 12, 034302.	2.8	279
88	Hybrid density functional study of oxygen vacancies in KTaO ₃ and NaTaO ₃ . <i>Physical Review B</i> , 2011, 83, .	1.1	26
89	Atomistic structure and energetics of interface between Mn-doped $\hat{3}$ -Ga ₂ O ₃ and MgAl ₂ O ₄ . <i>Journal of Materials Science</i> , 2011, 46, 4169-4175.	1.7	12
90	Epitaxial Growth and Characterization of Rocksalt ZnO Thin Films with Low-Level NiO Alloying. <i>Japanese Journal of Applied Physics</i> , 2011, 50, 075503.	0.8	3

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91	Epitaxial growth of Mn-doped Ga_2O_3 on spinel substrate. Journal of Materials Research, 2011, 26, 578-583.	1.2	46
92	Non-Fermi-Liquid Behavior on an Iron-Based Itinerant Electron Magnet $\text{Fe}_3\text{Mo}_3\text{N}$. Journal of the Physical Society of Japan, 2010, 79, 043701.	0.7	17
93	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. Physical Review B, 2010, 81, .	1.1	61
94	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.	0.7	1
95	Classification of spinel structures based on first-principles cluster expansion analysis. Physical Review B, 2010, 81, .	1.1	38
96	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. Journal of Materials Chemistry, 2010, 20, 10335.	6.7	7
97	Native defects in oxide semiconductors: a density functional approach. Journal of Physics Condensed Matter, 2010, 22, 384211.	0.7	47
98	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. Physical Review B, 2009, 80, .	1.1	6
99	First-principles study of defect-induced potentials in Ca_2Mn_5 . Physical Review B, 2009, 80, .	1.1	5
100	Role of Ti Antisitelike Defects in SrTiO_3 . Physical Review Letters, 2009, 103, 185502.	2.9	109
101	^{27}Al NMR Chemical Shifts in Oxide Crystals: A First-Principles Study. Journal of Physical Chemistry C, 2009, 113, 3869-3873.	1.5	53
102	First Principles Thermodynamics Calculations of Atomic Scale Modifications. Materia Japan, 2009, 48, 299-302.	0.1	0
103	First-principles investigation of $\text{R}_2\text{O}_3(\text{ZnO})_3$ (R=Al, Ga, and In) in homologous series of compounds. Journal of Solid State Chemistry, 2008, 181, 137-142.	1.4	14
104	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. Physical Review B, 2008, 77, .	1.1	655
105	First-principles study of native defects and lanthanum impurities in NaTaO_3 . Physical Review B, 2008, 78, .	1.1	58
106	Structure and Stability of a Homologous Series of Tin Oxides. Physical Review Letters, 2008, 100, 045702.	2.9	146
107	First-principles calculations of the ferroelastic transition between rutile-type and CaCl_2 type structures in CaCl_2 and SiO_2 at high pressures. Physical Review B, 2008, 78, .	1.1	4,498
108	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. Physical Review B, 2008, 78, .	1.1	210

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109	First principles calculations for modern ceramic science and engineering. Journal of Physics Condensed Matter, 2008, 20, 064215.	0.7	4
110	First Principles Calculations of Advanced Nitrides, Oxides and Alloys. Key Engineering Materials, 2008, 403, 73-76.	0.4	0
111	Effects of crystal structure on Co- $L_{2,3}$ absorption near-edge structure and electron-energy-loss near-edge structure of trivalent cobalt oxides. Physical Review B, 2008, 77, .	1.1	37
112	Transition pathway of C_{2O} crystals under high pressures. Physical Review B, 2008, 77, .	1.1	65
113	First-principles-based phase diagram of the cubic BNC ternary system. Physical Review B, 2008, 77, .	1.1	36
114	First Principles Calculation of CO and H ₂ Adsorption on Strained Pt Surface. Materials Transactions, 2008, 49, 2484-2490.	0.4	6
115	Atomic structures of supersaturated ZnO-Al ₂ O ₃ solid solutions. Journal of Applied Physics, 2008, 103, 014309.	1.1	68
116	First-principles study of defect equilibria in lithium zinc nitride. Journal of Physics Condensed Matter, 2007, 19, 046201.	0.7	6
117	Microstructure of Mn-doped $\hat{3}$ -Ga ₂ O ₃ epitaxial film on sapphire (0001) with room temperature ferromagnetism. Journal of Applied Physics, 2007, 101, 063526.	1.1	46
118	Awaking of ferromagnetism in GaMnN through control of Mn valence. Applied Physics Letters, 2007, 90, 012504.	1.5	15
119	Ordering and segregation of aCu ₇₅ Pt ₂₅ (111)surface: A first-principles cluster expansion study. Physical Review B, 2007, 76, .	1.1	31
120	Atomic-Scale Processes of Grain-Boundary Faceting in a Zirconia Bicrystal. Materials Science Forum, 2007, 558-559, 955-958.	0.3	0
121	Structures and energetics of Ga ₂ O ₃ polymorphs. Journal of Physics Condensed Matter, 2007, 19, 346211.	0.7	253
122	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
123	Coexistence of Mn ²⁺ and Mn ³⁺ in ferromagnetic GaMnN. Journal of Physics Condensed Matter, 2006, 18, 4615-4621.	0.7	43
124	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. Physical Review B, 2006, 74, .	1.1	67
125	First-principles calculations of native defects in tin monoxide. Physical Review B, 2006, 74, .	1.1	276
126	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

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127	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	218
128	Carbon supersaturation due to paraequilibrium carburization: Stainless steels with greatly improved mechanical properties. <i>Acta Materialia</i> , 2006, 54, 1597-1606.	3.8	161
129	Room temperature ferromagnetism in Mn-doped $\hat{3}$ -Ga ₂ O ₃ with spinel structure. <i>Applied Physics Letters</i> , 2006, 89, 181903.	1.5	97
130	First-principles study of cation disordering in MgAl ₂ O ₄ spinel with cluster expansion and Monte Carlo simulation. <i>Physical Review B</i> , 2006, 73, .	1.1	47
131	Structure Units of $\langle 100 \rangle$ Zirconia Grain Boundary. <i>Materia Japan</i> , 2006, 45, 842-842.	0.1	0
132	Structure of Oxide Interfaces Viewed at An Atomistic and Electronic Level. <i>Materia Japan</i> , 2005, 44, 687-690.	0.1	0
133	Epitaxial Growth of Cuprous Oxide Electrodeposited onto Semiconductor and Metal Substrates. <i>Journal of the American Ceramic Society</i> , 2005, 88, 253-270.	1.9	63
134	Atomic and electronic structure of $[0001]_{\text{ZnO}} \parallel [11\bar{2}0]_{\text{MgO}}$ symmetric tilt grain boundary in ZnO bicrystal with linear current-voltage characteristic. <i>Journal of Materials Science</i> , 2005, 40, 3059-3066.	1.7	32
135	Effect of boundary plane on the atomic structure of $[0001]_{\text{ZnO}} \parallel [11\bar{2}0]_{\text{MgO}}$ tilt grain boundaries in ZnO. <i>Journal of Materials Science</i> , 2005, 40, 3067-3074.	1.7	13
136	Grain Boundary Dependence of Dopant Segregation and Electrical Property in ZnO. <i>Materia Japan</i> , 2005, 44, 965-965.	0.1	0
137	Current-Voltage Characteristic and Grain Boundary Structure in Undoped and Pr and Co Doped ZnO Bicrystals. <i>Materials Science Forum</i> , 2005, 475-479, 3867-3870.	0.3	1
138	Identification of Mg Vacancy in MgO by Positron Lifetime Measurements and First-Principles Calculations. <i>Defect and Diffusion Forum</i> , 2005, 242-244, 1-8.	0.4	1
139	Local environment of Mn dopant in ZnO by near-edge x-ray absorption fine structure analysis. <i>Applied Physics Letters</i> , 2005, 86, 121902.	1.5	49
140	General Rule for Displacive Phase Transitions in Perovskite Compounds Revisited by First Principles Calculations. <i>Physical Review Letters</i> , 2005, 94, 035502.	2.9	43
141	Arrangement of multiple structural units in a $[0001]_{\text{ZnO}} \parallel [11\bar{2}0]_{\text{MgO}}$ tilt grain boundary in ZnO. <i>Physical Review B</i> , 2005, 72, .	1.1	31
142	Pressure-induced phase transition in ZnO and ZnO-MgO pseudobinary system: A first-principles lattice dynamics study. <i>Physical Review B</i> , 2005, 72, .	1.1	98
143	Epitaxial Electrodeposition of High-Aspect-Ratio Cu ₂ O(110) Nanostructures on InP(111). <i>Chemistry of Materials</i> , 2005, 17, 725-729.	3.2	74
144	Grain boundary dependency of nonlinear current-voltage characteristics in Pr and Co Doped ZnO Bicrystals. <i>Journal of Applied Physics</i> , 2004, 95, 1258-1264.	1.1	41

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145	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
146	Effectiveness of BaZrO ₃ buffer layer in SmBa ₂ Cu ₃ O _y epitaxial growth on MgO substrate: A first-principles study. Journal of Applied Physics, 2004, 95, 2309-2318.	1.1	6
147	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
148	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
149	Atomic structure of [0001]-tilt grain boundaries in ZnO: a high-resolution TEM study of fiber-textured thin films. Physical Review B, 2004, 70, .	1.1	61
150	Atomic Structure of Tilt Grain Boundaries in ZnO. Materia Japan, 2004, 43, 985-985.	0.1	0
151	Al-doped ZnO ceramics fabricated by mechanical alloying and high-pressure sintering technique. Journal of Materials Science Letters, 2003, 22, 1201-1204.	0.5	4
152	Non-linear current-voltage characteristics related to native defects in SrTiO ₃ and ZnO bicrystals. Science and Technology of Advanced Materials, 2003, 4, 605-611.	2.8	12
153	First principles calculations of the formation energy of Cr/Al vacancies in spinel-type MgCr ₂ O ₄ and MgAl ₂ O ₄ . International Journal of Quantum Chemistry, 2003, 91, 208-210.	1.0	3
154	Current-Voltage Characteristics of Cobalt-Doped Inversion Boundaries in Zinc Oxide Bicrystals. Journal of the American Ceramic Society, 2003, 86, 1616-1618.	1.9	22
155	Improvement of superconducting properties of SmBa ₂ Cu ₃ O _y films on MgO substrate by using BaZrO ₃ buffer layer. Physica C: Superconductivity and Its Applications, 2003, 392-396, 835-840.	0.6	15
156	Epitaxial electrodeposition of Cu ₂ O films onto InP(001). Applied Physics Letters, 2003, 83, 1944-1946.	1.5	49
157	Shape Control in Epitaxial Electrodeposition: Cu ₂ O Nanocubes on InP(001). Chemistry of Materials, 2003, 15, 4882-4885.	3.2	115
158	Electronic states associated with bond disorder at ZnO grain boundaries. Advances in Quantum Chemistry, 2003, 42, 175-186.	0.4	0
159	First-Principles Calculations of Silicon Nitrides and SiAlONs. Key Engineering Materials, 2003, 247, 149-154.	0.4	0
160	Grain-boundary faceting at a = 3, [110]/{112} grain boundary in a cubic zirconia bicrystal. Philosophical Magazine, 2003, 83, 2221-2246.	0.7	28
161	Mechanism for Improvement of In-Plane Alignment of SmBa ₂ Cu ₃ O _y Films by BaZrO ₃ Buffer Layer on MgO Substrate. Nippon Kinzoku Gakkaihi/Journal of the Japan Institute of Metals, 2003, 67, 295-301.	0.2	6
162	Formation energy of Cr/Al vacancies in spinel MgCr ₂ O ₄ and MgAl ₂ O ₄ by first-principles calculations. Physical Review B, 2002, 65, .	1.1	21

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163	Atomic structure and solute segregation of a $\hat{\epsilon} = 3$, $[110]/\{111\}$ grain boundary in an yttria-stabilized cubic zirconia bicrystal. Philosophical Magazine Letters, 2002, 82, 393-400.	0.5	40
164	Hardness of cubic silicon nitride. Journal of Materials Research, 2002, 17, 731-733.	1.2	64
165	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. Materials Transactions, 2002, 43, 1426-1429.	0.4	101
166	First-Principles Calculations of Co Impurities and Native Defects in ZnO. Materials Transactions, 2002, 43, 1439-1443.	0.4	20
167	Current-Voltage Characteristics Across Small Angle Symmetric Tilt Boundaries in Nb-Doped SrTiO ₃ Bicrystals. Materials Transactions, 2002, 43, 1537-1541.	0.4	10
168	Current-Voltage Characteristics across (0001) Twist Boundaries in Zinc Oxide Bicrystals. Journal of the American Ceramic Society, 2002, 85, 2142-2144.	1.9	33
169	Theoretical Prediction of Post-spinel Phases of Silicon Nitride. Journal of the American Ceramic Society, 2002, 85, 7-10.	1.9	29
170	First-Principles Calculations of Anion Vacancies in Oxides and Nitrides. Journal of the American Ceramic Society, 2002, 85, 68-74.	1.9	51
171	Effective Doping in Cubic Si ₃ N ₄ and Ge ₃ N ₄ : A First-Principles Study. Journal of the American Ceramic Society, 2002, 85, 97-100.	1.9	32
172	Energetics of native defects in ZnO. Journal of Applied Physics, 2001, 90, 824-828.	1.1	360
173	Electron-energy-loss near edge structures of six-fold-coordinated Zn in MgO. Ultramicroscopy, 2001, 86, 363-370.	0.8	38
174	n- and p-type dopants for cubic silicon nitride. Applied Physics Letters, 2001, 78, 1577-1579.	1.5	22
175	Ab initio study of symmetric tilt boundaries in ZnO. Physical Review B, 2001, 63, .	1.1	52
176	Atomic and Electronic Structure of Symmetric Tilt Boundaries in ZnO. Materials Research Society Symposia Proceedings, 2000, 654, 121.	0.1	1
177	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
178	Geometry and electronic structure of $[0001]/\langle 100 \rangle$ $\hat{\epsilon} = 7$ symmetric tilt boundary in ZnO. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2000, 80, 1567-1581.	0.8	40
179	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
180	Electronic Structure and Chemical Bondings of MgCr ₂ O ₄ . Japanese Journal of Applied Physics, 2000, 39, 513-516.	0.8	6

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