

Akihide Kuwabara

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

154
papers

3,874
citations

34
h-index

56
g-index

171
ext. papers

4,526
ext. citations

5.3
avg, IF

5.35
L-index

#	Paper	IF	Citations
154	Kinetic Control of Anion Stoichiometry in Hexagonal BaTiO ₃ . <i>Inorganics</i> , 2022 , 10, 73	2.9	
153	Accelerated lithium ions diffusion at the interface between LiFePO ₄ electrode and electrolyte by surface-nitride treatment. <i>Solid State Ionics</i> , 2021 , 373, 115792	3.3	1
152	On-Chip Electrochemical Analysis Combined with Liquid-Phase Electron Microscopy of Zinc Deposition/Dissolution. <i>Journal of the Electrochemical Society</i> , 2021 , 168, 112511	3.9	1
151	Influence of Ag Clusters on the Electronic Structures of β -GaO Photocatalyst Surfaces.. <i>ACS Omega</i> , 2021 , 6, 33701-33707	3.9	
150	Dehydration of Electrochemically Protonated Oxide: SrCoO with Square Spin Tubes. <i>Journal of the American Chemical Society</i> , 2021 , 143, 17517-17525	16.4	4
149	Structural phase transitions of LaScO ₃ from first principles. <i>Materials Today Communications</i> , 2021 , 26, 102048	2.5	2
148	Anion ordering enables fast H conduction at low temperatures. <i>Science Advances</i> , 2021 , 7,	14.3	7
147	Alkali-Rich Antiperovskite MFCh (M = Li, Na; Ch = S, Se, Te): The Role of Anions in Phase Stability and Ionic Transport. <i>Journal of the American Chemical Society</i> , 2021 , 143, 10668-10675	16.4	3
146	In situ electron microscopy analysis of electrochemical Zn deposition onto an electrode. <i>Journal of Power Sources</i> , 2021 , 481, 228831	8.9	13
145	Ionic conduction mechanism in Ca-doped lanthanum oxychloride. <i>Dalton Transactions</i> , 2021 , 50, 151-156	4.3	5
144	Nanoscale Defluorination Mechanism and Solid Electrolyte Interphase of a MgF ₂ Anode in Fluoride-Shuttle Batteries. <i>ACS Applied Energy Materials</i> , 2021 , 4, 996-1003	6.1	1
143	Hydride-based antiperovskites with soft anionic sublattices as fast alkali ionic conductors. <i>Nature Communications</i> , 2021 , 12, 201	17.4	19
142	Effects of Nitrogen/Fluorine Codoping on Photocatalytic Rutile TiO ₂ Crystal Studied by First-Principles Calculations. <i>Inorganic Chemistry</i> , 2021 , 60, 2381-2389	5.1	3
141	Core/Shell Double Doping of Zn and Ca on β -Ga ₂ O ₃ Photocatalysts for Remarkable Water Splitting. <i>ACS Catalysis</i> , 2021 , 11, 1911-1919	13.1	10
140	Theoretical investigation of tetrahedral distortion of four-coordinate iron(II) centres in FePd(CN). <i>Dalton Transactions</i> , 2021 , 50, 1990-1994	4.3	
139	A computational search for wurtzite-structured ferroelectrics with low coercive voltages. <i>APL Materials</i> , 2020 , 8, 121102	5.7	5
138	Dopant arrangements in Y-doped BaZrO ₃ under processing conditions and their impact on proton conduction: a large-scale first-principles thermodynamics study. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 12674-12686	13	8

137	Flux Crystal Growth, Crystal Structure, and Optical Properties of New Germanate Garnet CeCaMgGeO. <i>Frontiers in Chemistry</i> , 2020 , 8, 91	5	
136	Direct Measurement of Electronic Band Structures at Oxide Grain Boundaries. <i>Nano Letters</i> , 2020 , 20, 2530-2536	11.5	15
135	Flux Crystal Growth, Structure, and Optical Properties of the New Germanium Oxysulfide La ₄ (GeS ₂ O ₂) ₃ . <i>Crystal Growth and Design</i> , 2020 , 20, 4054-4061	3.5	1
134	Microscopic characterization of the C _B bonds in fluorine-graphite intercalation compounds. <i>Journal of Power Sources</i> , 2020 , 445, 227320	8.9	10
133	Responsive Four-Coordinate Iron(II) Nodes in FePd(CN). <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 19254-19259	16.4	6
132	Atomic-Scale Analysis of Biphasic Boundaries in the Lithium-Ion Battery Cathode Material LiFePO ₄ . <i>ACS Applied Energy Materials</i> , 2020 , 3, 8009-8016	6.1	3
131	Oxygen Affinity: The Missing Link Enabling Prediction of Proton Conductivities in Doped Barium Zirconates. <i>Chemistry of Materials</i> , 2020 , 32, 7292-7300	9.6	8
130	In situ electron microscopic observation of electrochemical Li-intercalation into MoS ₂ . <i>Solid State Ionics</i> , 2020 , 357, 115488	3.3	2
129	Synthesis and H conductivity of a new oxyhydride BaYHO with anion-ordered rock-salt layers. <i>Chemical Communications</i> , 2020 , 56, 10373-10376	5.8	14
128	Responsive Four-Coordinate Iron(II) Nodes in FePd(CN) ₄ . <i>Angewandte Chemie</i> , 2020 , 132, 19416-19421	3.6	
127	Hidden Ladder in SrMoO ₃ /SrTiO ₃ Superlattices: Experiments and Theoretical Calculations. <i>Journal of the Physical Society of Japan</i> , 2020 , 89, 074801	1.5	
126	Oxygen loss and surface degradation during electrochemical cycling of lithium-ion battery cathode material LiMn ₂ O ₄ . <i>Journal of Materials Chemistry A</i> , 2019 , 7, 8845-8854	13	33
125	First-principles study of the ferroelectric phase of AgNbO ₃ 2019 , 137-159		
124	Application of machine learning-based selective sampling to determine BaZrO ₃ grain boundary structures. <i>Computational Materials Science</i> , 2019 , 164, 57-65	3.2	4
123	BaScHO: H Conductive Layered Oxyhydride with H Site Selectivity. <i>Inorganic Chemistry</i> , 2019 , 58, 4431-4436	3.6	15
122	Hydride Conductivity in an Anion-Ordered Fluorite Structure LnHO with an Enlarged Bottleneck. <i>Chemistry of Materials</i> , 2019 , 31, 7360-7366	9.6	28
121	Transition-Metal Distribution in Brownmillerite CaFeCoO. <i>Inorganic Chemistry</i> , 2019 , 58, 10209-10216	5.1	3
120	Equilibrium hydrogen pressures in the VH system from first principles. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 28909-28918	6.7	5

119	Selective Hydride Occupation in BaVO ₃ ·xH ₂ O (0.3 ≤ x ≤ 0.8) with Face- and Corner-Shared Octahedra. <i>Chemistry of Materials</i> , 2018 , 30, 1566-1574	9.6	20
118	Exploring a potential energy surface by machine learning for characterizing atomic transport. <i>Physical Review B</i> , 2018 , 97,	3.3	22
117	Microscopic mechanism of biphasic interface relaxation in lithium iron phosphate after delithiation. <i>Nature Communications</i> , 2018 , 9, 2863	17.4	20
116	Chemical Pressure-Induced Anion Order-Disorder Transition in LnHO Enabled by Hydride Size Flexibility. <i>Journal of the American Chemical Society</i> , 2018 , 140, 11170-11173	16.4	43
115	Polarization fluctuations in the perovskite-structured ferroelectric AgNbO ₃ . <i>Physical Review B</i> , 2018 , 97,	3.3	13
114	Negative-pressure-induced helimagnetism in ferromagnetic cubic perovskites Sr _{1-x} BaxCoO ₃ . <i>Physical Review Materials</i> , 2018 , 2,	3.2	5
113	High Rate Performance of Dual-Substituted LiFePO ₄ Based on Controlling Metastable Intermediate Phase. <i>ACS Applied Energy Materials</i> , 2018 , 1, 6736-6740	6.1	5
112	Systematic analysis of electron energy-loss near-edge structures in Li-ion battery materials. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25052-25061	3.6	7
111	Competing structural instabilities in Bi ₂ SiO ₅ . <i>Physical Review B</i> , 2018 , 98,	3.3	16
110	Density functional study of the phase stability and Raman spectra of YbO, YbSiO and YbSiO under pressure. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 16518-16527	3.6	18
109	Atomic level changes during capacity fade in highly oriented thin films of cathode material LiCoPO ₄ . <i>Journal of Materials Chemistry A</i> , 2017 , 5, 9329-9338	13	20
108	Theoretical investigation of solid solution states of Ti _{1-x} VxH ₂ . <i>Acta Materialia</i> , 2017 , 134, 274-282	8.4	2
107	Lattice dynamics and ferroelectric properties of the nitride perovskite LaWN ₃ . <i>Physical Review B</i> , 2017 , 95,	3.3	20
106	On Hydride Diffusion in Transition Metal Perovskite Oxyhydrides Investigated via Deuterium Exchange. <i>Chemistry of Materials</i> , 2017 , 29, 8187-8194	9.6	20
105	Why is sodium-intercalated graphite unstable?. <i>RSC Advances</i> , 2017 , 7, 36550-36554	3.7	129
104	Effect of oxygen vacancy segregation in Au or Pt/oxide hetero-interfaces on electronic structures. <i>RSC Advances</i> , 2017 , 7, 36034-36037	3.7	2
103	Quantitative analysis of Li distributions in battery material Li _{1-x} FePO ₄ using Fe M _{2,3} -edge and valence electron energy loss spectra. <i>Journal of Electron Microscopy</i> , 2017 , 66, 254-260		4
102	ZnTaON: Stabilized High-Temperature LiNbO ₃ -type Structure. <i>Journal of the American Chemical Society</i> , 2016 , 138, 15950-15955	16.4	22

101	Machine-learning-based selective sampling procedure for identifying the low-energy region in a potential energy surface: A case study on proton conduction in oxides. <i>Physical Review B</i> , 2016 , 93,	3.3	47
100	Isolated energy level in the band gap of Yb ₂ Si ₂ O ₇ identified by electron energy-loss spectroscopy. <i>Physical Review B</i> , 2016 , 93,	3.3	4
99	Theoretical and experimental studies of formation and migration of oxygen vacancies in BaM _x Ti _{1-x} O ₃ (M = Zr, Ge). <i>Japanese Journal of Applied Physics</i> , 2016 , 55, 10TB02	1.4	7
98	Heterovalent Pb-substitution in ferroelectric bismuth silicate Bi ₂ SiO ₅ . <i>Journal of Materials Chemistry C</i> , 2016 , 4, 3168-3174	7.1	13
97	Mechanism of polarization switching in wurtzite-structured zinc oxide thin films. <i>Applied Physics Letters</i> , 2016 , 109, 102903	3.4	16
96	The electric field induced ferroelectric phase transition of AgNbO ₃ . <i>Journal of Applied Physics</i> , 2016 , 119, 064102	2.5	24
95	First-Principles-Based Phonon Calculation and Raman Spectroscopy Measurement of RuGa ₂ and RuAl ₂ with High Thermoelectric Power Factors. <i>Materials Transactions</i> , 2016 , 57, 1050-1054	1.3	2
94	Crystalline Grain Interior Configuration Affects Lithium Migration Kinetics in Li-Rich Layered Oxide. <i>Nano Letters</i> , 2016 , 16, 2907-15	11.5	83
93	Crystal and electronic structure changes during the charge-discharge process of Na ₄ Co ₃ (PO ₄) ₂ P ₂ O ₇ . <i>Journal of Power Sources</i> , 2016 , 326, 220-225	8.9	25
92	Cation ordering in A-site-deficient Li-ion conducting perovskites La _(1-x) /3Li _x NbO ₃ . <i>Journal of Materials Chemistry A</i> , 2015 , 3, 3351-3359	13	30
91	First-Principles Based Phonon Calculation and Raman Spectroscopy Measurement of RuGa ₂ and RuAl ₂ with High Thermoelectric Power Factor. <i>Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals</i> , 2015 , 79, 591-596	0.4	
90	Domain boundaries and their influence on Li migration in solid-state electrolyte (La,Li)TiO ₃ . <i>Journal of Power Sources</i> , 2015 , 276, 203-207	8.9	53
89	An alternative description of mass transfer through thick oxide films. <i>Scripta Materialia</i> , 2015 , 100, 66-69, 6	5.6	1
88	Impact of local strain on Ti-L _{2,3} electron energy-loss near-edge structures of BaTiO ₃ : a first-principles multiplet study. <i>Microscopy (Oxford, England)</i> , 2014 , 63, 249-54	1.3	9
87	Domain boundary structures in lanthanum lithium titanates. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 843-852	13	46
86	Surface design of alloy protection against CO-poisoning from first principles. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 355006	1.8	2
85	A Density Functional Study of Oxygen Adatoms on a Step-Doubled Platinum Surface. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 23675-23681	3.8	3
84	Epitaxial Growth of LiMn ₂ O ₄ Thin Films by Chemical Solution Deposition for Multilayer Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 19540-19547	3.8	22

83	An Improved Method for Quantitatively Predicting the Electrochemical Stabilities of Organic Liquid Electrolytes Using Ab Initio Calculations. <i>Journal of the Electrochemical Society</i> , 2014 , 161, G7-G14	3.9	11
82	Systematic calculations of On (n = 1 to 6) polytypes of LiCoO ₂ . <i>Physica Status Solidi - Rapid Research Letters</i> , 2014 , 8, 545-548	2.5	3
81	Ferroelectricity in wurtzite structure simple chalcogenide. <i>Applied Physics Letters</i> , 2014 , 104, 242909	3.4	36
80	Structural Distortion and Compositional Gradients Adjacent to Epitaxial LiMn ₂ O ₄ Thin Film Interfaces. <i>Advanced Materials Interfaces</i> , 2014 , 1, 1400143	4.6	24
79	Photo-induced change of dielectric response in BaCoSiO ₄ stuffed tridymite. <i>Journal of Applied Physics</i> , 2014 , 115, 164103	2.5	13
78	A density functional study of vacancy formation in grain boundaries of undoped Alumina. <i>Acta Materialia</i> , 2014 , 69, 365-371	8.4	18
77	Defect Chemistry of Rutile TiO ₂ from First Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5919-5930	3.8	39
76	Antiphase inversion domains in lithium cobaltite thin films deposited on single-crystal sapphire substrates. <i>Acta Materialia</i> , 2013 , 61, 7671-7678	8.4	24
75	Impact of lithium-ion ordering on surface electronic states of Li(x)CoO ₂ . <i>Physical Review Letters</i> , 2013 , 111, 126104	7.4	27
74	First-Principles Study of Point Defect Formation in AgNbO ₃ . <i>Japanese Journal of Applied Physics</i> , 2013 , 52, 09KF08	1.4	15
73	Chemical Expansion and Change in Lattice Constant of Y-Doped BaZrO ₃ by Hydration/Dehydration Reaction and Final Heat-Treating Temperature. <i>Journal of the American Ceramic Society</i> , 2013 , 96, 879-884	3.8	58
72	Adsorption and Diffusion of Oxygen Atoms on a Pt(211) Stepped Surface. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 9772-9778	3.8	22
71	Lithium Atom and A-Site Vacancy Distributions in Lanthanum Lithium Titanate. <i>Chemistry of Materials</i> , 2013 , 25, 1607-1614	9.6	77
70	Accelerated Materials Design of Lithium Superionic Conductors Based on First-Principles Calculations and Machine Learning Algorithms. <i>Advanced Energy Materials</i> , 2013 , 3, 980-985	21.8	139
69	First-principles calculations of lithium-ion migration at a coherent grain boundary in a cathode material, LiCoO(2). <i>Advanced Materials</i> , 2013 , 25, 618-22	24	118
68	Ferroelectricity driven by twisting of silicate tetrahedral chains. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 8088-92	16.4	50
67	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO ₃ . <i>Japanese Journal of Applied Physics</i> , 2012 , 51, 09LE01	1.4	6
66	The influence of charge ordering on the phase stability of spinel LiNi ₂ O ₄ . <i>RSC Advances</i> , 2012 , 2, 12940	3.7	10

65	On the structural origin of the catalytic properties of inherently strained ultrasmall decahedral gold nanoparticles. <i>Nano Letters</i> , 2012 , 12, 2027-31	11.5	86
64	Theoretical and experimental analysis for site preference of rare earth elements in BaTiO ₃ . <i>Ceramics International</i> , 2012 , 38, S25-S28	5.1	17
63	Local structural arrangements around oxygen and hydrogen-related defects in proton conducting LaP3O9 investigated by first principles calculations. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 7995-8003	6.7	10
62	Defects at the (1 1 0) surface of rutile TiO ₂ from ab initio calculations. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 8110-8117	6.7	12
61	A First-Principles Study of the Ferroelectric Phase of AgNbO ₃ . <i>Japanese Journal of Applied Physics</i> , 2012 , 51, 09LE02	1.4	7
60	A High-Coincidence Twin Boundary in Lithium Battery Material LiCoO ₂ . <i>Nanoscience and Nanotechnology Letters</i> , 2012 , 4, 165-168	0.8	11
59	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO ₃ . <i>Japanese Journal of Applied Physics</i> , 2012 , 51, 09LE01	1.4	3
58	A First-Principles Study of the Ferroelectric Phase of AgNbO ₃ . <i>Japanese Journal of Applied Physics</i> , 2012 , 51, 09LE02	1.4	9
57	First-principles calculations of lattice dynamics in CdTiO ₃ and CaTiO ₃ : Phase stability and ferroelectricity. <i>Physical Review B</i> , 2011 , 84,	3.3	47
56	Computer simulation of coherent BaZrO ₃ /MgO interfaces. <i>Journal of the Ceramic Society of Japan</i> , 2011 , 119, 861-866	1	1
55	Oxygen-Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. <i>Angewandte Chemie</i> , 2011 , 123, 3109-3113	3.6	11
54	Oxygen-vacancy ordering at surfaces of lithium manganese(III,IV) oxide spinel nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 3053-7	16.4	111
53	Ab-initio multiplet calculation of oxygen vacancy effect on Ti-L _{2,3} electron energy loss near edge structures of BaTiO ₃ . <i>Applied Physics Letters</i> , 2011 , 99, 233109	3.4	7
52	Anisotropic Permittivity of Tetragonal BaTiO ₃ : A First-Principles Study. <i>Japanese Journal of Applied Physics</i> , 2011 , 50, 09NE02	1.4	16
51	First-Principles Calculations of Phase Transition in CaTiO ₃ under Negative Static Pressure. <i>Journal of the Korean Physical Society</i> , 2011 , 59, 2497-2502	0.6	5
50	Anisotropic Permittivity of Tetragonal BaTiO ₃ : A First-Principles Study. <i>Japanese Journal of Applied Physics</i> , 2011 , 50, 09NE02	1.4	5
49	Quantitative Evaluation of Electrochemical Potential Windows of Electrolytes for Electric Double-Layer Capacitors Using Ab Initio Calculations. <i>Journal of the Electrochemical Society</i> , 2010 , 157, A696	3.9	21
48	Cr diffusion in α -Al ₂ O ₃ : Secondary ion mass spectroscopy and first-principles study. <i>Physical Review B</i> , 2010 , 82,	3.3	8

47	First-Principles Calculations of Electronic Structure and Solution Energies of Mn-Doped BaTiO ₃ . <i>Japanese Journal of Applied Physics</i> , 2010 , 49, 09MC01	1.4	26
46	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. <i>Journal of Materials Chemistry</i> , 2010 , 20, 10335		7
45	Effects of Off-Stoichiometry of LiC ₆ on the Lithium Diffusion Mechanism and Diffusivity by First Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 2375-2379	3.8	84
44	A combined conductivity and DFT study of protons in PbZrO ₃ and alkaline earth zirconate perovskites. <i>Solid State Ionics</i> , 2010 , 181, 130-137	3.3	49
43	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. <i>Physical Review B</i> , 2009 , 80,	3.3	4
42	First-Principles Calculations of Rare-Earth Dopants in BaTiO ₃ . <i>Japanese Journal of Applied Physics</i> , 2009 , 48, 09KC03	1.4	18
41	Magnetic Properties of Ni Alloys for Superconducting Wire Substrates: A First-Principles Study. <i>Japanese Journal of Applied Physics</i> , 2009 , 48, 083003	1.4	3
40	Local condensation around oxygen vacancies in t-LaNbO ₄ from first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 5550-3	3.6	23
39	SYNTHESIS AND ELECTRICAL CONDUCTIVITY OF TETRA-VALENT CERIUM POLYPHOSPHATE BULKS. <i>Phosphorus Research Bulletin</i> , 2009 , 23, 20-24	0.3	7
38	Geometric ferroelectricity in rare-earth compounds RGaO ₃ and RInO ₃ . <i>Physical Review B</i> , 2009 , 79,	3.3	36
37	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. <i>Physical Review B</i> , 2008 , 78,	3.3	160
36	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. <i>Physical Review B</i> , 2008 , 78,	3.3	71
35	First Principles Calculations of Advanced Nitrides, Oxides and Alloys. <i>Key Engineering Materials</i> , 2008 , 403, 73-76	0.4	
34	First Principles Calculation of CO and H ₂ Adsorption on Strained Pt Surface. <i>Materials Transactions</i> , 2008 , 49, 2484-2490	1.3	4
33	First-principles investigation of R ₂ O ₃ (ZnO) ₃ (R=Al, Ga, and In) in homologous series of compounds. <i>Journal of Solid State Chemistry</i> , 2008 , 181, 137-142	3.3	10
32	First-principles study of vacancy formation in hydroxyapatite. <i>Physical Review B</i> , 2007 , 75,	3.3	92
31	Structures and energetics of Ga ₂ O ₃ polymorphs. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 346211	1.8	182
30	Theoretical investigation to thermal equilibrium concentration of point defect through first-principles calculation. <i>Science and Technology of Advanced Materials</i> , 2007 , 8, 519-523	7.1	14

29	First-principles study of defect equilibria in lithium zinc nitride. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 046201	1.8	6
28	Ordering and segregation of a Cu ₇₅ Pt ₂₅ (111) surface: A first-principles cluster expansion study. <i>Physical Review B</i> , 2007 , 76,	3.3	28
27	?????????????????. <i>Electrochemistry</i> , 2007 , 75, 421-425	1.2	
26	Near-infrared analysis of protein secondary structure in aqueous solutions and freeze-dried solids. <i>Journal of Pharmaceutical Sciences</i> , 2006 , 95, 781-9	3.9	49
25	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,	3.3	42
24	Prediction of ground-state structures and order-disorder phase transitions in II-III spinel oxides: A combined cluster-expansion method and first-principles study. <i>Physical Review B</i> , 2006 , 73,	3.3	72
23	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. <i>Physical Review B</i> , 2006 , 74,	3.3	65
22	First-principles calculations of migration energy of lithium ions in halides and chalcogenides. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 8258-62	3.4	22
21	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. <i>Physical Review B</i> , 2006 , 73,	3.3	181
20	Ab initio lattice dynamics and phase transformations of ZrO ₂ . <i>Physical Review B</i> , 2005 , 71,	3.3	90
19	Pressure-induced phase transition in ZnO and ZnO/MgO pseudobinary system: A first-principles lattice dynamics study. <i>Physical Review B</i> , 2005 , 72,	3.3	91
18	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. <i>Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals</i> , 2005 , 69, 835-840	0.4	
17	High temperature plastic flow and grain boundary chemistry in oxide ceramics. <i>Journal of Materials Science</i> , 2005 , 40, 3129-3135	4.3	10
16	General rule for displacive phase transitions in perovskite compounds revisited by first principles calculations. <i>Physical Review Letters</i> , 2005 , 94, 035502	7.4	36
15	Cubic and orthorhombic structures of aluminum hydride AlH ₃ predicted by a first-principles study. <i>Physical Review B</i> , 2005 , 71,	3.3	65
14	Superplastic Behavior in Small Amount of Ge-Ti Co-Doped TZP. <i>Materials Science Forum</i> , 2004 , 447-448, 365-372	0.4	1
13	Superplastic flow stress and electronic structure in yttria-stabilized tetragonal zirconia polycrystals doped with GeO ₂ and TiO ₂ . <i>Acta Materialia</i> , 2004 , 52, 5563-5569	8.4	24
12	First Principles Calculation of Defect Formation Energies in Sr- and Mg-Doped LaGaO ₃ . <i>Journal of Physical Chemistry B</i> , 2004 , 108, 9168-9172	3.4	36

11	Grain Boundary Energy and Tensile Ductility in Superplastic Cation-doped TZP. <i>Materials Transactions</i> , 2004 , 45, 2144-2149	1.3	6
10	Effects of Dislocations on the Oxygen Ionic Conduction in Yttria Stabilized Zirconia. <i>Materials Transactions</i> , 2004 , 45, 2042-2047	1.3	24
9	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. <i>Materials Transactions</i> , 2004 , 45, 2106-2111	1.3	3
8	Dislocation-enhanced ionic conductivity of yttria-stabilized zirconia. <i>Applied Physics Letters</i> , 2003 , 82, 877-879	3.4	63
7	Influence of Interaction between Neighboring Oxygen Ions on Phase Stability in Cubic Zirconia. <i>Journal of the American Ceramic Society</i> , 2002 , 85, 2557-2561	3.8	12
6	Local Bonding States of Titanium and Germanium-doped Tetragonal Zirconia Polycrystal and Their Correlation to High Temperature Ductility. <i>Materials Transactions</i> , 2002 , 43, 2468-2472	1.3	10
5	The instability and resulting phase transition of cubic zirconia. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2001 , 312, 90-98	5.3	29
4	Effect of Chemical Bonding States on the Tensile Ductility in Glass-Doped TZP. <i>Materials Science Forum</i> , 2001 , 357-359, 399-404	0.4	14
3	Structure and chemistry of grain boundaries in SiO ₂ -doped TZP. <i>Science and Technology of Advanced Materials</i> , 2001 , 2, 411-424	7.1	20
2	Ceramic Materials. Analysis of Phase Stability in Cubic Zirconia Solid Solutions by First Principle Molecular Orbital Method.. <i>Zairyo/Journal of the Society of Materials Science, Japan</i> , 2001 , 50, 619-624	0.1	
1	First-Principles Calculations of Point Defect Formation and Anion Diffusion Mechanisms in the Oxyhydride Ba ₂ ScHO ₃		2