Akihide Kuwabara

List of Publications by Year
in descending order

192	5,427	79946	103101
papers	citations	39 h-index	66 g-index

211	211	211	8357
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Appraisal of awareness and usage of digital technologies for sustainable wellbeing among construction workers in a developing economy. International Journal of Construction Management, 2024, 24, 521-529.	3.2	3
2	Interatomic potentials for cubic zirconia and yttria-stabilized zirconia optimized by genetic algorithm. Computational Materials Science, 2024, 233, 112722.	3.1	1
3	Strongly Enhanced Polarization in a Ferroelectric Crystal by Conduction-Proton Flow. Journal of the American Chemical Society, 2024, 146, 1476-1483.	14.6	2
4	Double-Layered Perovskite Oxyfluoride Cathodes with High Capacity Involving Oâ€“O Bond Formation for Fluoride-Ion Batteries. Journal of the American Chemical Society, 2024, 146, 3844-3853.	14.6	6
5	Composite anode for fluoride-ion batteries using alloy formation and phase separation in charge and discharge processes. Journal of Materials Chemistry A, 2024, 12, 8350-8358.	10.5	1
6	Correction to â€œAtomic-Scale Observations of Oxygen Release Degradation in Sulfide-Based All-Solid-State Batteries with Layered Oxide Cathodesâ€• ACS Applied Materials & Interfaces, 2023, 15, 7635-7637.	8.3	0
7	A new family of anti-perovskite oxyhydrides with tetrahedral GaO₄ polyanions. Dalton Transactions, 2023, 52, 15420-15425.	3.4	0
8	Potassium-rich antiperovskites K₃HTe and K₃FTe and their structural relation to lithium and sodium counterparts. Dalton Transactions, 2023, 52, 9026-9031.	3.4	0
9	Electropositive Metal Doping into Lanthanum Hydride for H^{â”} Conducting Solid Electrolyte Use at Room Temperature. Advanced Energy Materials, 2023, 13, .	22.2	2
10	Discovery of Unconventional Protonâ€Conducting Inorganic Solids via Defectâ€Chemistryâ€Trained, Interpretable Machine Learning. Advanced Energy Materials, 2023, 13, .	22.2	3
11	Mechanisms of point defect formation and ionic conduction in divalent cation-doped lanthanum oxybromide: first-principles and experimental study. Dalton Transactions, 2023, 52, 14822-14829.	3.4	0
12	First-Principles Calculations of Fluoride-Ion Migration in Fluorine-Ion Battery Electrolyte Material K₂BiF₅. ECS Meeting Abstracts, 2023, MA2023-02, 679-679.	0.0	0
13	Dependence of Proton Diffusivity on Dopant Concentration in Yttrium-Doped Barium Zirconate; First-Principles Study. ECS Meeting Abstracts, 2023, MA2023-02, 2229-2229.	0.0	0
14	First-Principles Calculations on Diffusion and Association Behavior of Fluoride Ions in Ba-Doped LaF₃ Solid Electrolyte. ECS Meeting Abstracts, 2023, MA2023-02, 584-584.	0.0	0
15	Oxide-ion diffusion in brownmillerite-type Ca₂AlMnO_{5+Î´} from first-principles calculations. Physical Chemistry Chemical Physics, 2022, 24, 1503-1509.	2.9	4
16	Atomic-Level Changes during Electrochemical Cycling of Oriented LiMn₂O₄ Cathodic Thin Films. ACS Applied Materials & Interfaces, 2022, 14, 6507-6517.	8.3	12
17	An extended computational approach for point-defect equilibria in semiconductor materials. Npj Computational Materials, 2022, 8, .	9.1	4
18	Design and fabrication of an electrochemical chip for liquid-phase transmission electron microscopy. Microscopy (Oxford, England), 2022, 71, 238-241.	1.4	2

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19	Kinetic Control of Anion Stoichiometry in Hexagonal BaTiO3. Inorganics, 2022, 10, 73.	2.8	0
20	Lone-Pair-Induced Intra- and Interlayer Polarizations in SillÃ©n-Aurivillius Layered Perovskite Bi₄NbO₈Br. Inorganic Chemistry, 2022, 61, 9816-9822.	4.2	10
21	Lithium Lanthanum Titanate Single Crystals: Dependence of Lithium-Ion Conductivity on Crystal Domain Orientation. Nano Letters, 2022, 22, 5516-5522.	9.5	13
22	Reliable electrochemical setup for in situ observations with an atmospheric SEM. Microscopy (Oxford, England), 2022, 71, 311-314.	1.4	2
23	Anion Redox in an Amorphous Titanium Polysulfide. ACS Applied Materials & Interfaces, 2022, 14, 33191-33199.	8.3	2
24	Na₃H(ZnH₄) Antiperovskite: A Large Octahedral Distortion with an Off-Centering Hydride Anion Coupled to Molecular Hydride. Chemistry of Materials, 2022, 34, 6815-6823.	7.1	8
25	Facilitating ab initio configurational sampling of multicomponent solids using an on-lattice neural network model and active learning. Journal of Chemical Physics, 2022, 157, .	3.1	7
26	Atomic-Scale Observations of Oxygen Release Degradation in Sulfide-Based All-Solid-State Batteries with Layered Oxide Cathodes. ACS Applied Materials & Interfaces, 2022, 14, 39459-39466.	8.3	19
27	Atomic-level characterization of the oxygen storage material YBaCo₄O_{7+Î´} synthesized at low temperature. Journal of Materials Chemistry A, 2022, 10, 23087-23094.	10.5	0
28	Atomic-Scale Strucural Analysis of Pt-Based Nanoparticles Using Scanning Transmission Electron Microscopy. ECS Meeting Abstracts, 2022, MA2022-02, 1445-1445.	0.0	0
29	In situ electron microscopy analysis of electrochemical Zn deposition onto an electrode. Journal of Power Sources, 2021, 481, 228831.	8.0	42
30	Ionic conduction mechanism in Ca-doped lanthanum oxychloride. Dalton Transactions, 2021, 50, 151-156.	3.4	9
31	Nanoscale Defluorination Mechanism and Solid Electrolyte Interphase of a MgF₂ Anode in Fluoride-Shuttle Batteries. ACS Applied Energy Materials, 2021, 4, 996-1003.	5.3	7
32	Hydride-based antiperovskites with soft anionic sublattices as fast alkali ionic conductors. Nature Communications, 2021, 12, 201.	13.2	49
33	Effects of Nitrogen/Fluorine Codoping on Photocatalytic Rutile TiO₂ Crystal Studied by First-Principles Calculations. Inorganic Chemistry, 2021, 60, 2381-2389.	4.2	10
34	Coreâ€“Shell Double Doping of Zn and Ca on Î²-Ga₂O₃ Photocatalysts for Remarkable Water Splitting. ACS Catalysis, 2021, 11, 1911-1919.	11.7	35
35	Theoretical investigation of tetrahedral distortion of four-coordinate iron(<scp>ii</scp>) centres in FePd(CN)₄. Dalton Transactions, 2021, 50, 1990-1994.	3.4	2
36	Structural phase transitions of LaScO3 from first principles. Materials Today Communications, 2021, 26, 102048.	2.0	8

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37	Defect Engineering and Anisotropic Modulation of Ionic Transport in Perovskite Solid Electrolyte LixLa(1â^'x)/3NbO3. Molecules, 2021, 26, 3559.	3.9	7
38	Anion ordering enables fast H ^{â^'} conduction at low temperatures. Science Advances, 2021, 7, .	10.9	33
39	Alkali-Rich Antiperovskite M₃FCh (M = Li, Na; Ch = S, Se, Te): The Role of Anions in Phase Stability and Ionic Transport. Journal of the American Chemical Society, 2021, 143, 10668-10675.	14.6	24
40	Dehydration of Electrochemically Protonated Oxide: SrCoO₂ with Square Spin Tubes. Journal of the American Chemical Society, 2021, 143, 17517-17525.	14.6	19
41	Accelerated lithium ions diffusion at the interface between LiFePO4 electrode and electrolyte by surface-nitride treatment. Solid State Ionics, 2021, 373, 115792.	2.9	2
42	On-Chip Electrochemical Analysis Combined with Liquid-Phase Electron Microscopy of Zinc Deposition/Dissolution. Journal of the Electrochemical Society, 2021, 168, 112511.	2.9	10
43	Influence of Ag Clusters on the Electronic Structures of Î²-Ga₂O₃ Photocatalyst Surfaces. ACS Omega, 2021, 6, 33701-33707.	3.6	1
44	Microscopic characterization of the Câ€“F bonds in fluorineâ€“graphite intercalation compounds. Journal of Power Sources, 2020, 445, 227320.	8.0	29
45	Responsive Fourâ€Coordinate Iron(II) Nodes in FePd(CN)₄. Angewandte Chemie - International Edition, 2020, 59, 19254-19259.	14.8	20
46	Atomic-Scale Analysis of Biphasic Boundaries in the Lithium-Ion Battery Cathode Material LiFePO₄. ACS Applied Energy Materials, 2020, 3, 8009-8016.	5.3	11
47	Oxygen Affinity: The Missing Link Enabling Prediction of Proton Conductivities in Doped Barium Zirconates. Chemistry of Materials, 2020, 32, 7292-7300.	7.1	27
48	In situ electron microscopic observation of electrochemical Li-intercalation into MoS2. Solid State Ionics, 2020, 357, 115488.	2.9	11
49	Synthesis and H^{â^'} conductivity of a new oxyhydride Ba₂YHO₃ with anion-ordered rock-salt layers. Chemical Communications, 2020, 56, 10373-10376.	4.2	32
50	Responsive Fourâ€Coordinate Iron(II) Nodes in FePd(CN) 4. Angewandte Chemie, 2020, 132, 19416-19421.	2.1	0
51	Hidden Ladder in SrMoO3/SrTiO3 Superlattices: Experiments and Theoretical Calculations. Journal of the Physical Society of Japan, 2020, 89, 074801.	1.6	0
52	A computational search for wurtzite-structured ferroelectrics with low coercive voltages. APL Materials, 2020, 8, .	4.8	27
53	Dopant arrangements in Y-doped BaZrO₃ under processing conditions and their impact on proton conduction: a large-scale first-principles thermodynamics study. Journal of Materials Chemistry A, 2020, 8, 12674-12686.	10.5	26
54	Optical enhancement of dielectric permittivity in reduced lanthanum aluminate. Physical Review B, 2020, 101, .	3.3	1

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55	Flux Crystal Growth, Crystal Structure, and Optical Properties of New Germanate Garnet Ce2CaMg2Ge3O12. Frontiers in Chemistry, 2020, 8, 91.	3.7	2
56	Direct Measurement of Electronic Band Structures at Oxide Grain Boundaries. Nano Letters, 2020, 20, 2530-2536.	9.5	46
57	Flux Crystal Growth, Structure, and Optical Properties of the New Germanium Oxysulfide La₄(GeS₂O₂)₃. Crystal Growth and Design, 2020, 20, 4054-4061.	3.2	5
58	Transition-Metal Distribution in Brownmillerite Ca₂FeCoO₅. Inorganic Chemistry, 2019, 58, 10209-10216.	4.2	3
59	Equilibrium hydrogen pressures in the Vâ€“H system from first principles. International Journal of Hydrogen Energy, 2019, 44, 28909-28918.	7.2	11
60	Oxygen loss and surface degradation during electrochemical cycling of lithium-ion battery cathode material LiMn₂O₄. Journal of Materials Chemistry A, 2019, 7, 8845-8854.	10.5	69
61	ANID-SEoKELM: Adaptive network intrusion detection based on selective ensemble of kernel ELMs with random features. Knowledge-Based Systems, 2019, 177, 104-116.	7.4	31
62	First-principles study of the ferroelectric phase of AgNbO3. , 2019, , 137-159.		0
63	Application of machine learning-based selective sampling to determine BaZrO3 grain boundary structures. Computational Materials Science, 2019, 164, 57-65.	3.1	4
64	Ba₂ScHO₃: H^{â€“} Conductive Layered Oxyhydride with H^{â€“} Site Selectivity. Inorganic Chemistry, 2019, 58, 4431-4436.	4.2	42
65	PALEOENVIRONMENTAL AND BIOSTRATIGRAPHIC IMPLICATIONS OF ECHINODERM OSSICLES TRAPPED WITHIN BURMESE AMBER. Palaios, 2019, 34, 652-656.	1.4	7
66	Selective Hydride Occupation in BaVO_{3â€“x}H_x (0.3 â‰¤ x â‰¤ 0.8) with Face- and Corner-Shared Octahedra. Chemistry of Materials, 2018, 30, 1566-1574.	7.1	26
67	Exploring a potential energy surface by machine learning for characterizing atomic transport. Physical Review B, 2018, 97, .	3.3	29
68	Extracellular Adenosine Stimulates Vacuolar ATPaseâ€“Dependent Proton Secretion in Medullary Intercalated Cells. Journal of the American Society of Nephrology: JASN, 2018, 29, 545-556.	0.5	22
69	High Rate Performance of Dual-Substituted LiFePO₄ Based on Controlling Metastable Intermediate Phase. ACS Applied Energy Materials, 2018, 1, 6736-6740.	5.3	9
70	Systematic analysis of electron energy-loss near-edge structures in Li-ion battery materials. Physical Chemistry Chemical Physics, 2018, 20, 25052-25061.	2.9	18
71	TAP: a targeted clinical genomics pipeline for detecting transcript variants using RNA-seq data. BMC Medical Genomics, 2018, 11, 79.	1.5	12
72	Density functional study of the phase stability and Raman spectra of Yb₂O₃, Yb₂SiO₅ and Yb₂Si₂O₇ under pressure. Physical Chemistry Chemical Physics, 2018, 20, 16518-16527.	2.9	33

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73	Microscopic mechanism of biphasic interface relaxation in lithium iron phosphate after delithiation. Nature Communications, 2018, 9, 2863.	13.2	29
74	Chemical Pressure-Induced Anion Orderâ€“Disorder Transition in LnHO Enabled by Hydride Size Flexibility. Journal of the American Chemical Society, 2018, 140, 11170-11173.	14.6	70
75	Polarization fluctuations in the perovskite-structured ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>AgNb</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 97, .	3.3	23
76	Extensive supraglottic swelling. Laryngo- Rhino- Otologie, 2018, 97, .	0.2	0
77	Atomic level changes during capacity fade in highly oriented thin films of cathode material LiCoPO₄. Journal of Materials Chemistry A, 2017, 5, 9329-9338.	10.5	30
78	Theoretical investigation of solid solution states of Ti1âˆ’V H2. Acta Materialia, 2017, 134, 274-282.	8.0	5
79	Lattice dynamics and ferroelectric properties of the nitride perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaWN</mml:mi><mml:mn>3</mml:mn></mml:msub><... Physical Review B, 2017, 95, .	3.3	45
80	On Hydride Diffusion in Transition Metal Perovskite Oxyhydrides Investigated via Deuterium Exchange. Chemistry of Materials, 2017, 29, 8187-8194.	7.1	34
81	Why is sodium-intercalated graphite unstable?. RSC Advances, 2017, 7, 36550-36554.	3.7	217
82	Quantitative analysis of Li distributions in battery material Li1-xFePO4 using Fe M2,3-edge and valence electron energy loss spectra. Journal of Electron Microscopy, 2017, 66, 254-260.	1.0	4
83	Mechanism of polarization switching in wurtzite-structured zinc oxide thin films. Applied Physics Letters, 2016, 109, .	3.2	36
84	Peculiarities of the interaction of a structure with moving ice. Doklady Physics, 2016, 61, 555-557.	0.8	2
85	The electric field induced ferroelectric phase transition of AgNbO3. Journal of Applied Physics, 2016, 119, .	2.3	32
86	Advanced Aero-Engines Technology Enablers: An Overview of the European Project E-BREAK. , 2016, , .		2
87	First-Principles-Based Phonon Calculation and Raman Spectroscopy Measurement of RuGa₂ and RuAl₂ with High Thermoelectric Power Factors. Materials Transactions, 2016, 57, 1050-1054.	1.3	3
88	Crystalline Grain Interior Configuration Affects Lithium Migration Kinetics in Li-Rich Layered Oxide. Nano Letters, 2016, 16, 2907-2915.	9.5	121
89	A computational model of the attention process in risky choice.. Decision, 2016, 3, 254-280.	0.5	17
90	Crystal and electronic structure changes during the charge-discharge process of Na4Co3(PO4)2P2O7. Journal of Power Sources, 2016, 326, 220-225.	8.0	33

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91	Structural Characterization of Pine Kraft Lignin: BioChoice Lignin vs Indulin AT. Journal of Wood Chemistry and Technology, 2016, 36, 432-446.	1.8	118
92	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. Physical Review B, 2016, 93, .	3.3	56
93	Isolated energy level in the band gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Yb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo>⁢</mml:mo><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math>identified by electron energy-loss spectroscopy. Physical Review B, 2016, 93, .	3.3	8
94	High and abrupt breakdown voltage In0.15Ga0.85As0.14Sb0.86/GaSb junctions grown by LPE. Infrared Physics and Technology, 2016, 79, 32-35.	3.0	1
95	Theoretical and experimental studies of formation and migration of oxygen vacancies in BaM_xTi_{1â”'} _xO₃ (M = Zr, Ge). Japanese Journal of Applied Physics, 2016, 55, 10TB02.	1.6	8
96	Heterovalent Pb-substitution in ferroelectric bismuth silicate Bi₂SiO₅. Journal of Materials Chemistry C, 2016, 4, 3168-3174.	5.6	15
97	Domain boundaries and their influence on Li migration in solid-state electrolyte (La,Li)TiO3. Journal of Power Sources, 2015, 276, 203-207.	8.0	76
98	An alternative description of mass transfer through thick oxide films. Scripta Materialia, 2015, 100, 66-69.	5.3	1
99	Cation ordering in A-site-deficient Li-ion conducting perovskites La_{(1â”'x)/3}Li_xNbO₃. Journal of Materials Chemistry A, 2015, 3, 3351-3359.	10.5	37
100	2nd FCCA Symposium/Annual Forum for Young Glyco-Scientists 2015. Trends in Glycoscience and Glycotechnology, 2015, 27, J63-J64.	0.0	0
101	Atomic-Level Characterization of Interfaces in LiCoO2. ECS Transactions, 2014, 58, 1-11.	0.6	1
102	An Improved Method for Quantitatively Predicting the Electrochemical Stabilities of Organic Liquid Electrolytes Using Ab Initio Calculations. Journal of the Electrochemical Society, 2014, 161, G7-G14.	2.9	16
103	Systematic calculations of On (n = 1 to 6) polytypes of LiCoO₂. Physica Status Solidi - Rapid Research Letters, 2014, 8, 545-548.	2.5	4
104	Ferroelectricity in wurtzite structure simple chalcogenide. Applied Physics Letters, 2014, 104, .	3.2	60
105	Structural Distortion and Compositional Gradients Adjacent to Epitaxial LiMn₂O₄ Thin Film Interfaces. Advanced Materials Interfaces, 2014, 1, 1400143.	4.1	30
106	Photo-induced change of dielectric response in BaCoSiO4 stuffed tridymite. Journal of Applied Physics, 2014, 115, .	2.3	22
107	A density functional study of vacancy formation in grain boundaries of undoped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si28.gif" overflow="scroll"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math>-alumina. Acta Materialia, 2014, 69, 365-371.	8.0	23
108	Impact of local strain on Ti-L_{2,3}electron energy-loss near-edge structures of BaTiO₃: a first-principles multiplet study. Microscopy (Oxford, England), 2014, 63, 249-254.	1.4	10

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109	Domain boundary structures in lanthanum lithium titanates. Journal of Materials Chemistry A, 2014, 2, 843-852.	10.5	68
110	Surface design of alloy protection against CO-poisoning from first principles. Journal of Physics Condensed Matter, 2014, 26, 355006.	1.9	2
111	A Density Functional Study of Oxygen Adatoms on a Step-Doubled Platinum Surface. Journal of Physical Chemistry C, 2014, 118, 23675-23681.	3.3	3
112	Epitaxial Growth of LiMn₂O₄Thin Films by Chemical Solution Deposition for Multilayer Lithium-Ion Batteries. Journal of Physical Chemistry C, 2014, 118, 19540-19547.	3.3	26
113	Defect Chemistry of Rutile TiO₂ from First Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 5919-5930.	3.3	46
114	First-Principles Study of Point Defect Formation in AgNbO₃. Japanese Journal of Applied Physics, 2013, 52, 09KF08.	1.6	24
115	Chemical Expansion and Change in Lattice Constant of Yâ€Doped <scp><scp>BaZrO</scp></scp>₃ by Hydration/Dehydration Reaction and Final Heatâ€Treating Temperature. Journal of the American Ceramic Society, 2013, 96, 879-884.	3.8	70
116	Adsorption and Diffusion of Oxygen Atoms on a Pt(211) Stepped Surface. Journal of Physical Chemistry C, 2013, 117, 9772-9778.	3.3	25
117	Lithium Atom and A-Site Vacancy Distributions in Lanthanum Lithium Titanate. Chemistry of Materials, 2013, 25, 1607-1614.	7.1	99
118	Accelerated Materials Design of Lithium Superionic Conductors Based on Firstâ€Principles Calculations and Machine Learning Algorithms. Advanced Energy Materials, 2013, 3, 980-985.	22.2	189
119	Firstâ€Principles Calculations of Lithiumâ€Ion Migration at a Coherent Grain Boundary in a Cathode Material, LiCoO₂. Advanced Materials, 2013, 25, 618-622.	24.3	154
120	Ferroelectricity Driven by Twisting of Silicate Tetrahedral Chains. Angewandte Chemie - International Edition, 2013, 52, 8088-8092.	14.8	64
121	A First-Principles Study of the Ferroelectric Phase of AgNbO₃. Japanese Journal of Applied Physics, 2012, 51, 09LE02.	1.6	9
122	A High-Coincidence Twin Boundary in Lithium Battery Material LiCoO₂. Nanoscience and Nanotechnology Letters, 2012, 4, 165-168.	0.4	13
123	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO$_{3}$. Japanese Journal of Applied Physics, 2012, 51, 09LE01.	1.6	6
124	The influence of charge ordering on the phase stability of spinel LiNi2O4. RSC Advances, 2012, 2, 12940.	3.7	14
125	On the Structural Origin of the Catalytic Properties of Inherently Strained Ultrasmall Decahedral Gold Nanoparticles. Nano Letters, 2012, 12, 2027-2031.	9.5	105
126	Local structural arrangements around oxygen and hydrogen-related defects in proton conducting LaP3O9 investigated by first principles calculations. International Journal of Hydrogen Energy, 2012, 37, 7995-8003.	7.2	10

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127	Defects at the (1 1 0) surface of rutile TiO2 from ab initio calculations. International Journal of Hydrogen Energy, 2012, 37, 8110-8117.	7.2	13
128	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO3. Japanese Journal of Applied Physics, 2012, 51, 09LE01.	1.6	3
129	A First-Principles Study of the Ferroelectric Phase of AgNbO₃. Japanese Journal of Applied Physics, 2012, 51, 09LE02.	1.6	9
130	First-principles calculations of lattice dynamics in CdTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and CaTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: Phase stability and ferroelectricity. Physical Review B, 2011, 84, .	3.3	60
131	Computer simulation of coherent BaZrO3/MgO interfaces. Journal of the Ceramic Society of Japan, 2011, 119, 861-866.	1.3	1
132	Young age, increased tumor proliferation and FOXM1 expression predict early metastatic relapse only for endocrine-dependent breast cancers. Breast Cancer Research and Treatment, 2011, 126, 803-810.	2.5	29
133	Oxygenâ€Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. Angewandte Chemie, 2011, 123, 3109-3113.	2.1	13
134	Oxygenâ€Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. Angewandte Chemie - International Edition, 2011, 50, 3053-3057.	14.8	129
135	Detection and manipulation of nuclear spin states in fermionic strontium. Physical Review A, 2011, 84, .	2.5	60
136	Anisotropic Permittivity of Tetragonal BaTiO₃: A First-Principles Study. Japanese Journal of Applied Physics, 2011, 50, 09NE02.	1.6	17
137	Intracortical lesions by 3T magnetic resonance imaging and correlation with cognitive impairment in multiple sclerosis. Multiple Sclerosis Journal, 2011, 17, 1122-1129.	3.3	105
138	Anisotropic Permittivity of Tetragonal BaTiO₃: A First-Principles Study. Japanese Journal of Applied Physics, 2011, 50, 09NE02.	1.6	5
139	A combined conductivity and DFT study of protons in PbZrO3 and alkaline earth zirconate perovskites. Solid State Ionics, 2010, 181, 130-137.	2.9	58
140	Quantitative Evaluation of Electrochemical Potential Windows of Electrolytes for Electric Double-Layer Capacitors Using Ab Initio Calculations. Journal of the Electrochemical Society, 2010, 157, A696.	2.9	26
141	Cr diffusion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:msub><mml:mrow><mml:mtext>-Al</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>O3: Secondary ion mass spectroscopy and first-principles study. Physical Review B, 2010, 82, .	3.3	10
142	First-Principles Calculations of Electronic Structure and Solution Energies of Mn-Doped BaTiO₃. Japanese Journal of Applied Physics, 2010, 49, 09MC01.	1.6	29
143	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. Journal of Materials Chemistry, 2010, 20, 10335.	6.7	7
144	Effects of Off-Stoichiometry of LiC₆ on the Lithium Diffusion Mechanism and Diffusivity by First Principles Calculations. Journal of Physical Chemistry C, 2010, 114, 2375-2379.	3.3	114

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145	SYNTHESIS AND ELECTRICAL CONDUCTIVITY OF TETRA-VALENT CERIUM POLYPHOSPHATE BULKS. Phosphorus Research Bulletin, 2009, 23, 20-24.	0.6	8
146	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. Physical Review B, 2009, 80, .	3.3	6
147	First-Principles Calculations of Rare-Earth Dopants in BaTiO3. Japanese Journal of Applied Physics, 2009, 48, 09KC03.	1.6	22
148	Magnetic Properties of Ni Alloys for Superconducting Wire Substrates: A First-Principles Study. Japanese Journal of Applied Physics, 2009, 48, 083003.	1.6	3
149	Local condensation around oxygen vacancies in t-LaNbO4 from first principles calculations. Physical Chemistry Chemical Physics, 2009, 11, 5550.	2.9	25
150	Geometric ferroelectricity in rare-earth compounds<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mrow><mml:mtext>GaO</mml:mtext></mml:mrow><mml:mn><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mrow><mml:mtext>InO</mml:mtext></mml:mrow><mml:mn>3 Physical Review B, 2009, 79, .	3.3	42
151	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.	3.0	14
152	Diffusing Supply Chain Innovations at Hewlett-Packard Company: Applications of Performance Technology. Performance Improvement Quarterly, 2008, 13, 6-15.	1.2	2
153	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. Physical Review B, 2008, 78, .	3.3	224
154	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. Physical Review B, 2008, 78, .	3.3	83
155	First Principles Calculations of Advanced Nitrides, Oxides and Alloys. Key Engineering Materials, 2008, 403, 73-76.	0.2	0
156	First Principles Calculation of CO and H₂ Adsorption on Strained Pt Surface. Materials Transactions, 2008, 49, 2484-2490.	1.3	6
157	Ordering and segregation of aCu75Pt25(111)surface: A first-principles cluster expansion study. Physical Review B, 2007, 76, .	3.3	31
158	First-Principles Study on Segregation and Surface Structures of Pt-Rh Alloys. ECS Transactions, 2007, 11, 749-758.	0.6	0
159	â€˜Breast Cancer on Long Islandâ€™: The Emergence of a New Object Through Mapping Practices. BioSocieties, 2007, 2, 193-218.	1.3	1
160	ç„¡æ©Ÿçµæ™¶ã,ã,ªãƒ³ä¼å°Žä½“ã®é‡åæ–™è¨ˆ. Electrochemistry, 2007, 75, 421-425.	1.4	0
161	First-principles study of vacancy formation in hydroxyapatite. Physical Review B, 2007, 75, .	3.3	124
162	Theoretical investigation to thermal equilibrium concentration of point defect through first-principles calculation. Science and Technology of Advanced Materials, 2007, 8, 519-523.	6.1	16

#	Article	IF	Citations
163	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	94
164	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. Physical Review B, 2006, 74, .	3.3	67
165	First-Principles Calculations of Migration Energy of Lithium Ions in Halides and Chalcogenides. Journal of Physical Chemistry B, 2006, 110, 8258-8262.	2.7	27
166	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. Physical Review B, 2006, 73, .	3.3	234
167	First-principles study of cation disordering inMgAl2O4spinel with cluster expansion and Monte Carlo simulation. Physical Review B, 2006, 73, .	3.3	51
168	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2005, 69, 835-840.	0.6	0
169	Cubic and orthorhombic structures of aluminum hydrideAlH3predicted by a first-principles study. Physical Review B, 2005, 71, .	3.3	67
170	Ab initiolattice dynamics and phase transformations ofZrO2. Physical Review B, 2005, 71, .	3.3	109
171	Pressure-induced phase transition in ZnO andZnOâ^'MgOpseudobinary system: A first-principles lattice dynamics study. Physical Review B, 2005, 72, .	3.3	101
172	Superplastic Behavior in Small Amount of Ge-Ti Co-Doped TZP. Materials Science Forum, 2004, 447-448, 365-372.	0.2	1
173	Superplastic flow stress and electronic structure in yttria-stabilized tetragonal zirconia polycrystals doped with GeO2 and TiO2. Acta Materialia, 2004, 52, 5563-5569.	8.0	25
174	First Principles Calculation of Defect Formation Energies in Sr- and Mg-Doped LaGaO3. Journal of Physical Chemistry B, 2004, 108, 9168-9172.	2.7	38
175	Grain Boundary Energy and Tensile Ductility in Superplastic Cation-doped TZP. Materials Transactions, 2004, 45, 2144-2149.	1.3	7
176	Effects of Dislocations on the Oxygen Ionic Conduction in Yttria Stabilized Zirconia. Materials Transactions, 2004, 45, 2042-2047.	1.3	34
177	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. Materials Transactions, 2004, 45, 2106-2111.	1.3	3
178	Dislocation-enhanced ionic conductivity of yttria-stabilized zirconia. Applied Physics Letters, 2003, 82, 877-879.	3.2	82
179	Local Bonding States of Titanium and Germanium-doped Tetragonal Zirconia Polycrystal and Their Correlation to High Temperature Ductility. Materials Transactions, 2002, 43, 2468-2472.	1.3	13
180	Influence of Interaction between Neighboring Oxygen Ions on Phase Stability in Cubic Zirconia. Journal of the American Ceramic Society, 2002, 85, 2557-2561.	3.8	13

#	Article	IF	Citations
181	Structure and chemistry of grain boundaries in SiO2-doped TZP. Science and Technology of Advanced Materials, 2001, 2, 411-424.	6.1	26
182	Effect of Chemical Bonding States on the Tensile Ductility in Glass-Doped TZP. Materials Science Forum, 2001, 357-359, 399-404.	0.2	14
183	Ceramic Materials. Analysis of Phase Stability in Cubic Zirconia Solid Solutions by First Principle Molecular Orbital Method.. Zairyo/Journal of the Society of Materials Science, Japan, 2001, 50, 619-624.	0.2	0
184	Panendoscopy as a screening procedure for simultaneous primary tumors in head and neck cancer. European Archives of Oto-Rhino-Laryngology, 1996, 253, 319-324.	1.8	23
185	Mood influences on health-related judgments: Appraisal of own health versus appraisal of unhealthy behaviours. European Journal of Social Psychology, 1993, 23, 613-625.	2.2	40
186	Dynamic Analysis of a Universal Joint With Manufacturing Tolerances. Journal of Mechanisms, Transmissions, and Automation in Design, 1986, 108, 524-532.	0.2	14
187	Defect structures and dopant solution states of Hfâ€doped Si ₃ N ₄ ceramics. International Journal of Applied Ceramic Technology, 0, , .	2.1	0
188	A novel analytical model of particle size distributions in granular materials. Engineering With Computers, 0, , .	5.8	0
189	Atomic-Scale and Nanoscale Structural Changes in LiCoO₂ Due to Irreversible Delithiation Accompanied by Oxygen Release. Chemistry of Materials, 0, , .	7.1	0
190	Experimental Visualization of F-Ion Diffusion Pathways and Geometric Frustration-Induced Positional Disorder in CaF₂â€“BaF₂ Solid Electrolytes. ACS Applied Energy Materials, 0, , .	5.3	0
191	Robustly Boosting Thermoelectric Performance of Nâ€Type PbSe via Lattice Plainification and Dynamic Doping. Small, 0, , .	11.2	0
192	Fluoride Ion Storage and Conduction Mechanism in Fluoride Ion Battery Positive Electrode, Ruddlesdenâ€“Popper-Type Layered Perovskite La_{1.2}Sr_{1.8}Mn₂O₇ Crystal. Inorganic Chemistry, 0, , .	4.2	0