Akihide Kuwabara

List of Publications by Year
in descending order

164	5,210	94381	106281
papers	citations	37 h-index	65 g-index

171	171	171	6840
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structures and energetics of Ga₂O₃polymorphs. Journal of Physics Condensed Matter, 2007, 19, 346211.	0.7	253
2	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. Physical Review B, 2006, 73, .	1.1	218
3	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. Physical Review B, 2008, 78, .	1.1	210
4	Why is sodium-intercalated graphite unstable?. RSC Advances, 2017, 7, 36550-36554.	1.7	194
5	Accelerated Materials Design of Lithium Superionic Conductors Based on Firstâ€Principles Calculations and Machine Learning Algorithms. Advanced Energy Materials, 2013, 3, 980-985.	10.2	178
6	Firstâ€Principles Calculations of Lithiumâ€Ion Migration at a Coherent Grain Boundary in a Cathode Material, LiCoO₂. Advanced Materials, 2013, 25, 618-622.	11.1	149
7	Oxygenâ€Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. Angewandte Chemie - International Edition, 2011, 50, 3053-3057.	7.2	127
8	First-principles study of vacancy formation in hydroxyapatite. Physical Review B, 2007, 75, .	1.1	119
9	Crystalline Grain Interior Configuration Affects Lithium Migration Kinetics in Li-Rich Layered Oxide. Nano Letters, 2016, 16, 2907-2915.	4.5	115
10	Ab initiolattice dynamics and phase transformations ofZrO2. Physical Review B, 2005, 71, .	1.1	109
11	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.	1.5	109
12	On the Structural Origin of the Catalytic Properties of Inherently Strained Ultrasmall Decahedral Gold Nanoparticles. Nano Letters, 2012, 12, 2027-2031.	4.5	102
13	Pressure-induced phase transition in ZnO andZnOâ^'MgOpseudobinary system: A first-principles lattice dynamics study. Physical Review B, 2005, 72, .	1.1	98
14	Lithium Atom and A-Site Vacancy Distributions in Lanthanum Lithium Titanate. Chemistry of Materials, 2013, 25, 1607-1614.	3.2	97
15	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
16	Dislocation-enhanced ionic conductivity of yttria-stabilized zirconia. Applied Physics Letters, 2003, 82, 877-879.	1.5	81
17	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. Physical Review B, 2008, 78, .	1.1	79
18	Domain boundaries and their influence on Li migration in solid-state electrolyte (La,Li)TiO3. Journal of Power Sources, 2015, 276, 203-207.	4.0	75

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19	Cubic and orthorhombic structures of aluminum hydrideAlH3predicted by a first-principles study. Physical Review B, 2005, 71, .	1.1	67
20	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. Physical Review B, 2006, 74, .	1.1	67
21	Domain boundary structures in lanthanum lithium titanates. Journal of Materials Chemistry A, 2014, 2, 843-852.	5.2	66
22	Chemical Expansion and Change in Lattice Constant of Yâ€Ðoped <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.	1.9	65
23	Chemical Pressure-Induced Anion Orderâ€“Disorder Transition in LnHO Enabled by Hydride Size Flexibility. Journal of the American Chemical Society, 2018, 140, 11170-11173.	6.6	65
24	Ferroelectricity Driven by Twisting of Silicate Tetrahedral Chains. Angewandte Chemie - International Edition, 2013, 52, 8088-8092.	7.2	62
25	Oxygen loss and surface degradation during electrochemical cycling of lithium-ion battery cathode material LiMn₂O₄. Journal of Materials Chemistry A, 2019, 7, 8845-8854.	5.2	61
26	Near-infrared analysis of protein secondary structure in aqueous solutions and freeze-dried solids. Journal of Pharmaceutical Sciences, 2006, 95, 781-789.	1.6	59
27	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, .	1.1	58
28	A combined conductivity and DFT study of protons in PbZrO3 and alkaline earth zirconate perovskites. Solid State Ionics, 2010, 181, 130-137.	1.3	57
29	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, .	1.1	55
30	Ferroelectricity in wurtzite structure simple chalcogenide. Applied Physics Letters, 2014, 104, .	1.5	52
31	Hydride Conductivity in an Anion-Ordered Fluorite Structure LnHO with an Enlarged Bottleneck. Chemistry of Materials, 2019, 31, 7360-7366.	3.2	52
32	First-principles study of cation disordering inMgAl2O4spinel with cluster expansion and Monte Carlo simulation. Physical Review B, 2006, 73, .	1.1	47
33	Hydride-based antiperovskites with soft anionic sublattices as fast alkali ionic conductors. Nature Communications, 2021, 12, 201.	5.8	46
34	Defect Chemistry of Rutile TiO₂ from First Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 5919-5930.	1.5	45
35	General Rule for Displacive Phase Transitions in Perovskite Compounds Revisited by First Principles Calculations. Physical Review Letters, 2005, 94, 035502.	2.9	43
36	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></m Physical Review B, 2017, 95, .	1.1	43

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37	Ferroelectric 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>3</mml:mn></mml:msub></mml:mrow></mml:math><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</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 79, .	1.1	42
38	Ba₂ScHO₃: H^{â€“} Conductive Layered Oxyhydride with H^{â€“} Site Selectivity. Inorganic Chemistry, 2019, 58, 4431-4436.	1.9	41
39	First Principles Calculation of Defect Formation Energies in Sr- and Mg-Doped LaGaO3. Journal of Physical Chemistry B, 2004, 108, 9168-9172.	1.2	38
40	Direct Measurement of Electronic Band Structures at Oxide Grain Boundaries. Nano Letters, 2020, 20, 2530-2536.	4.5	38
41	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.	5.2	37
42	The instability and resulting phase transition of cubic zirconia. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2001, 312, 90-98.	2.6	34
43	Effects of Dislocations on the Oxygen Ionic Conduction in Yttria Stabilized Zirconia. Materials Transactions, 2004, 45, 2042-2047.	0.4	34
44	On Hydride Diffusion in Transition Metal Perovskite Oxyhydrides Investigated via Deuterium Exchange. Chemistry of Materials, 2017, 29, 8187-8194.	3.2	33
45	In situ electron microscopy analysis of electrochemical Zn deposition onto an electrode. Journal of Power Sources, 2021, 481, 228831.	4.0	33
46	Crystal and electronic structure changes during the charge-discharge process of Na4Co3(PO4)2P2O7. Journal of Power Sources, 2016, 326, 220-225.	4.0	32
47	Anion ordering enables fast H ^{â^'} conduction at low temperatures. Science Advances, 2021, 7, .	4.7	32
48	Ordering and segregation of aCu75Pt25(111)surface: A first-principles cluster expansion study. Physical Review B, 2007, 76, .	1.1	31
49	The electric field induced ferroelectric phase transition of AgNbO3. Journal of Applied Physics, 2016, 119, .	1.1	31
50	Mechanism of polarization switching in wurtzite-structured zinc oxide thin films. Applied Physics Letters, 2016, 109, .	1.5	30
51	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.	1.3	30
52	Synthesis and H^{â^'} conductivity of a new oxyhydride Ba₂YHO₃ with anion-ordered rock-salt layers. Chemical Communications, 2020, 56, 10373-10376.	2.2	30
53	Antiphase inversion domains in lithium cobaltite thin films deposited on single-crystal sapphire substrates. Acta Materialia, 2013, 61, 7671-7678.	3.8	29
54	Impact of Lithium-Ion Ordering on Surface Electronic States of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Li</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi>CoO</mml:mi></mml:msub></mml:math>. Physical Review Letters, 2013, 111, 126104.	2.9	29

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55	Structural Distortion and Compositional Gradients Adjacent to Epitaxial LiMn₂O₄ Thin Film Interfaces. Advanced Materials Interfaces, 2014, 1, 1400143.	1.9	29
56	Exploring a potential energy surface by machine learning for characterizing atomic transport. Physical Review B, 2018, 97, .	1.1	29
57	Atomic level changes during capacity fade in highly oriented thin films of cathode material LiCoPO₄. Journal of Materials Chemistry A, 2017, 5, 9329-9338.	5.2	28
58	Coreâ€“Shell Double Doping of Zn and Ca on Î²-Ga₂O₃ Photocatalysts for Remarkable Water Splitting. ACS Catalysis, 2021, 11, 1911-1919.	5.5	28
59	First-Principles Calculations of Electronic Structure and Solution Energies of Mn-Doped BaTiO3. Japanese Journal of Applied Physics, 2010, 49, 09MC01.	0.8	27
60	Microscopic mechanism of biphasic interface relaxation in lithium iron phosphate after delithiation. Nature Communications, 2018, 9, 2863.	5.8	27
61	Microscopic characterization of the Câ€“F bonds in fluorineâ€“graphite intercalation compounds. Journal of Power Sources, 2020, 445, 227320.	4.0	27
62	Structure and chemistry of grain boundaries in SiO2-doped TZP. Science and Technology of Advanced Materials, 2001, 2, 411-424.	2.8	26
63	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
64	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.	1.3	26
65	ZnTaO₂N: Stabilized High-Temperature LiNbO₃-type Structure. Journal of the American Chemical Society, 2016, 138, 15950-15955.	6.6	26
66	Superplastic flow stress and electronic structure in yttria-stabilized tetragonal zirconia polycrystals doped with GeO2 and TiO2. Acta Materialia, 2004, 52, 5563-5569.	3.8	25
67	Epitaxial Growth of LiMn2O4 Thin Films by Chemical Solution Deposition for Multilayer Lithium-Ion Batteries. Journal of Physical Chemistry C, 2014, 118, 19540-19547.	1.5	25
68	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.	3.2	25
69	Oxygen Affinity: The Missing Link Enabling Prediction of Proton Conductivities in Doped Barium Zirconates. Chemistry of Materials, 2020, 32, 7292-7300.	3.2	25
70	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.	5.2	25
71	Local condensation around oxygen vacancies in t-LaNbO4 from first principles calculations. Physical Chemistry Chemical Physics, 2009, 11, 5550.	1.3	24
72	Adsorption and Diffusion of Oxygen Atoms on a Pt(211) Stepped Surface. Journal of Physical Chemistry C, 2013, 117, 9772-9778.	1.5	24

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73	A density functional study of vacancy formation in grain boundaries of undoped Î±-alumina. Acta Materialia, 2014, 69, 365-371.	3.8	23
74	First-Principles Calculations of Rare-Earth Dopants in BaTiO3. Japanese Journal of Applied Physics, 2009, 48, 09KC03.	0.8	22
75	First-Principles Study of Point Defect Formation in AgNbO₃. Japanese Journal of Applied Physics, 2013, 52, 09KF08.	0.8	22
76	Theoretical and experimental analysis for site preference of rare earth elements in BaTiO3. Ceramics International, 2012, 38, S25-S28.	2.3	21
77	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.	6.6	21
78	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, .	1.1	20
79	Photo-induced change of dielectric response in BaCoSiO4 stuffed tridymite. Journal of Applied Physics, 2014, 115, .	1.1	19
80	Competing structural instabilities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>1</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2018, 98, .	1.1	19
81	A computational search for wurtzite-structured ferroelectrics with low coercive voltages. APL Materials, 2020, 8, .	2.2	19
82	Systematic analysis of electron energy-loss near-edge structures in Li-ion battery materials. Physical Chemistry Chemical Physics, 2018, 20, 25052-25061.	1.3	18
83	Responsive Fourâ€Coordinate Iron(II) Nodes in FePd(CN)₄. Angewandte Chemie - International Edition, 2020, 59, 19254-19259.	7.2	18
84	Anisotropic Permittivity of Tetragonal BaTiO₃: A First-Principles Study. Japanese Journal of Applied Physics, 2011, 50, 09NE02.	0.8	17
85	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.	1.3	16
86	Heterovalent Pb-substitution in ferroelectric bismuth silicate Bi₂SiO₅. Journal of Materials Chemistry C, 2016, 4, 3168-3174.	2.7	15
87	Dehydration of Electrochemically Protonated Oxide: SrCoO₂ with Square Spin Tubes. Journal of the American Chemical Society, 2021, 143, 17517-17525.	6.6	15
88	Effect of Chemical Bonding States on the Tensile Ductility in Glass-Doped TZP. Materials Science Forum, 2001, 357-359, 399-404.	0.3	14
89	Theoretical investigation to thermal equilibrium concentration of point defect through first-principles calculation. Science and Technology of Advanced Materials, 2007, 8, 519-523.	2.8	14
90	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.	1.4	14

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91	The influence of charge ordering on the phase stability of spinel LiNi2O4. RSC Advances, 2012, 2, 12940.	1.7	14
92	Local Bonding States of Titanium and Germanium-doped Tetragonal Zirconia Polycrystal and Their Correlation to High Temperature Ductility. Materials Transactions, 2002, 43, 2468-2472.	0.4	13
93	Influence of Interaction between Neighboring Oxygen Ions on Phase Stability in Cubic Zirconia. Journal of the American Ceramic Society, 2002, 85, 2557-2561.	1.9	13
94	A High-Coincidence Twin Boundary in Lithium Battery Material LiCoO₂. Nanoscience and Nanotechnology Letters, 2012, 4, 165-168.	0.4	13
95	Defects at the (1 1 0) surface of rutile TiO2 from ab initio calculations. International Journal of Hydrogen Energy, 2012, 37, 8110-8117.	3.8	13
96	High temperature plastic flow and grain boundary chemistry in oxide ceramics. Journal of Materials Science, 2005, 40, 3129-3135.	1.7	12
97	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> Secondary ion mass spectroscopy and first-principles study. Physical Review B, 2010, 82, .	1.1	10
98	Ab-initio multiplet calculation of oxygen vacancy effect on Ti-L2,3 electron energy loss near edge structures of BaTiO3. Applied Physics Letters, 2011, 99, 233109.	1.5	10
99	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.	3.8	10
100	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.	0.7	10
101	In situ electron microscopic observation of electrochemical Li-intercalation into MoS2. Solid State Ionics, 2020, 357, 115488.	1.3	10
102	High Rate Performance of Dual-Substituted LiFePO₄ Based on Controlling Metastable Intermediate Phase. ACS Applied Energy Materials, 2018, 1, 6736-6740.	2.5	9
103	Effects of Nitrogen/Fluorine Codoping on Photocatalytic Rutile TiO₂ Crystal Studied by First-Principles Calculations. Inorganic Chemistry, 2021, 60, 2381-2389.	1.9	9
104	A First-Principles Study of the Ferroelectric Phase of AgNbO₃. Japanese Journal of Applied Physics, 2012, 51, 09LE02.	0.8	9
105	Atomic-Level Changes during Electrochemical Cycling of Oriented LiMn₂O₄ Cathodic Thin Films. ACS Applied Materials & Interfaces, 2022, 14, 6507-6517.	4.0	9
106	Lithium Lanthanum Titanate Single Crystals: Dependence of Lithium-Ion Conductivity on Crystal Domain Orientation. Nano Letters, 2022, 22, 5516-5522.	4.5	9
107	A First-Principles Study of the Ferroelectric Phase of AgNbO₃. Japanese Journal of Applied Physics, 2012, 51, 09LE02.	0.8	8
108	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.	0.8	8

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109	Structural phase transitions of LaScO3 from first principles. Materials Today Communications, 2021, 26, 102048.	0.9	8
110	On-Chip Electrochemical Analysis Combined with Liquid-Phase Electron Microscopy of Zinc Deposition/Dissolution. Journal of the Electrochemical Society, 2021, 168, 112511.	1.3	8
111	Grain Boundary Energy and Tensile Ductility in Superplastic Cation-doped TZP. Materials Transactions, 2004, 45, 2144-2149.	0.4	7
112	SYNTHESIS AND ELECTRICAL CONDUCTIVITY OF TETRA-VALENT CERIUM POLYPHOSPHATE BULKS. Phosphorus Research Bulletin, 2009, 23, 20-24.	0.1	7
113	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. Journal of Materials Chemistry, 2010, 20, 10335.	6.7	7
114	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: 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, .	1.1	7
115	Ionic conduction mechanism in Ca-doped lanthanum oxychloride. Dalton Transactions, 2021, 50, 151-156.	1.6	7
116	Nanoscale Defluorination Mechanism and Solid Electrolyte Interphase of a MgF₂ Anode in Fluoride-Shuttle Batteries. ACS Applied Energy Materials, 2021, 4, 996-1003.	2.5	7
117	Defect Engineering and Anisotropic Modulation of Ionic Transport in Perovskite Solid Electrolyte LixLa(1â^'x)/3NbO3. Molecules, 2021, 26, 3559.	1.7	7
118	Lone-Pair-Induced Intra- and Interlayer Polarizations in SillÃ©n-Aurivillius Layered Perovskite Bi₄NbO₈Br. Inorganic Chemistry, 2022, 61, 9816-9822.	1.9	7
119	First-principles study of defect equilibria in lithium zinc nitride. Journal of Physics Condensed Matter, 2007, 19, 046201.	0.7	6
120	First Principles Calculation of CO and H₂ Adsorption on Strained Pt Surface. Materials Transactions, 2008, 49, 2484-2490.	0.4	6
121	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. Physical Review B, 2009, 80, .	1.1	6
122	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO$_{3}$. Japanese Journal of Applied Physics, 2012, 51, 09LE01.	0.8	6
123	Equilibrium hydrogen pressures in the Vâ€“H system from first principles. International Journal of Hydrogen Energy, 2019, 44, 28909-28918.	3.8	6
124	Negative-pressure-induced helimagnetism in ferromagnetic cubic perovskites Sr1â^'xBaxCoO3. Physical Review Materials, 2018, 2, .	0.9	6
125	First-Principles Calculations of Phase Transition in CaTiO3 under Negative Static Pressure. Journal of the Korean Physical Society, 2011, 59, 2497-2502.	0.3	6
126	Atomic-Scale Analysis of Biphasic Boundaries in the Lithium-Ion Battery Cathode Material LiFePO₄. ACS Applied Energy Materials, 2020, 3, 8009-8016.	2.5	5

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127	Anisotropic Permittivity of Tetragonal BaTiO₃: A First-Principles Study. Japanese Journal of Applied Physics, 2011, 50, 09NE02.	0.8	5
128	Systematic calculations of On (n = 1 to 6) polytypes of LiCoO₂. Physica Status Solidi - Rapid Research Letters, 2014, 8, 545-548.	1.2	4
129	Theoretical investigation of solid solution states of Ti1âˆ'V H2. Acta Materialia, 2017, 134, 274-282.	3.8	4
130	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.	0.9	4
131	Application of machine learning-based selective sampling to determine BaZrO3 grain boundary structures. Computational Materials Science, 2019, 164, 57-65.	1.4	4
132	Flux Crystal Growth, Structure, and Optical Properties of the New Germanium Oxysulfide La₄(GeS₂O₂)₃. Crystal Growth and Design, 2020, 20, 4054-4061.	1.4	4
133	Oxide-ion diffusion in brownmillerite-type Ca₂AlMnO_{5+Î´} from first-principles calculations. Physical Chemistry Chemical Physics, 2022, 24, 1503-1509.	1.3	4
134	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. Materials Transactions, 2004, 45, 2106-2111.	0.4	3
135	Magnetic Properties of Ni Alloys for Superconducting Wire Substrates: A First-Principles Study. Japanese Journal of Applied Physics, 2009, 48, 083003.	0.8	3
136	A Density Functional Study of Oxygen Adatoms on a Step-Doubled Platinum Surface. Journal of Physical Chemistry C, 2014, 118, 23675-23681.	1.5	3
137	First-Principles-Based Phonon Calculation and Raman Spectroscopy Measurement of RuGa₂ and RuAl₂ with High Thermoelectric Power Factors. Materials Transactions, 2016, 57, 1050-1054.	0.4	3
138	Transition-Metal Distribution in Brownmillerite Ca₂FeCoO₅. Inorganic Chemistry, 2019, 58, 10209-10216.	1.9	3
139	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO3. Japanese Journal of Applied Physics, 2012, 51, 09LE01.	0.8	3
140	An extended computational approach for point-defect equilibria in semiconductor materials. Npj Computational Materials, 2022, 8, .	3.5	3
141	Surface design of alloy protection against CO-poisoning from first principles. Journal of Physics Condensed Matter, 2014, 26, 355006.	0.7	2
142	Effect of oxygen vacancy segregation in Au or Pt/oxide hetero-interfaces on electronic structures. RSC Advances, 2017, 7, 36034-36037.	1.7	2
143	Theoretical investigation of tetrahedral distortion of four-coordinate iron(<scp>ii</scp>) centres in FePd(CN)₄. Dalton Transactions, 2021, 50, 1990-1994.	1.6	2
144	Accelerated lithium ions diffusion at the interface between LiFePO4 electrode and electrolyte by surface-nitride treatment. Solid State Ionics, 2021, 373, 115792.	1.3	2

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145	Design and Fabrication of an Electrochemical Chip for Liquid-Phase Transmission Electron Microscopy. Microscopy (Oxford, England), 2022, , .	0.7	2
146	Reliable electrochemical setup for <i>in situ</i> observations with an atmospheric SEM. Microscopy (Oxford, England), 2022, 71, 311-314.	0.7	2
147	Superplastic Behavior in Small Amount of Ge-Ti Co-Doped TZP. Materials Science Forum, 2004, 447-448, 365-372.	0.3	1
148	Computer simulation of coherent BaZrO3/MgO interfaces. Journal of the Ceramic Society of Japan, 2011, 119, 861-866.	0.5	1
149	Atomic-Level Characterization of Interfaces in LiCoO2. ECS Transactions, 2014, 58, 1-11.	0.3	1
150	An alternative description of mass transfer through thick oxide films. Scripta Materialia, 2015, 100, 66-69.	2.6	1
151	Optical enhancement of dielectric permittivity in reduced lanthanum aluminate. Physical Review B, 2020, 101, .	1.1	1
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