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	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. Physical Review B, 2006, 73, .	3.3	234
2	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. Physical Review B, 2008, 78, .	3.3	224
3	Why is sodium-intercalated graphite unstable?. RSC Advances, 2017, 7, 36550-36554.	3.7	217
4	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
5	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
6	Oxygenâ€Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. Angewandte Chemie - International Edition, 2011, 50, 3053-3057.	14.8	129
7	First-principles study of vacancy formation in hydroxyapatite. Physical Review B, 2007, 75, .	3.3	124
8	Crystalline Grain Interior Configuration Affects Lithium Migration Kinetics in Li-Rich Layered Oxide. Nano Letters, 2016, 16, 2907-2915.	9.5	121
9	Structural Characterization of Pine Kraft Lignin: BioChoice Lignin vs Indulin AT. Journal of Wood Chemistry and Technology, 2016, 36, 432-446.	1.8	118
10	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
11	Ab initiolattice dynamics and phase transformations ofZrO2. Physical Review B, 2005, 71, .	3.3	109
12	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
13	On the Structural Origin of the Catalytic Properties of Inherently Strained Ultrasmall Decahedral Gold Nanoparticles. Nano Letters, 2012, 12, 2027-2031.	9.5	105
14	Pressure-induced phase transition in ZnO andZnOâ^'MgOpseudobinary system: A first-principles lattice dynamics study. Physical Review B, 2005, 72, .	3.3	101
15	Lithium Atom and A-Site Vacancy Distributions in Lanthanum Lithium Titanate. Chemistry of Materials, 2013, 25, 1607-1614.	7.1	99
16	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
17	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. Physical Review B, 2008, 78, .	3.3	83
18	Dislocation-enhanced ionic conductivity of yttria-stabilized zirconia. Applied Physics Letters, 2003, 82, 877-879.	3.2	82

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19	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
20	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
21	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
22	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
23	Domain boundary structures in lanthanum lithium titanates. Journal of Materials Chemistry A, 2014, 2, 843-852.	10.5	68
24	Cubic and orthorhombic structures of aluminum hydrideAlH3predicted by a first-principles study. Physical Review B, 2005, 71, .	3.3	67
25	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. Physical Review B, 2006, 74, .	3.3	67
26	Ferroelectricity Driven by Twisting of Silicate Tetrahedral Chains. Angewandte Chemie - International Edition, 2013, 52, 8088-8092.	14.8	64
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, .	3.3	60
28	Detection and manipulation of nuclear spin states in fermionic strontium. Physical Review A, 2011, 84, .	2.5	60
29	Ferroelectricity in wurtzite structure simple chalcogenide. Applied Physics Letters, 2014, 104, .	3.2	60
30	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
31	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
32	First-principles study of cation disordering inMgAl2O4spinel with cluster expansion and Monte Carlo simulation. Physical Review B, 2006, 73, .	3.3	51
33	Hydride-based antiperovskites with soft anionic sublattices as fast alkali ionic conductors. Nature Communications, 2021, 12, 201.	13.2	49
34	Defect Chemistry of Rutile TiO₂ from First Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 5919-5930.	3.3	46
35	Direct Measurement of Electronic Band Structures at Oxide Grain Boundaries. Nano Letters, 2020, 20, 2530-2536.	9.5	46
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, .	3.3	45

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37	Ba₂ScHO₃: H^{â€“} Conductive Layered Oxyhydride with H^{â€“} Site Selectivity. Inorganic Chemistry, 2019, 58, 4431-4436.	4.2	42
38	In situ electron microscopy analysis of electrochemical Zn deposition onto an electrode. Journal of Power Sources, 2021, 481, 228831.	8.0	42
39	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:mi><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> Physical Review B, 2009, 79, .	3.3	42
40	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
41	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
42	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
43	Mechanism of polarization switching in wurtzite-structured zinc oxide thin films. Applied Physics Letters, 2016, 109, .	3.2	36
44	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
45	Effects of Dislocations on the Oxygen Ionic Conduction in Yttria Stabilized Zirconia. Materials Transactions, 2004, 45, 2042-2047.	1.3	34
46	On Hydride Diffusion in Transition Metal Perovskite Oxyhydrides Investigated via Deuterium Exchange. Chemistry of Materials, 2017, 29, 8187-8194.	7.1	34
47	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
48	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
49	Anion ordering enables fast H ^{â^'} conduction at low temperatures. Science Advances, 2021, 7, .	10.9	33
50	The electric field induced ferroelectric phase transition of AgNbO3. Journal of Applied Physics, 2016, 119, .	2.3	32
51	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
52	Ordering and segregation of aCu75Pt25(111)surface: A first-principles cluster expansion study. Physical Review B, 2007, 76, .	3.3	31
53	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
54	Structural Distortion and Compositional Gradients Adjacent to Epitaxial LiMn₂O₄ Thin Film Interfaces. Advanced Materials Interfaces, 2014, 1, 1400143.	4.1	30

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55	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
56	First-Principles Calculations of Electronic Structure and Solution Energies of Mn-Doped BaTiO₃. Japanese Journal of Applied Physics, 2010, 49, 09MC01.	1.6	29
57	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
58	Exploring a potential energy surface by machine learning for characterizing atomic transport. Physical Review B, 2018, 97, .	3.3	29
59	Microscopic mechanism of biphasic interface relaxation in lithium iron phosphate after delithiation. Nature Communications, 2018, 9, 2863.	13.2	29
60	Microscopic characterization of the Câ€“F bonds in fluorineâ€“graphite intercalation compounds. Journal of Power Sources, 2020, 445, 227320.	8.0	29
61	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
62	Oxygen Affinity: The Missing Link Enabling Prediction of Proton Conductivities in Doped Barium Zirconates. Chemistry of Materials, 2020, 32, 7292-7300.	7.1	27
63	A computational search for wurtzite-structured ferroelectrics with low coercive voltages. APL Materials, 2020, 8, .	4.8	27
64	Structure and chemistry of grain boundaries in SiO2-doped TZP. Science and Technology of Advanced Materials, 2001, 2, 411-424.	6.1	26
65	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
66	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
67	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
68	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
69	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
70	Local condensation around oxygen vacancies in t-LaNbO4 from first principles calculations. Physical Chemistry Chemical Physics, 2009, 11, 5550.	2.9	25
71	Adsorption and Diffusion of Oxygen Atoms on a Pt(211) Stepped Surface. Journal of Physical Chemistry C, 2013, 117, 9772-9778.	3.3	25
72	First-Principles Study of Point Defect Formation in AgNbO₃. Japanese Journal of Applied Physics, 2013, 52, 09KF08.	1.6	24

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73	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
74	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
75	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
76	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
77	First-Principles Calculations of Rare-Earth Dopants in BaTiO3. Japanese Journal of Applied Physics, 2009, 48, 09KC03.	1.6	22
78	Photo-induced change of dielectric response in BaCoSiO4 stuffed tridymite. Journal of Applied Physics, 2014, 115, .	2.3	22
79	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
80	Responsive Fourâ€Coordinate Iron(II) Nodes in FePd(CN)₄. Angewandte Chemie - International Edition, 2020, 59, 19254-19259.	14.8	20
81	Dehydration of Electrochemically Protonated Oxide: SrCoO₂ with Square Spin Tubes. Journal of the American Chemical Society, 2021, 143, 17517-17525.	14.6	19
82	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
83	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
84	Anisotropic Permittivity of Tetragonal BaTiO₃: A First-Principles Study. Japanese Journal of Applied Physics, 2011, 50, 09NE02.	1.6	17
85	A computational model of the attention process in risky choice.. Decision, 2016, 3, 254-280.	0.5	17
86	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
87	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
88	Heterovalent Pb-substitution in ferroelectric bismuth silicate Bi₂SiO₅. Journal of Materials Chemistry C, 2016, 4, 3168-3174.	5.6	15
89	Dynamic Analysis of a Universal Joint With Manufacturing Tolerances. Journal of Mechanisms, Transmissions, and Automation in Design, 1986, 108, 524-532.	0.2	14
90	Effect of Chemical Bonding States on the Tensile Ductility in Glass-Doped TZP. Materials Science Forum, 2001, 357-359, 399-404.	0.2	14

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91	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
92	The influence of charge ordering on the phase stability of spinel LiNi2O4. RSC Advances, 2012, 2, 12940.	3.7	14
93	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
94	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
95	Oxygenâ€Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. Angewandte Chemie, 2011, 123, 3109-3113.	2.1	13
96	A High-Coincidence Twin Boundary in Lithium Battery Material LiCoO₂. Nanoscience and Nanotechnology Letters, 2012, 4, 165-168.	0.4	13
97	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
98	Lithium Lanthanum Titanate Single Crystals: Dependence of Lithium-Ion Conductivity on Crystal Domain Orientation. Nano Letters, 2022, 22, 5516-5522.	9.5	13
99	TAP: a targeted clinical genomics pipeline for detecting transcript variants using RNA-seq data. BMC Medical Genomics, 2018, 11, 79.	1.5	12
100	Atomic-Level Changes during Electrochemical Cycling of Oriented LiMn₂O₄ Cathodic Thin Films. ACS Applied Materials & Interfaces, 2022, 14, 6507-6517.	8.3	12
101	Equilibrium hydrogen pressures in the Vâ€“H system from first principles. International Journal of Hydrogen Energy, 2019, 44, 28909-28918.	7.2	11
102	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
103	In situ electron microscopic observation of electrochemical Li-intercalation into MoS2. Solid State Ionics, 2020, 357, 115488.	2.9	11
104	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 Secondary ion mass spectroscopy and first-principles study. Physical Review B, 2010, 82, .	3.8	10
105	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
106	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
107	Effects of Nitrogen/Fluorine Codoping on Photocatalytic Rutile TiO₂ Crystal Studied by First-Principles Calculations. Inorganic Chemistry, 2021, 60, 2381-2389.	4.2	10
108	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

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109	Lone-Pair-Induced Intra- and Interlayer Polarizations in SillÃ©n-Aurivillius Layered Perovskite Bi₄NbO₈Br. Inorganic Chemistry, 2022, 61, 9816-9822.	4.2	10
110	A First-Principles Study of the Ferroelectric Phase of AgNbO₃. Japanese Journal of Applied Physics, 2012, 51, 09LE02.	1.6	9
111	High Rate Performance of Dual-Substituted LiFePO₄ Based on Controlling Metastable Intermediate Phase. ACS Applied Energy Materials, 2018, 1, 6736-6740.	5.3	9
112	Ionic conduction mechanism in Ca-doped lanthanum oxychloride. Dalton Transactions, 2021, 50, 151-156.	3.4	9
113	A First-Principles Study of the Ferroelectric Phase of AgNbO₃. Japanese Journal of Applied Physics, 2012, 51, 09LE02.	1.6	9
114	SYNTHESIS AND ELECTRICAL CONDUCTIVITY OF TETRA-VALENT CERIUM POLYPHOSPHATE BULKS. Phosphorus Research Bulletin, 2009, 23, 20-24.	0.6	8
115	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:mi mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:mrow></mml:math>identified by electron energy-loss spectroscopy. Physical Review B, 2016, 93, .	3.3	8
116	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
117	Structural phase transitions of LaScO3 from first principles. Materials Today Communications, 2021, 26, 102048.	2.0	8
118	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
119	Grain Boundary Energy and Tensile Ductility in Superplastic Cation-doped TZP. Materials Transactions, 2004, 45, 2144-2149.	1.3	7
120	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. Journal of Materials Chemistry, 2010, 20, 10335.	6.7	7
121	PALEOENVIRONMENTAL AND BIOSTRATIGRAPHIC IMPLICATIONS OF ECHINODERM OSSICLES TRAPPED WITHIN BURMESE AMBER. Palaios, 2019, 34, 652-656.	1.4	7
122	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
123	Defect Engineering and Anisotropic Modulation of Ionic Transport in Perovskite Solid Electrolyte LixLa(1â^'x)/3NbO3. Molecules, 2021, 26, 3559.	3.9	7
124	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
125	First Principles Calculation of CO and H₂ Adsorption on Strained Pt Surface. Materials Transactions, 2008, 49, 2484-2490.	1.3	6
126	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. Physical Review B, 2009, 80, .	3.3	6

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127	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO$_{3}$. Japanese Journal of Applied Physics, 2012, 51, 09LE01.	1.6	6
128	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
129	Theoretical investigation of solid solution states of Ti1âˆ’V H2. Acta Materialia, 2017, 134, 274-282.	8.0	5
130	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
131	Anisotropic Permittivity of Tetragonal BaTiO₃: A First-Principles Study. Japanese Journal of Applied Physics, 2011, 50, 09NE02.	1.6	5
132	Systematic calculations of On (n = 1 to 6) polytypes of LiCoO₂. Physica Status Solidi - Rapid Research Letters, 2014, 8, 545-548.	2.5	4
133	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
134	Application of machine learning-based selective sampling to determine BaZrO3 grain boundary structures. Computational Materials Science, 2019, 164, 57-65.	3.1	4
135	Oxide-ion diffusion in brownmillerite-type Ca₂AlMnO_{5+Î´} from first-principles calculations. Physical Chemistry Chemical Physics, 2022, 24, 1503-1509.	2.9	4
136	An extended computational approach for point-defect equilibria in semiconductor materials. Npj Computational Materials, 2022, 8, .	9.1	4
137	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. Materials Transactions, 2004, 45, 2106-2111.	1.3	3
138	Magnetic Properties of Ni Alloys for Superconducting Wire Substrates: A First-Principles Study. Japanese Journal of Applied Physics, 2009, 48, 083003.	1.6	3
139	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
140	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
141	Transition-Metal Distribution in Brownmillerite Ca₂FeCoO₅. Inorganic Chemistry, 2019, 58, 10209-10216.	4.2	3
142	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO3. Japanese Journal of Applied Physics, 2012, 51, 09LE01.	1.6	3
143	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
144	Discovery of Unconventional Protonâ€Conducting Inorganic Solids via Defectâ€Chemistryâ€Trained, Interpretable Machine Learning. Advanced Energy Materials, 2023, 13, .	22.2	3

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145	Diffusing Supply Chain Innovations at Hewlett-Packard Company: Applications of Performance Technology. Performance Improvement Quarterly, 2008, 13, 6-15.	1.2	2
146	Surface design of alloy protection against CO-poisoning from first principles. Journal of Physics Condensed Matter, 2014, 26, 355006.	1.9	2
147	Peculiarities of the interaction of a structure with moving ice. Doklady Physics, 2016, 61, 555-557.	0.8	2
148	Advanced Aero-Engines Technology Enablers: An Overview of the European Project E-BREAK. , 2016, , .		2
149	Flux Crystal Growth, Crystal Structure, and Optical Properties of New Germanate Garnet Ce2CaMg2Ge3O12. Frontiers in Chemistry, 2020, 8, 91.	3.7	2
150	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
151	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
152	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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