Isao Tanaka

List of Publications by Year in descending order

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419 papers	27,289 citations	17405 63 h-index	6630 156 g-index
424 all docs	424 docs citations	424 times ranked	21471 citing authors

#	Article	IF	Citations
1	First principles phonon calculations in materials science. Scripta Materialia, 2015, 108, 1-5.	2.6	7,324
2	First-principles calculations of the ferroelastic transition between rutile-type and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaCl</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu high pressures. Physical Review B, 2008, 78, .	1.1	4,498
3	Distributions of phonon lifetimes in Brillouin zones. Physical Review B, 2015, 91, .	1.1	963
4	High-Density Electron Anions in a Nanoporous Single Crystal: [Ca24Al28O64]4+(4e-). Science, 2003, 301, 626-629.	6.0	744
5	Band structure diagram paths based on crystallography. Computational Materials Science, 2017, 128, 140-184.	1.4	457
6	First-principles phonon calculations of thermal expansion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ti</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ti</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub Physical Review B, 2010, 81, .	1.1	429
7	Phonon-phonon interactions in transition metals. Physical Review B, 2011, 84, .	1.1	363
8	Prediction of Low-Thermal-Conductivity Compounds with First-Principles Anharmonic Lattice-Dynamics Calculations and Bayesian Optimization. Physical Review Letters, 2015, 115, 205901.	2.9	343
9	Point defects in ZnO: an approach from first principles. Science and Technology of Advanced Materials, 2011, 12, 034302.	2.8	279
10	Prediction model of band gap for inorganic compounds by combination of density functional theory calculations and machine learning techniques. Physical Review B, 2016, 93, .	1.1	252
11	Machine learning with systematic density-functional theory calculations: Application to melting temperatures of single- and binary-component solids. Physical Review B, 2014, 89, .	1.1	243
12	Representation of compounds for machine-learning prediction of physical properties. Physical Review B, 2017, 95, .	1.1	220
13	Lithium Iron Borates as Highâ€Capacity Battery Electrodes. Advanced Materials, 2010, 22, 3583-3587.	11.1	218
14	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212
15	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. Physical Review B, 2008, 78, .	1.1	210
16	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. Nature Communications, 2016, 7, 11962.	5.8	208
17	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
18	First-principles calculations of ELNES and XANES of selected wide-gap materials: Dependence on crystal structure and orientation. Physical Review B, 2004, 70, .	1.1	162

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19	First-principles study on lithium removal from Li2MnO3. Journal of Power Sources, 2009, 189, 798-801.	4.0	158
20	Design and synthesis of a magnesium alloy for room temperature hydrogen storage. Acta Materialia, 2018, 149, 88-96.	3.8	157
21	Pure H ^{â€“} conduction in oxyhydrides. Science, 2016, 351, 1314-1317.	6.0	155
22	Defect Chemistry in Layered LiMO₂ (M = Co, Ni, Mn, and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 627 Td (Li<su 3886-3894.	3.2	128
23	Cluster expansion method for multicomponent systems based on optimal selection of structures for density-functional theory calculations. Physical Review B, 2009, 80, .	1.1	116
24	Soft longitudinal modes in spin-singletCuGeO3. Physical Review B, 1994, 50, 1278-1281.	1.1	112
25	XANES and ELNES in Ceramic Science. Journal of the American Ceramic Society, 2005, 88, 2013-2029.	1.9	111
26	Broadening Mechanism of Resistive Transition under Magnetic Field in Single Crystalline (La1-xSrx)2CuO4. Japanese Journal of Applied Physics, 1989, 28, L555-L556.	0.8	109
27	Ab initiolattice dynamics and phase transformations ofZrO2. Physical Review B, 2005, 71, .	1.1	109
28	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
29	Accelerated discovery of cathode materials with prolonged cycle life for lithium-ion battery. Nature Communications, 2014, 5, 4553.	5.8	108
30	First-principles XANES simulations of spinel zinc ferrite with a disordered cation distribution. Physical Review B, 2007, 75, .	1.1	105
31	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. Computer Physics Communications, 2017, 221, 221-234.	3.0	105
32	Antiferromagnetic superexchange via<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>states of titanium in EuTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>as seen from hybrid Hartree-Fock density functional calculations. Physical Review B, 2011, 83, .	1.1	104
33	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. Materials Transactions, 2002, 43, 1426-1429.	0.4	101
34	Decomposition reactions forNaAlH4,Na3AlH6, and NaH: First-principles study. Physical Review B, 2005, 71, .	1.1	97
35	Unconventional lattice stiffening in superconductingLa2â^'xSrxCuO4single crystals. Physical Review B, 1995, 52, 570-580.	1.1	96
36	Ab initiocharge transfer multiplet calculations on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:mn> and ELNES of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>transition metal oxides. Physical Review B, 2011, 83, .	1.1	94

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37	Antiâ€ferrodistortiveâ€Like Oxygenâ€Octahedron Rotation Induced by the Oxygen Vacancy in Cubic SrTiO₃. Advanced Materials, 2013, 25, 86-90.	11.1	94
38	Structural Analysis and Superconducting Properties of F-Substituted NdOBiS₂ Single Crystals. Journal of the Physical Society of Japan, 2013, 82, 113701.	0.7	94
39	Raman-scattering study ofCuGeO3in the spin-Peierls phase. Physical Review B, 1994, 50, 16468-16474.	1.1	91
40	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. Journal of the American Ceramic Society, 2002, 85, 75-80.	1.9	90
41	Single crystal growth of superconducting La2-xSrxCuO4 by the TSFZ method. Journal of Crystal Growth, 1989, 96, 711-715.	0.7	89
42	Reduced SnO2 surfaces by first-principles calculations. Applied Physics Letters, 2004, 84, 909-911.	1.5	88
43	Complete elastic constants and giant softening ofc66in superconductingLa1.86Sr0.14CuO4. Physical Review Letters, 1990, 64, 2458-2461.	2.9	87
44	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. Physical Review B, 2017, 96, .	1.1	85
45	Growth and superconducting properties of F-substituted ROBiS2 (R=La, Ce, Nd) single crystals. Solid State Communications, 2014, 178, 33-36.	0.9	83
46	Sparse representation for a potential energy surface. Physical Review B, 2014, 90, .	1.1	81
47	Temperature dependence of anisotropic lower critical fields in (La1â^'xSrx)2CuO4. Physical Review B, 1990, 41, 4823-4826.	1.1	80
48	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. Journal of Chemical Physics, 2015, 143, 064710.	1.2	80
49	Crystal growth of Ca12Al14O33 by the floating zone method. Journal of Crystal Growth, 2002, 237-239, 801-805.	0.7	79
50	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. Physical Review B, 2008, 78, .	1.1	79
51	Theoretical ELNES using one-particle and multi-particle calculations. Micron, 2010, 41, 695-709.	1.1	79
52	Identification of ultradilute dopants in ceramics. Nature Materials, 2003, 2, 541-545.	13.3	78
53	First-Principles Study on Relaxor-Type Ferroelectric Behavior without Chemical Inhomogeneity in BaTaO₂N and SrTaO₂N. Chemistry of Materials, 2012, 24, 4343-4349.	3.2	78
54	Evolution of crystal structures in metallic elements. Physical Review B, 2013, 87, .	1.1	78

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55	High-pressure torsion of titanium at cryogenic and room temperatures: Grain size effect on allotropic phase transformations. Acta Materialia, 2014, 68, 207-213.	3.8	78
56	Crystal structure, defect chemistry and oxygen ion transport of the ferroelectric perovskite, Na_{0.5}Bi_{0.5}TiO₃: insights from first-principles calculations. Journal of Materials Chemistry A, 2015, 3, 16574-16582.	5.2	72
57	New nanostructured phases with reversible hydrogen storage capability in immiscible magnesiumâ€“zirconium system produced by high-pressure torsion. Acta Materialia, 2016, 108, 293-303.	3.8	72
58	First-principles interatomic potentials for ten elemental metals via compressed sensing. Physical Review B, 2015, 92, .	1.1	71
59	Interplay between lattice softening and high-Tcsuperconductivity inLa1.86Sr0.14CuO4. Physical Review Letters, 1993, 70, 3447-3450.	2.9	70
60	Ionization potentials of (112) and (11<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq0 0 0 rgBT /Overlock 10 of CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and CuGaSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><m	1.1	70
61	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. Entropy, 2018, 20, 655.	1.1	69
62	Cubic and orthorhombic structures of aluminum hydrideAlH3predicted by a first-principles study. Physical Review B, 2005, 71, .	1.1	67
63	First-Principles Insight into the Hydration Ability and Proton Conduction of the Solid State Proton Conductor, Y and Sn Co-Doped BaZrO₃. Chemistry of Materials, 2015, 27, 901-908.	3.2	67
64	Electron Carrier Generation in a Refractory Oxide 12CaOÂ·7Al2O3by Heating in Reducing Atmosphere: Conversion from an Insulator to a Persistent Conductor. Journal of the American Ceramic Society, 2006, 89, 3294-3298.	1.9	65
65	Transition pathway of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>crystals under high pressures. Physical Review B, 2008, 77, .	1.1	65
66	Lattice thermal conductivities of two <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm polymorphs by first-principles calculations and the phonon Boltzmann transport equation. Physical Review B, 2018, 97, .	1.1	65
67	Ultra-severe plastic deformation: Evolution of microstructure, phase transformation and hardness in immiscible magnesium-based systems. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2017, 701, 158-166.	2.6	62
68	Nanoporous Crystal 12CaOÂ·7Al2O3:Â A Playground for Studies of Ultraviolet Optical Absorption of Negative Ions. Journal of Physical Chemistry B, 2007, 111, 1946-1956.	1.2	61
69	Electronic and structural properties of the oxygen vacancy in BaTiO3. Applied Physics Letters, 2011, 98, .	1.5	61
70	Superconducting Double Perovskite Bismuth Oxide Prepared by a Lowâ€Temperature Hydrothermal Reaction. Angewandte Chemie - International Edition, 2014, 53, 3599-3603.	7.2	61
71	Inversion Symmetry Breaking by Oxygen Octahedral Rotations in the Ruddlesden-Popper<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Na</mml:mi><mml:mi>R</mml:mi><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mr Physical Review Letters, 2014, 112, 187602.	2.9	60
72	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. Physical Review B, 2017, 95, .	1.1	59

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73	First-principles study of native defects and lanthanum impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>NaTaO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: Physical Review B, 2008, 78, .	1.1	58
74	Crystal structures of LaO1â^'xFxBiS2 (x~0.23, 0.46): Effect of F doping on distortion of Biâ€“S plane. Journal of Solid State Chemistry, 2014, 212, 213-217.	1.4	58
75	First Principles Calculation of Fe L_{2,3}-edge X-ray Absorption Near Edge Structures of Iron Oxides. Materials Transactions, 2004, 45, 1414-1418.	0.4	56
76	Unconventional Superconductivity in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>BiS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mr -Based Layered Superconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NdO</mml:mi></mml:mrow><mml:mrow><mml:mn>0.71</mml:mn> mathvariant="nor. Physical Review Letters, 2017, 118, 167002.	2.9	55
77	Crystal and Electronic Structure and Magnetic Properties of Divalent Europium Perovskite Oxides EuMO₃ (M = Ti, Zr, and Hf): Experimental and First-Principles Approaches. Inorganic Chemistry, 2012, 51, 4560-4567.	1.9	54
78	²⁷Al NMR Chemical Shifts in Oxide Crystals: A First-Principles Study. Journal of Physical Chemistry C, 2009, 113, 3869-3873.	1.5	53
79	First principles study of dopant solubility and defect chemistry in LiCoO₂. Journal of Materials Chemistry A, 2014, 2, 11235-11245.	5.2	52
80	Direct evidence of hidden local spin polarization in a centrosymmetric superconductor LaO0.55 F0.45BiS2. Nature Communications, 2017, 8, 1919.	5.8	52
81	Firstâ€Principles Calculations of Anion Vacancies in Oxides and Nitrides. Journal of the American Ceramic Society, 2002, 85, 68-74.	1.9	51
82	Core-hole effect on dipolar and quadrupolar transitions ofSrTiO3andBaTiO3at TiKedge. Physical Review B, 2005, 71, .	1.1	50
83	Band offsets of CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/CdS and CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/ZnS (110) interfaces: A hybrid density functional theory study. Physical Review B, 2013, 88, .	1.1	50
84	First-Principles Calculations of Oxygen Vacancy Formation and Metallic Behavior at a Î²-MnO₂ Grain Boundary. ACS Applied Materials & Interfaces, 2015, 7, 1726-1734.	4.0	50
85	Synthesis and electrochemistry of monoclinic Li(MnxFe1â^'x)BO3: a combined experimental and computational study. Journal of Materials Chemistry, 2011, 21, 10690.	6.7	49
86	Thermal contraction at the spin-Peierls transition inCuGeO3. Physical Review B, 1994, 50, 12606-12610.	1.1	48
87	Relation between structure and doping in La2â^'xSrxCuO4+Î´ a neutron diffraction study on single crystals. Physica C: Superconductivity and Its Applications, 1994, 223, 396-416.	0.6	48
88	Double thermoelectric power factor of a 2D electron system. Nature Communications, 2018, 9, 2224.	5.8	48
89	Epitaxial growth of Mn-doped Î³-Ga₂O₃ on spinel substrate. Journal of Materials Research, 2011, 26, 578-583.	1.2	46
90	Defect chemistry of a BaZrO3 Î£3 (111) grain boundary by first principles calculations and spaceâ€“charge theory. Physical Chemistry Chemical Physics, 2012, 14, 12339.	1.3	46

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91	Mode decomposition based on crystallographic symmetry in the band-unfolding method. Physical Review B, 2017, 95, .	1.1	46
92	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. Journal of Physical Chemistry C, 2017, 121, 18947-18953.	1.5	44
93	Conceptual and practical bases for the high accuracy of machine learning interatomic potentials: Application to elemental titanium. Physical Review Materials, 2017, 1, .	0.9	44
94	Atomic Structure of Luminescent Centers in High-Efficiency Ce-doped w-AlN Single Crystal. Scientific Reports, 2014, 4, 3778.	1.6	43
95	Categorization of surface polarity from a crystallographic approach. Computational Materials Science, 2016, 113, 221-230.	1.4	43
96	Coexistence of superconductivity and charge-density wave in the quasi-one-dimensional material HfTe3. Scientific Reports, 2017, 7, 45217.	1.6	43
97	Proton-Conducting Network in Lanthanum Orthophosphate. Journal of Physical Chemistry C, 2012, 116, 19117-19124.	1.5	42
98	Mn L2,3-edge X-ray absorption spectroscopic studies on charge-discharge mechanism of Li2MnO3. Applied Physics Letters, 2014, 104, .	1.5	42
99	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> 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, .	1.1	42
100	Superoxide Ion Encaged in Nanoporous Crystal 12CaOÂ·7Al2O3 Studied by Continuous Wave and Pulsed Electron Paramagnetic Resonance. Journal of Physical Chemistry B, 2004, 108, 18557-18568.	1.2	41
101	Strong Spinâ€Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. Advanced Functional Materials, 2013, 23, 1864-1872.	7.8	41
102	Distribution of solute atoms inÎ²- and spinelSi6â^'zAlzOzN8â^'zby AlK-edge x-ray absorption near-edge structure. Physical Review B, 2005, 71, .	1.1	40
103	Functional Complex Point-Defect Structure in a Huge-Size-Mismatch System. Physical Review Letters, 2013, 110, 065504.	2.9	40
104	Evaluation of Migration Energy of Lithium Ions in Chalcogenides and Halides by First Principles Calculation. Materials Transactions, 2002, 43, 1460-1463.	0.4	39
105	Theoretical Study on the Chemistry of Intergranular Glassy Film in Si₃N₄â€“SiO₂ Ceramics. Journal of the American Ceramic Society, 2002, 85, 109-112.	1.9	39
106	Thermal annealing effect on magnetism and cation distribution in disordered ZnFe2O4 thin films deposited on glass substrates. Journal of Magnetism and Magnetic Materials, 2007, 310, 2543-2545.	1.0	39
107	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP₂, CdSnP₂, and Zn_{1-x}Cd_xSnP₂Alloys. Applied Physics Express, 2013, 6, 061201.	1.1	39
108	Oxygen Vacancy Formation and Reduction Properties of Î²-MnO₂ Grain Boundaries and the Potential for High Electrochemical Performance. ACS Applied Materials & Interfaces, 2014, 6, 17776-17784.	4.0	39

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109	Matrix- and tensor-based recommender systems for the discovery of currently unknown inorganic compounds. Physical Review Materials, 2018, 2, .	0.9	39
110	Classification of spinel structures based on first-principles cluster expansion analysis. Physical Review B, 2010, 81, .	1.1	38
111	Electronic structures of dynamically stable As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>	1.1	38
112	Protonic Conduction in the BaNdInO₄ Structure Achieved by Acceptor Doping. Chemistry of Materials, 2021, 33, 2139-2146.	3.2	37
113	Solubility of Si₃N₄ in Liquid SiO₂. Journal of the American Ceramic Society, 2002, 85, 25-32.	1.9	36
114	Electronic States of Sulfur Doped TiO₂ by First Principles Calculations. Materials Transactions, 2004, 45, 1987-1990.	0.4	36
115	First-principles-based phase diagram of the cubic BNC ternary system. Physical Review B, 2008, 77, .	1.1	36
116	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. Physical Review B, 2014, 90, .	1.1	36
117	Characterization and structural analysis of twinned La2â^'xSrxCuO4Â±Î´ crystals by neutron diffraction. Physica C: Superconductivity and Its Applications, 1992, 191, 455-468.	0.6	34
118	Theoretical Fingerprints of Transition Metal L_{2,3} XANES and ELNES for Lithium Transition Metal Oxides by ab Initio Multiplet Calculations. Journal of Physical Chemistry C, 2011, 115, 11871-11879.	1.5	34
119	Proximity to Fermi surface topological change in superconducting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>La</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>0.54</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:mrow><mml:mn>0.46</mml:mn></mml:mrow></mml:msub><mml:mi>Bi</mml:mi><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2014, 90, .	1.1	34
120	Zr coordination change during crystallization of MgOâ€“Al2O3â€“SiO2â€“ZrO2 glass ceramics. Journal of Non-Crystalline Solids, 2014, 384, 47-54.	1.5	34
121	Structures and energetics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Bi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>in a defective fluorite family derived by systematic first-principles lattice dynamics calculations. Physical Review B, 2010, 81, .	1.1	33
122	Conventional s-Wave Superconductivity in BiS₂-Based NdO_{0.71}F_{0.29}BiS₂ Revealed by Thermal Transport Measurements. Journal of the Physical Society of Japan, 2016, 85, 073707.	0.7	33
123	Compositional descriptor-based recommender system for the materials discovery. Journal of Chemical Physics, 2018, 148, 241719.	1.2	33
124	Effective Doping in Cubic Si₃N₄ and Ge₃N₄: A Firstâ€Principles Study. Journal of the American Ceramic Society, 2002, 85, 97-100.	1.9	32
125	Free-Energy Calculation of Precipitate Nucleation in an Fe-Cu-Ni Alloy. Materials Transactions, 2004, 45, 1978-1981.	0.4	32
126	Proton trapping in Y and Sn Co-doped BaZrO₃. Journal of Materials Chemistry A, 2015, 3, 10045-10051.	5.2	32

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127	Structure, Superconductivity, and Magnetism of Ce(O,F)BiS2 Single Crystals. Crystal Growth and Design, 2015, 15, 39-44.	1.4	32
128	Muon spin relaxation study on magnetism in high quality single crystal of a high transition temperature superconductor La2â^'xSrxCuO4â^'ï*f* (0.11â‰¤xâ‰¤0.14). Hyperfine Interactions, 1991, 63, 271-277.	0.2	31
129	Superconductivity in CeOBiS2 with cerium valence fluctuation. Solid State Communications, 2016, 245, 11-14.	0.9	31
130	Group-theoretical high-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential. Physical Review B, 2019, 99, .	1.1	31
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