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	Investigation of Superconductivity in Ce-Doped (La,Pr)OBiS2 Single Crystals. Materials, 2022, 15, 2977.	1.3	0
2	Growth and characterization of Bi₂Sr₂Ca_{1â€“x}Y _x Cu₂O_{8+Î´} single-crystal whiskers. Japanese Journal of Applied Physics, 2022, 61, 063001.	0.8	1
3	Growth and characterization of Li₇La₃Zr₂O₁₂ single crystals by using floating zone method for use as fast Li-ion conductorâ€. Journal of Physics: Conference Series, 2021, 1718, 012012.	0.3	0
4	NaInX2 (Xâ€‰=â€‰S, Se) layered materials for energy harvesting applications: first-principles insights into optoelectronic and thermoelectric properties. Journal of Materials Science: Materials in Electronics, 2021, 32, 3878-3893.	1.1	9
5	Influence of Se doping on recently synthesized NaInS2-xSex solid solutions for potential thermo-mechanical applications studied via first-principles method. Materials Today Communications, 2021, 26, 101988.	0.9	9
6	Protonic Conduction in the BaNdInO₄ Structure Achieved by Acceptor Doping. Chemistry of Materials, 2021, 33, 2139-2146.	3.2	37
7	Combination of recommender system and single-particle diagnosis for accelerated discovery of novel nitrides. Journal of Chemical Physics, 2021, 154, 224117.	1.2	3
8	Effect of Li concentration on the ionic conductivity of Li<i>_x</i>La_{(1â^'}<i>_x</i><sub>)/3</s solid solutions. Journal of the Ceramic Society of Japan, 2021, 129, 535-539.	1.1	2
9	Cooperative Oxide-Ion Transport in Pyrochlore Y₂Ti₂O₇: A First-Principles Molecular Dynamics Study. Journal of Physical Chemistry C, 2021, 125, 20460-20467.	1.5	3
10	Cd additive effect on self-flux growth of Cs-intercalated NbS2 superconducting single crystals. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2021, .	0.3	0
11	Investigating the combined effects of mirror tilting and position on rutile crystal growth using the infrared convergent-heating floating zone method. Journal of Crystal Growth, 2021, 571, 126257.	0.7	0
12	Fluorine solubility and superconducting properties of Sm(O,F)BiS2 single crystals. Journal of Alloys and Compounds, 2021, 883, 160812.	2.8	1
13	Finding well-optimized special quasirandom structures with decision diagram. Physical Review Materials, 2021, 5, .	0.9	0
14	Phonon structure of titanium under shear deformation along <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>{</mml:mo><mml:mn>10</mml:mn><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo>Â¯</mml:mo></mml:mover><mml:mn>2</mml:mn><mml:mo>}</mml:mo></mml:mro twinning mode. Physical Review B, 2020, 102, .	1.1	2
15	Enumeration of nonequivalent substitutional structures using advanced data structure of binary decision diagram. Journal of Chemical Physics, 2020, 153, 104109.	1.2	2
16	First-Principles Study on the Stability of Weberite-Type, Pyrochlore, and Defect-Fluorite Structures of A₂³⁺B₂⁴⁺O₇ (A =) Tj ETQq0 0 0 rgBT /Overlock	1.5	10
17	Growth and anisotropy evaluation of NbBiCh3 (Ch = S, Se) misfit-layered superconducting single crystals. Solid State Communications, 2020, 321, 114051.	0.9	12
18	Lithium-ionic conductivity of Li La(1â^')/3NbO3 single crystals grown by the TSFZ method. Solid State Ionics, 2020, 350, 115330.	1.3	4

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19	Fast material search of lithium ion conducting oxides using a recommender system. Journal of Materials Chemistry A, 2020, 8, 11582-11588.	5.2	19
20	Growth of Cr2N single crystals by the floating zone method. Journal of Crystal Growth, 2020, 546, 125782.	0.7	1
21	Growth and Characterization of ROBiS₂ High-Entropy Superconducting Single Crystals. ACS Omega, 2020, 5, 16819-16825.	1.6	16
22	Flux Growth and Superconducting Properties of (Ce,Pr)OBiS2 Single Crystals. Frontiers in Chemistry, 2020, 8, 44.	1.8	14
23	Effects of the Mirror Tilt Angle on the Growth of LiCoO2 Single Crystals by the Traveling Solvent Floating Zone (TSFZ) Technique Using a Tilting-Mirror-type Image Furnace. Crystal Growth and Design, 2020, 20, 3413-3416.	1.4	6
24	Application of machine learning potentials to predict grain boundary properties in fcc elemental metals. Physical Review Materials, 2020, 4, .	0.9	20
25	Group-theoretical high-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential. Physical Review B, 2019, 99, .	1.1	31
26	Growth and characterization of (La,Ce)OBiS₂ single crystals. Japanese Journal of Applied Physics, 2019, 58, 063001.	0.8	5
27	Growth of Superconducting Sm(O,F)BiS₂ Single Crystals. Crystal Growth and Design, 2019, 19, 6136-6140.	1.4	7
28	Crystal Growth and Characterization of LixLa(1â€“x)/3NbO3 by the Traveling Solvent Floating Zone Method. Crystal Growth and Design, 2019, 19, 6291-6295.	1.4	8
29	Bulk superconductivity in a four-layer-type Bi-based compound La2O2Bi3Ag0.6Sn0.4S5.7Se0.3. Scientific Reports, 2019, 9, 13346.	1.6	10
30	Self-Combustion Synthesis of Novel Metastable Ternary Molybdenum Nitrides. , 2019, 1, 64-70.		20
31	Growth and transport properties under high pressure of PrOBiS2 single crystals. Solid State Communications, 2019, 296, 17-20.	0.9	5
32	Vibrational Effects in X-ray Absorption Spectra of Two-Dimensional Layered Materials. Journal of Physical Chemistry C, 2019, 123, 9688-9692.	1.5	14
33	Pressure-induced insulator to metal transition of mixed valence compound Ce(O,F)SbS2. Journal of Applied Physics, 2019, 125, .	1.1	8
34	Solution effect on improved structural compatibility of NiTi-based alloys by systematic first-principles calculations. Journal of Applied Physics, 2019, 125, .	1.1	4
35	Recommender System of Successful Processing Conditions for New Compounds Based on a Parallel Experimental Data Set. Chemistry of Materials, 2019, 31, 9984-9992.	3.2	11
36	Growth of LiCoO₂ Single Crystals by the TSFZ Method. Crystal Growth and Design, 2019, 19, 415-420.	1.4	8

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37	Growth and physical properties of Ce(O,F)Sb(S,Se)2 single crystals with site-selected chalcogen atoms. Solid State Communications, 2019, 289, 38-42.	0.9	5
38	Determination of the phase relation of a Li La(1â˜)/3NbO3 system by the slow cooling floating zone method. Journal of Crystal Growth, 2019, 507, 251-254.	0.7	4
39	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>A</mml:mi></mml:math> -site cation size effect on oxygen octahedral rotations in acentric Ruddlesden-Popper alkali rare-earth titanates. Physical Review Materials, 2019, 3, .	0.9	7
40	Impact of interstitial C on phase stability and stacking-fault energy of the CrMnFeCoNi high-entropy alloy. Physical Review Materials, 2019, 3, .	0.9	30
41	Design and synthesis of a magnesium alloy for room temperature hydrogen storage. Acta Materialia, 2018, 149, 88-96.	3.8	157
42	Crystal Structure and Superconductivity of Tetragonal and Monoclinic Ce_{1â€“x}Pr_xOBiS₂. Inorganic Chemistry, 2018, 57, 5364-5370.	1.9	14
43	Firstâ€principles study in an interâ€granular glassy film model of silicon nitride. Journal of the American Ceramic Society, 2018, 101, 2673-2688.	1.9	23
44	Position effects of mirrorâ€“lamp system on the growth of rutile crystal based on the infrared convergent-heating floating zone method. Journal of Crystal Growth, 2018, 496-497, 69-73.	0.7	1
45	Compositional descriptor-based recommender system for the materials discovery. Journal of Chemical Physics, 2018, 148, 241719.	1.2	33
46	Synthesis, crystal structure and optical absorption of NaInS2-Se. Journal of Alloys and Compounds, 2018, 750, 409-413.	2.8	8
47	Temperature-dependent phonon spectra of magnetic random solid solutions. Npj Computational Materials, 2018, 4, .	3.5	19
48	Crystal growth of La 2/3- x Li 3 x TiO 3 by the TSFZ method. Royal Society Open Science, 2018, 5, 181445.	1.1	8
49	High Rate Performance of Dual-Substituted LiFePO₄ Based on Controlling Metastable Intermediate Phase. ACS Applied Energy Materials, 2018, 1, 6736-6740.	2.5	9
50	Synthesis of Bi₂(O,F)S₂ superconductors by NaF treatment. Journal of the Ceramic Society of Japan, 2018, 126, 591-593.	0.5	2
51	Data-centric science for materials innovation. MRS Bulletin, 2018, 43, 659-663.	1.7	26
52	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
53	Linearized machine-learning interatomic potentials for non-magnetic elemental metals: Limitation of pairwise descriptors and trend of predictive power. Journal of Chemical Physics, 2018, 148, 234106.	1.2	20
54	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

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55	Double thermoelectric power factor of a 2D electron system. Nature Communications, 2018, 9, 2224.	5.8	48
56	Matrix- and tensor-based recommender systems for the discovery of currently unknown inorganic compounds. Physical Review Materials, 2018, 2, .	0.9	39
57	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	24
58	Thermoelectric phase diagram of the SrTiO3â€“SrNbO3 solid solution system. Journal of Applied Physics, 2017, 121, .	1.1	22
59	Theoretical investigation of solid solution states of Ti1âˆ’V H2. Acta Materialia, 2017, 134, 274-282.	3.8	4
60	Growth and superconducting properties of Cd-doped La(O,F)BiS2 single crystals. Solid State Communications, 2017, 261, 32-36.	0.9	3
61	First-Principles Selection of Solute Elements for Er-Stabilized Bi₂O₃ Oxide-Ion Conductor with Improved Long-Term Stability at Moderate Temperatures. Chemistry of Materials, 2017, 29, 3763-3768.	3.2	26
62	Mode decomposition based on crystallographic symmetry in the band-unfolding method. Physical Review B, 2017, 95, .	1.1	46
63	Competing Structural Instabilities in the Ruddlesdenâ€“Popper Derivatives HRTiO₄ (R = Rare) Tj ETQq1 1 0.784314 rgBT /O Centrosymmetricity. Chemistry of Materials, 2017, 29, 656-665.	3.2	22
64	Band structure diagram paths based on crystallography. Computational Materials Science, 2017, 128, 140-184.	1.4	457
65	Thermodynamics of Meissner effect and flux pinning behavior in the bulk of single-crystal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mrow><mml:mn>2</mml:mn>		

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73	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. Journal of Physical Chemistry C, 2017, 121, 18947-18953.	1.5	44
74	Ce 4f electronic states of CeO1â”xFxBiS2 studied by soft x-ray photoemission spectroscopy. Physical Review B, 2017, 95, .	1.1	5
75	First-principles screening of structural properties of intermetallic compounds on martensitic transformation. Npj Computational Materials, 2017, 3, .	3.5	12
76	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
77	Coexistence of superconductivity and charge-density wave in the quasi-one-dimensional material HfTe3. Scientific Reports, 2017, 7, 45217.	1.6	43
78	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. Physical Review B, 2017, 95, .	1.1	59
79	Control of the solid-liquid interface during growth of a Ce-doped Gd 2 Si 2 O 7 crystal by the traveling solvent floating zone method. Journal of Crystal Growth, 2017, 468, 465-468.	0.7	3
80	Discovery of a Novel Sn(II)â€Based Oxide Î²â€SnMoO₄ for Daylightâ€Driven Photocatalysis. Advanced Science, 2017, 4, 1600246.	5.6	22
81	Effects of growth parameters on silicon molten zone formed by infrared convergent-heating floating zone method. Journal of Crystal Growth, 2017, 459, 105-111.	0.7	5
82	New Approaches to Computational Materials Science Using First Principles Methods. Materia Japan, 2017, 56, 234-237.	0.1	0
83	Direct evidence of hidden local spin polarization in a centrosymmetric superconductor LaO0.55 F0.45BiS2. Nature Communications, 2017, 8, 1919.	5.8	52
84	Materials Design Using First-Principles Calculations for Lithium-Ion Batteries. Materia Japan, 2017, 56, 430-433.	0.1	0
85	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
86	Impacts of first principles calculations in engineering ceramics. Journal of the Ceramic Society of Japan, 2016, 124, 791-795.	0.5	3
87	First-principles calculations of high-pressure phase transition of TiO2 during decompression: From baddeleyite-type TiO2 to Î±-PbO2-type TiO2. Journal of Applied Physics, 2016, 120, 142108.	1.1	5
88	Floating Zone Growth and Characterization of (Ca_{1â€“x}Nd_x)₁₂Al₁₄O_{33+6x} (x â‰¤ 0.001) Single Crystals. ACS Omega, 2016, 1, 1157-1163.	2.6	5
89	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. APL Materials, 2016, 4, 104809.	2.2	12
90	Improper Inversion Symmetry Breaking and Piezoelectricity through Oxygen Octahedral Rotations in Layered Perovskite Family, LiRTiO₄ (R = Rare Earths). Advanced Electronic Materials, 2016, 2, 1500196.	2.6	28

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91	Growth and Structure of Ce(O,F)SbS₂ Single Crystals. Crystal Growth and Design, 2016, 16, 3037-3042.	1.4	23
92	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb₂O₆. Journal of Physical Chemistry C, 2016, 120, 9604-9611.	1.5	25
93	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
94	Bulk sensitive angle-resolved photoelectron spectroscopy on Nd(O,F)BiS2. Journal of Physics: Conference Series, 2016, 683, 012003.	0.3	4
95	Superconductivity in CeOBiS2 with cerium valence fluctuation. Solid State Communications, 2016, 245, 11-14.	0.9	31
96	Low phonon conductivity of layered BiCuOS, BiCuOSe, and BiCuOTe from first principles. Physical Review B, 2016, 94, .	1.1	28
97	Stability of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï‰</mml:mi></mml:math>structure of transition elements. Physical Review B, 2016, 93, .	1.1	17
98	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
99	Comparative ARPES studies of LaO_xF_{1â^'x}BiS₂(x = 0.23 and 0.46). Journal of Physics: Conference Series, 2016, 683, 012002.	0.3	3
100	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. Nature Communications, 2016, 7, 11962.	5.8	208
101	Correction to Structure, Superconductivity, and Magnetism of Ce(O,F)BiS₂ Single Crystals. Crystal Growth and Design, 2016, 16, 2459-2459.	1.4	0
102	Categorization of surface polarity from a crystallographic approach. Computational Materials Science, 2016, 113, 221-230.	1.4	43
103	Ï‰ structure in steel: A first-principles study. Journal of Alloys and Compounds, 2016, 684, 624-627.	2.8	20
104	Pure H ^{â€“} conduction in oxyhydrides. Science, 2016, 351, 1314-1317.	6.0	155
105	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
106	Toward Materials Discovery with First-Principles Datasets and Learning Methods. Springer Series in Materials Science, 2016, , 173-186.	0.4	0
107	Effects of tilt angle of mirrorâ€“lamp system on shape of solidâ€“liquid interface of silicon melt during floating zone growth using infrared convergent heating. Journal of Crystal Growth, 2016, 433, 24-30.	0.7	7
108	Crystal growth and anisotropy of high temperature thermoelectric properties of yttrium borosilicide single crystals. Journal of Solid State Chemistry, 2016, 233, 1-7.	1.4	18

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109	First-principles interatomic potentials for ten elemental metals via compressed sensing. Physical Review B, 2015, 92, .	1.1	71
110	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
111	Stability of 12CaO·7Al₂O₃ Crystal under High-Pressure: Experimental and First-Principles Approaches. Materials Transactions, 2015, 56, 1350-1353.	0.4	6
112	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
113	Selective fabrication of nâ€•and pâ€ŧype SnO films without doping. Physica Status Solidi - Rapid Research Letters, 2015, 9, 192-196.	1.2	18
114	Proton trapping in Y and Sn Co-doped BaZrO₃. Journal of Materials Chemistry A, 2015, 3, 10045-10051.	5.2	32
115	Axis symmetry of silicon molten zone interface shape under a mirror-shifting-type infrared convergent-heating floating-zone method. CrystEngComm, 2015, 17, 9452-9458.	1.3	4
116	Epitaxial growth of tin(II) niobate with a pyrochlore structure. Journal of Crystal Growth, 2015, 416, 126-129.	0.7	5
117	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
118	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
119	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
120	Distributions of phonon lifetimes in Brillouin zones. Physical Review B, 2015, 91, .	1.1	963
121	Li Intercalation into a Î²-MnO₂ Grain Boundary. ACS Applied Materials & Interfaces, 2015, 7, 8125-8131.	4.0	19
122	Special quasirandom structure in heterovalent ionic systems. Physical Review B, 2015, 91, .	1.1	6
123	YB48 the metal rich boundary of YB66; crystal growth and thermoelectric properties. Journal of Physics and Chemistry of Solids, 2015, 87, 221-227.	1.9	19
124	C-axis electrical resistivity of PrO_{1â^'}_aF_aBiS₂single crystals. Japanese Journal of Applied Physics, 2015, 54, 083101.	0.8	22
125	First principles phonon calculations in materials science. Scripta Materialia, 2015, 108, 1-5.	2.6	7,324
126	Structure, Superconductivity, and Magnetism of Ce(O,F)BiS2 Single Crystals. Crystal Growth and Design, 2015, 15, 39-44.	1.4	32

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127	Growth of Cu(In,Ga)S 2 single crystals using CsCl flux. Journal of Crystal Growth, 2015, 412, 16-19.	0.7	2
128	Superconducting Anisotropies of F-Substituted LaOBiSe₂ Single Crystals. Journal of the Physical Society of Japan, 2014, 83, 114709.	0.7	26
129	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:msub><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
130	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
131	Mn L2,3-edge X-ray absorption spectroscopic studies on charge-discharge mechanism of Li2MnO3. Applied Physics Letters, 2014, 104, .	1.5	42
132	Sparse representation for a potential energy surface. Physical Review B, 2014, 90, .	1.1	81
133	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
134	Cluster expansion of multicomponent ionic systems with controlled accuracy: importance of long-range interactions in heterovalent ionic systems. Journal of Physics Condensed Matter, 2014, 26, 115403.	0.7	17
135	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
136	Superconducting Double Perovskite Bismuth Oxide Prepared by a Lowâ€Temperature Hydrothermal Reaction. Angewandte Chemie - International Edition, 2014, 53, 3599-3603.	7.2	61
137	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
138	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.	7.9	60
139	Zr coordination change during crystallization of MgOâ€“Al2O3â€“SiO2â€“ZrO2 glass ceramics. Journal of Non-Crystalline Solids, 2014, 384, 47-54.	1.5	34
140	Photocatalytic activity of Î±-PbO₂-type TiO₂. Physica Status Solidi - Rapid Research Letters, 2014, 8, 822-826.	1.2	13
141	Local Structure and Energetics of Pr- and La-Doped SrTiO3 Grain Boundaries and the Influence on Coreâ€“Shell Structure Formation. Journal of Physical Chemistry C, 2014, 118, 25765-25778.	1.5	19
142	Efficient determination of alloy ground-state structures. Physical Review B, 2014, 90, .	1.1	11
143	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
144	Effects of lamp power and mirror position on the interface shape of the silicon molten zone during infrared convergent heating. CrystEngComm, 2014, 16, 4619-4623.	1.3	12

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145	First principles study of dopant solubility and defect chemistry in LiCoO₂. Journal of Materials Chemistry A, 2014, 2, 11235-11245.	5.2	52
146	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. Physical Review B, 2014, 90, .	1.1	36
147	Proton incorporation and trapping in ZrO₂grain boundaries. Journal of Materials Chemistry A, 2014, 2, 1400-1408.	5.2	20
148	Accelerated discovery of cathode materials with prolonged cycle life for lithium-ion battery. Nature Communications, 2014, 5, 4553.	5.8	108
149	Feed Size Dependence of Position Effects of Mirror-Lamp System on Shape of Silicon Crystal during Its Growth by Mirror-Shifting-Type Infrared Convergent-Heating Floating Zone Method. Crystal Growth and Design, 2014, 14, 5117-5121.	1.4	7
150	Significant Reduction in Hydration Energy for Yttria Stabilized Zirconia Grain Boundaries and the Consequences for Proton Conduction. Langmuir, 2014, 30, 10456-10464.	1.6	9
151	Surface design of alloy protection against CO-poisoning from first principles. Journal of Physics Condensed Matter, 2014, 26, 355006.	0.7	2
152	Protonic defects in yttria stabilized zirconia: incorporation, trapping and migration. Physical Chemistry Chemical Physics, 2014, 16, 4814.	1.3	15
153	Cytotoxicity of stoichiometric hydroxyapatites with different crystallite sizes. Journal of Asian Ceramic Societies, 2014, 2, 64-67.	1.0	10
154	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
155	Growth and superconducting properties of F-substituted ROBiS2 (R=La, Ce, Nd) single crystals. Solid State Communications, 2014, 178, 33-36.	0.9	83
156	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212
157	Atomic Structure of Luminescent Centers in High-Efficiency Ce-doped w-AlN Single Crystal. Scientific Reports, 2014, 4, 3778.	1.6	43
158	Effect of local coordination of Mn on Mn-L2,3 edge electron energy loss spectrum. Journal of Applied Physics, 2013, 114, .	1.1	21
159	Strong Spinâ€Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. Advanced Functional Materials, 2013, 23, 1864-1872.	7.8	41
160	Ground state of the singly ionized oxygen vacancy in rutile TiO2. Journal of Applied Physics, 2013, 114, .	1.1	23
161	First-principles study of valence band offsets at ZnSnP2/CdS, ZnSnP2/ZnS, and related chalcopyrite/zincblende heterointerfaces. Journal of Applied Physics, 2013, 114, .	1.1	24
162	Functional Complex Point-Defect Structure in a Huge-Size-Mismatch System. Physical Review Letters, 2013, 110, 065504.	2.9	40

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