Tamio Oguchi

List of Publications by Year
in descending order

205 papers	7,273 citations	66234 42 h-index	64668 79 g-index
205 all docs	205 docs citations	205 times ranked	5681 citing authors

#	Article	IF	Citations
1	Band theory of insulating transition-metal monoxides: Band-structure calculations. Physical Review B, 1984, 30, 4734-4747.	1.1	548
2	Prediction of Strongly Enhanced Two-Dimensional Ferromagnetic Moments on Metallic Overlayers, Interfaces, and Superlattices. Physical Review Letters, 1985, 54, 2700-2703.	2.9	525
3	Electronic band structure of the superconductorSr2RuO4. Physical Review B, 1995, 51, 1385-1388.	1.1	392
4	Transition-Metal Monoxides: Band or Mott Insulators. Physical Review Letters, 1984, 52, 1830-1833.	2.9	260
5	Origin of the metallic properties of heavily boron-doped superconducting diamond. Nature, 2005, 438, 647-650.	13.7	244
6	Magnetism of iron above the Curie temperature. Journal of Physics F: Metal Physics, 1983, 13, 145-160.	1.6	198
7	Band theory of the magnetic interaction in MnO, MnS, and NiO. Physical Review B, 1983, 28, 6443-6452.	1.1	156
8	Crystal structure, phase stability, and electronic structure of Ti-Al intermetallics:TiAl3. Physical Review B, 1990, 41, 12462-12467.	1.1	152
9	Electronic theory of the alloy phase stability of Cu-Ag, Cu-Au, and Ag-Au systems. Physical Review B, 1987, 35, 2169-2173.	1.1	151
10	Crystal structure, phase stability, and magnetism inNi3V. Physical Review B, 1987, 35, 6940-6943.	1.1	132
11	Peculiar Rashba Splitting Originating from the Two-Dimensional Symmetry of the Surface. Physical Review Letters, 2009, 103, 156801.	2.9	124
12	Solid-solution strengthening: Substitution of V inNi3Al and structural stability ofNi3(Al,V). Physical Review B, 1987, 36, 4186-4189.	1.1	123
13	First-Principles Predictions of Giant Electric Polarization. Japanese Journal of Applied Physics, 2005, 44, 7130-7133.	0.8	109
14	Crystal structure, phase stability, and electronic structure of Ti-Al intermetallics:Ti3Al. Physical Review B, 1991, 43, 1940-1947.	1.1	103
15	Origin of the Two-Peak Photoemission and Inverse-Photoemission Spectra in Ce and Ce Compounds. Physical Review Letters, 1984, 53, 1673-1676.	2.9	95
16	Crystal structure prediction accelerated by Bayesian optimization. Physical Review Materials, 2018, 2, .	0.9	94
17	Extremely Large Magnetoresistance in the Nonmagnetic Metal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>PdCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2013, 111, 056601.	2.9	89
18	Structural, electronic, and magnetic properties of Co: Evidence for magnetism-stabilizing structure. Physical Review B, 1986, 33, 7852-7854.	1.1	86

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19	Self-consistent electronic structures of magnetic semiconductors by a discrete variationalXÎ±calculation. III. Chalcopyrite CuFeS2. Physical Review B, 1981, 24, 3349-3353.	1.1	85
20	Implications of Band-Structure Calculations for High-TcRelated Oxides. Journal of the Physical Society of Japan, 1988, 57, 3445-3456.	0.7	83
21	Phase stability and magnetism ofNi3Al. Physical Review B, 1990, 41, 5010-5016.	1.1	78
22	Total-energy local-density studies of theÎ±-Î³phase transition in Ce. Physical Review B, 1986, 34, 369-378.	1.1	76
23	Magnetically induced tetragonal lattice distortion in antiferromagnetic fcc Mn. Journal of Magnetism and Magnetic Materials, 1984, 46, L1-L4.	1.0	75
24	Local density band approach to f-electron systems â€" heavy fermion superconductor UPt3. Journal of Magnetism and Magnetic Materials, 1985, 52, 174-178.	1.0	71
25	Ultrahigh-Resolution Photoemission Spectroscopy of Ni Borocarbides: Direct Observation of the Superconducting Gap and a Change in Gap Anisotropy by Impurity. Physical Review Letters, 2000, 85, 4952-4955.	2.9	70
26	Cohesion in AlB2-Type Diborides: A First-Principles Study. Journal of the Physical Society of Japan, 2002, 71, 1495-1500.	0.7	66
27	Tunable Spin Polarization in Bismuth Ultrathin Film on Si(111). Nano Letters, 2012, 12, 1776-1779.	4.5	65
28	Local density total energy description of ground and excited state properties of the rare earth metals. Journal of Magnetism and Magnetic Materials, 1986, 61, 139-150.	1.0	61
29	First-Principles Study of Lead-Free Piezoelectric SnTiO₃. Japanese Journal of Applied Physics, 2008, 47, 7735.	0.8	60
30	Angle-dependent magnetoresistance oscillation in the layered perovskiteSr2RuO4. Physical Review B, 1999, 59, 7263-7265.	1.1	58
31	The surface Rashba effect: akÂ·pperturbation approach. Journal of Physics Condensed Matter, 2009, 21, 092001.	0.7	58
32	First principles calculation of thermodynamic properties of noble-metal alloys. Acta Metallurgica, 1988, 36, 547-553.	2.1	57
33	Large out-of-plane spin polarization in a spin-splitting one-dimensional metallic surface state on Si(557)-Au. Physical Review B, 2010, 82, .	1.1	55
34	Signature of high Tc above 25â€‰K in high quality superconducting diamond. Applied Physics Letters, 2015, 106, 052601.	1.5	54
35	Topological proximity effect in a topological insulator hybrid. Nature Communications, 2015, 6, 6547.	5.8	53
36	First-principles study on the electronic structure of bismuth transition-metal oxides. Journal of Physics Condensed Matter, 2004, 16, S5677-S5683.	0.7	51

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37	Electronic Band Structure of the Pyrochlore Ruthenium OxidesA2Ru2O7(A=Bi, Tl and Y). Journal of the Physical Society of Japan, 2000, 69, 526-531.	0.7	49
38	Optical Reflectivity Spectrum of a CuFeS2 Single Crystal. Journal of the Physical Society of Japan, 1980, 48, 123-128.	0.7	47
39	Fermi-velocity effect on magnetoresistance in Fe/transition-metal multilayers. Journal of Magnetism and Magnetic Materials, 1993, 126, 519-520.	1.0	45
40	Orbital and spin magnetic moments ofTPt3(T=V, Cr, Mn, Fe, and Co). Physical Review B, 1996, 54, 1159-1162.	1.1	44
41	Quantum Oscillations of the Metallic Triangular-Lattice Antiferromagnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>PdCrO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2013, 111, 176405.	2.9	44
42	Local and non-local spin susceptibilities of transition metals. Journal of Physics F: Metal Physics, 1982, 12, 1661-1678.	1.6	43
43	Electronic Property of La2CuO4with Two Different Layered Structures. Japanese Journal of Applied Physics, 1987, 26, L417-L419.	0.8	40
44	Electronic States of Perovskite-Type Oxides and Ferroelectricity. Japanese Journal of Applied Physics, 2000, 39, 5679-5682.	0.8	40
45	Conversion of a conventional superconductor into a topological superconductor by topological proximity effect. Nature Communications, 2020, 11, 159.	5.8	40
46	First-principles calculation of the exchange interaction and the exchange force between magnetic Fe films. Physical Review B, 1997, 56, 3218-3221.	1.1	39
47	Coupling Ferroelectricity with Spin-Valley Physics in Oxide-Based Heterostructures. Physical Review Letters, 2015, 115, 037602.	2.9	38
48	Strong enhancement of piezoelectric constants in ScxAl1â^'xN: First-principles calculations. AIP Advances, 2016, 6, .	0.6	36
49	Effects of lattice parameters on piezoelectric constants in wurtzite materials: A theoretical study using first-principles and statistical-learning methods. Applied Physics Express, 2018, 11, 041201.	1.1	36
50	Electronic and structural properties of rare earth metals at normal and high pressures: Eu and Yb. Journal of Magnetism and Magnetic Materials, 1986, 59, 277-286.	1.0	35
51	Structural, electronic, and magnetic properties ofFe16N2. Physical Review B, 1994, 50, 10004-10008.	1.1	34
52	Li impurity in ZnSe: Electronic structure and the stability of the acceptor. Physical Review B, 1991, 43, 9362-9364.	1.1	33
53	First-Principles Studies of Antiferromagnetic MnO and NiO Surfaces. Journal of the Physical Society of Japan, 2003, 72, 588-593.	0.7	33
54	Tetrahedral tilting and ferroelectricity in Bi2AO5 (A=Si, Ge) from first principles calculations. Journal of Solid State Chemistry, 2016, 235, 68-75.	1.4	33

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55	Spin injection through energy-band symmetry matching with high spin polarization in atomically controlled ferromagnet/ferromagnet/semiconductor structures. NPG Asia Materials, 2020, 12, .	3.8	32
56	Electronic structure and spin polarisation of the transition metal thin film V(100). Journal of Physics F: Metal Physics, 1981, 11, 1643-1654.	1.6	31
57	Hartree-Fock study on the5forbital magnetic moment of US. Physical Review B, 1999, 59, 6813-6823.	1.1	31
58	Ab initiostudy of magnetic coupling in CaCu<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><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>B</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	1.1	31
59	Strain Engineering for Anion Arrangement in Perovskite Oxynitrides. ACS Nano, 2017, 11, 3860-3866.	7.3	31
60	Anisotropic superconductivity in UPt3. Physics Letters, Section A: General, Atomic and Solid State Physics, 1986, 117, 428-432.	0.9	30
61	Magnetic ground state of metallic hydrogen and lithium in the low-density limit. Physical Review B, 1986, 33, 324-329.	1.1	30
62	Low Temperature Specific Heat and Electrical Resistivity in Orthorhombic YBa2Cu3O6.8and Tetragonal YBa2Cu3O6.0. Japanese Journal of Applied Physics, 1987, 26, L1953-L1955.	0.8	30
63	Crystal structure predictions of Na C6O6 for sodium-ion batteries: First-principles calculations with an evolutionary algorithm. Electrochimica Acta, 2016, 195, 1-8.	2.6	30
64	Self-consistent electronic structures of magnetic semiconductors by a discrete variationalXÎ±calculation. I. Ferromagnetic spinels, CdCr2S4and CdCr2Se4. Physical Review B, 1980, 22, 872-879.	1.1	29
65	Hybridization, electronic structure and properties of uranium intermetallics: URu3, URh3, UPd3, UIr3 and UPt3. Journal of Magnetism and Magnetic Materials, 1986, 61, 233-245.	1.0	29
66	Magnetism in the heavy-electron superconductorsUPt3andURu2Si2. Physical Review B, 1988, 38, 11193-11198.	1.1	29
67	Molecular-dynamics simulations for molecular-beam epitaxy: Overlayer growth pattern in two-component Lennard-Jones systems. Physical Review B, 1989, 39, 9476-9485.	1.1	29
68	Atomic-Layer Alignment Tuning for Giant Perpendicular Magnetocrystalline Anisotropy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:math>Transition-Metal Thin Films. Physical Review Letters, 2013, 110, 267206.	2.9	29
69	Electronic structure and magnetic properties of the half-metallic ferrimagnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mn</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>by soft x-ray spectroscopies. Physical Review B, 2018, 97, .	1.1	29
70	Asymmetric Phosphorus Incorporation in Homoepitaxial P-Doped (111) Diamond Revealed by Photoelectron Holography. Nano Letters, 2019, 19, 5915-5919.	4.5	29
71	Density-Functional Molecular-Dynamics Method. Progress of Theoretical Physics Supplement, 1991, 103, 93-117.	0.2	28
72	Ultrathin Bismuth Film on 1T-TaS₂: Structural Transition and Charge-Density-Wave Proximity Effect. Nano Letters, 2018, 18, 3235-3240.	4.5	28

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73	Electronic band structure of YBa2Cu4O8. Physica C: Superconductivity and Its Applications, 1990, 172, 277-281.	0.6	27
74	Electronic Band Structure and Structural Properties of Zircon Nitride Chloride. Journal of the Physical Society of Japan, 2004, 73, 2771-2776.	0.7	27
75	First-principles exploration of ferromagnetic and ferroelectric double-perovskite transition-metal oxides. Physica B: Condensed Matter, 2006, 383, 9-12.	1.3	27
76	Bulk and surface electronic structures ofCePdX(X=As,Sb)studied by3dâ˜4fresonance photoemission. Physical Review B, 2000, 61, 4621-4628.	1.1	26
77	First-principles study on exchange force image of NiO(001) surface using a ferromagnetic Fe probe. Surface Science, 2005, 590, 42-50.	0.8	26
78	On the Phase Relation between Two Polymorphs of Ba1.8Y1.2Cu3O6.7-Î´and Their Oxygen Contents. Japanese Journal of Applied Physics, 1987, 26, L791-L793.	0.8	25
79	Surface structure of Cu(001)-c(2Ã—2)â€“Mg: a tensor low energy electron diffraction analysis and a first-principles calculation. Surface Science, 2000, 470, 53-61.	0.8	25
80	Local-density total-energy supercell description of excited-state properties of solids: Ce photoemission and inverse photoemission spectra. Physical Review B, 1986, 33, 8005-8015.	1.1	24
81	Electronic structure of UPd3 â€” A localized f compound. Journal of Magnetism and Magnetic Materials, 1987, 69, 27-33.	1.0	24
82	Band-theoretical prediction of magnetic anisotropy in uranium monochalcogenides. Physical Review B, 2000, 62, 11747-11750.	1.1	24
83	Cathode Properties of Perovskite-type NaMF3 (M= Fe, Mn, and Co) Prepared by Mechanical Ball Milling for Sodium-ion Battery. Electrochimica Acta, 2017, 245, 424-429.	2.6	24
84	First-Principles Study on Structural and Electronic Properties of Î±-S and Naâ€“S Crystals. Journal of the Physical Society of Japan, 2014, 83, 124713.	0.7	23
85	Transitionâ€metal monoxides: Itinerant versus localized picture of superexchange. Journal of Applied Physics, 1984, 55, 2318-2320.	1.1	22
86	Electronic structure, dynamic susceptibility, and NÃ©el temperature of the heavy-fermion magnetUCu5. Physical Review B, 1988, 38, 6818-6823.	1.1	22
87	Anomalous Hall conductivity and electronic structures of Si-substituted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mn</mml:mi><mml:mn>2</mml:mn></ epitaxial films. Physical Review B, 2018, 97, .	1.1	21
88	Electronic band structures of semiconducting ferromagnetic spinels CdCr2S4and CdCr2Se4. Journal of Physics C: Solid State Physics, 1980, 13, 1493-1511.	1.5	20
89	Electronic structure and magnetism of Cr/Sn multilayer systems. Journal of Magnetism and Magnetic Materials, 2001, 234, 126-132.	1.0	20
90	Fine-grained optimization method for crystal structure prediction. Npj Computational Materials, 2018, 4, .	3.5	20

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91	Theoretical study on the electronic structure of (Si)m/(Ge)nsuperlattices. Physical Review B, 1993, 48, 1571-1582.	1.1	19
92	Magnetoresistance in magnetic multilayers: A role of Fermi velocity. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1995, 31, 111-116.	1.7	19
93	Surface atomic forces and multilayer relaxation of W(001), W(110) and Fe/W(110). Surface Science, 1998, 417, 151-158.	0.8	19
94	Stability of Alkali-Metal Adsorption on fcc-Metal Surfaces: Cu(001)-(2Ã—1)-Li and Al(001)-c(2Ã—2)-Na. Journal of the Physical Society of Japan, 1998, 67, 978-982.	0.7	19
95	Relationship between Lattice Deformation and Polarization in BaTiO3. Japanese Journal of Applied Physics, 2001, 40, 5809-5811.	0.8	18
96	First-Principles Study on the Magnetic Anisotropy in Multiferroic PbVO₃ and BiCoO₃. Journal of the Physical Society of Japan, 2009, 78, 084709.	0.7	18
97	Local electronic states of Fe4N films revealed by x-ray absorption spectroscopy and x-ray magnetic circular dichroism. Journal of Applied Physics, 2015, 117, .	1.1	18
98	High-TcSuperconductor Ba0.5Y0.5Cu1Ox. Japanese Journal of Applied Physics, 1987, 26, L332-L333.	0.8	17
99	Electronic Structure of B-2pState in AlB2Single Crystal: Direct Observation ofpÏƒ andpÏ€ Density of States. Journal of the Physical Society of Japan, 2002, 71, 408-410.	0.7	17
100	Electronic structure of B-doped diamond: A first-principles study. Science and Technology of Advanced Materials, 2006, 7, S67-S70.	2.8	17
101	Why Are Garnets Not Ferroelectric? A Theoretical Investigation of Y₃Fe₅O₁₂. Chemistry of Materials, 2008, 20, 7545-7550.	3.2	17
102	Magnetic and transport properties of equiatomic quaternary Heusler CoFeVSi epitaxial films. Physical Review Materials, 2018, 2, .	0.9	17
103	Electronic and structural properties of Lu under pressure: Relation to structural phases of the rare-earth metals. Physical Review B, 1986, 34, 654-658.	1.1	15
104	Ultrathin Bismuth Film on High-Temperature Cuprate Superconductor Bi2Sr2CaCu2O8+Î´ as a Candidate of a Topological Superconductor. ACS Nano, 2018, 12, 10977-10983.	7.3	15
105	Theoretical Study of the Low-Temperature c(2Ã—2) Structure of Li Adsorbed Cu (001) Surface. Journal of the Physical Society of Japan, 1997, 66, 2751-2757.	0.7	14
106	Electronic Band Structure of SrCuO2. Journal of the Physical Society of Japan, 1997, 66, 1756-1761.	0.7	13
107	Giant converse magnetoelectric effect in a multiferroic heterostructure with polycrystalline Co2FeSi. NPG Asia Materials, 2022, 14, .	3.8	13
108	Electronic Band Structure and Gap Formation in CeRhAs. Journal of the Physical Society of Japan, 2004, 73, 145-151.	0.7	12

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109	Anisotropic s-wave superconductors studied by angle-resolved photoemission spectroscopy. Journal of Physics and Chemistry of Solids, 2006, 67, 277-281.	1.9	12
110	Role of van der Waals interaction in crystalline ammonia borane. Applied Physics Letters, 2011, 99, 181904.	1.5	12
111	Amorphous xNaF-FeSO₄ Systems (1 â‰¤ x â‰¤ 2) with Excellent Cathode Properties for Sodium-Ion Batteries. ACS Applied Energy Materials, 2019, 2, 5968-5974.	2.5	12
112	Half-metallicity of the ferrimagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">M</mml:mi><mml:msub><mml:mi mathvariant="normal">n</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>VAl</mml:mi></mml:mrow></mml:math> revealed by resonant inelastic soft x-ray scattering in a magnetic field. Physical Review B, 2019, 99, .	1.1	12
113	Insight into the diffusion mechanism of sodium ionâ€“polaron complexes in orthorhombic P2 layered cathode oxide Na_xMnO₂. Physical Chemistry Chemical Physics, 2020, 22, 18219-18228.	1.3	12
114	Magnetocaloric effect in MnCoGe alloys studied by first-principles calculations and Monte-Carlo simulation. Solid State Communications, 2021, 323, 114077.	0.9	12
115	Magnetism and electronic structure of bimetallic superlattices: Cr/Fe. Journal of Magnetism and Magnetic Materials, 1990, 86, 26-30.	1.0	11
116	FLAPW calculations of the magneto-optical Kerr effect of BCC Fe. Journal of Magnetism and Magnetic Materials, 1999, 192, 325-333.	1.0	11
117	First-Principles Investigation of Magneto-Optical Kerr Effect of Metallic Mutilayers. Journal of the Physical Society of Japan, 1999, 68, 1412-1422.	0.7	11
118	First-Principles Calculation of Spontaneous Polarization and Phase Stability in NaNO2. Journal of the Physical Society of Japan, 2002, 71, 336-339.	0.7	11
119	Discharge Reaction Mechanisms in Na/FeS₂ Batteries: First-Principles Calculations. Journal of the Physical Society of Japan, 2015, 84, 124709.	0.7	11
120	First-Principles Study on Cathode Properties of Li₂MTiO₄ (M = V,) Tj ETQq0 0 0 rgBT /Overlock 1 Japan, 2018, 87, 044805.	0.7	11
121	Firstâ€Principles Study of Naâ€Ion Battery Performance and Reaction Mechanism of Tin Sulfide as Negative Electrode. Chemical Record, 2019, 19, 811-816.	2.9	11
122	Electric-field tuning of the magnetic properties of bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>VI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:m : A first-principles study. Physical Review B, 2021, 104, .	1.1	11
123	Self-consistent electronic structures of magnetic semiconductors by a discrete variationalXÎ±calculation. II. HgCr2Se4. Physical Review B, 1981, 24, 3441-3444.	1.1	10
124	Selective and low temperature transition metal intercalation in layered tellurides. Nature Communications, 2016, 7, 13809.	5.8	10
125	Augmented-Plane-Wave Force Calculations for Transition-Metal Systems. Springer Series in Solid-state Sciences, 1993, , 33-41.	0.3	10
126	Theoretical Study of c(2Ã—2) Structure in Li/Al(001) System. Journal of the Physical Society of Japan, 2000, 69, 2192-2198.	0.7	10

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127	Electronic Band Structure of Magnetic Semiconductors with Spinel Structure. Japanese Journal of Applied Physics, 1980, 19, 223.	0.8	9
128	Alternating change of allowed and forbidden optical transitions in (Si)2m/(Ge)10â^'2msuperlattices with (001) stacking. Physical Review B, 1992, 45, 1496-1499.	1.1	9
129	Theory of the self-compensation in p-type ZnSe. Journal of Crystal Growth, 1992, 117, 625-633.	0.7	9
130	Near EF electronic structure of heavily boron-doped superconducting diamond. Journal of Physics and Chemistry of Solids, 2008, 69, 2978-2981.	1.9	9
131	Effect of atomic configuration on magnetic properties and electronic state of CoVMnAl quaternary heusler alloy. Journal of Alloys and Compounds, 2021, 855, 157389.	2.8	9
132	Electronic Band Structures of I-III-VI₂ Compounds. Japanese Journal of Applied Physics, 1980, 19, 107.	0.8	8
133	Possibility of measuring exchange force through force microscopy. Applied Surface Science, 1999, 140, 366-370.	3.1	8
134	First-principles calculation of exchange force on a magnetic Fe surface. Applied Surface Science, 1999, 142, 433-437.	3.1	8
135	High Resolution4d-4fResonance Photoemission Spectroscopy of CePdX (X=As, Sb). Journal of the Physical Society of Japan, 1999, 68, 1716-1724.	0.7	8
136	Contribution of Pb to Ferroelectricity in Perovskite-Type Oxides. Ferroelectrics, 2004, 301, 49-53.	0.3	8
137	First-principles study of electronic structure and thermoelectric properties of CeRhAs and related compounds. Physica B: Condensed Matter, 2004, 351, 316-318.	1.3	8
138	First-Principles Calculation of X-ray Absorption Spectra for the A-Site Ordered Perovskite CaCu₃Fe₄O₁₂. Journal of the Physical Society of Japan, 2013, 82, 094718.	0.7	8
139	Ab-initio Prediction of Magnetoelectricity in Infinite-Layer CaFeO₂and MgFeO₂. Journal of the Physical Society of Japan, 2014, 83, 094712.	0.7	8
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145	Theoretical study of the structural stability of CuPd and CuPt alloys: Pressure-induced phase transition of CuPt alloy. Physical Review B, 1991, 43, 947-955.	1.1	7
146	Polarization Performance of a New Spectrometer Based on a Multilayer-Coated Laminar Grating in the 150-190-eV Region. Optical Review, 2003, 10, 58-62.	1.2	7
147	Ab initiostudy on the electronic structure and vibration modes of alkali and alkaline-earth amides and alanates. Journal of Physics Condensed Matter, 2009, 21, 185501.	0.7	7
148	Geometrical Spin Frustration and Monoclinic-Distortion-Induced Spin Canting in the Double Perovskites Ln₂LiFeO₆ (Ln = La, Nd, Sm, and Eu) with Unusually High Valence Fe⁵⁺. Journal of the American Chemical Society, 2021, 143, 19207-19213.	6.6	7
149	Fermi-surface reconstruction involving two van Hove singularities across the antiferromagnetic transition in BaFe2As2. Solid State Communications, 2013, 157, 16-20.	0.9	6
150	Sparse modeling of chemical bonding in binary compounds. Science and Technology of Advanced Materials, 2019, 20, 1178-1188.	2.8	6
151	First-Principles Study of X-Ray Absorption Spectra in NaFeSO₄F for Exploring Na-Ion Battery Reactions. Journal of the Physical Society of Japan, 2019, 88, 124709.	0.7	6
152	Significant role of oxygen redox reaction with O2-release in Li-excess cation-disordered rock-salt cathodes Li2+2Mn1â^'Ti1â^'O4: First-principles calculations. Electrochimica Acta, 2020, 330, 135286.	2.6	6
153	Manipulation of Dirac Cone in Topological Insulator/Topological Insulator Heterostructure. ACS Applied Electronic Materials, 2021, 3, 1080-1085.	2.0	6
154	Adjusting the descriptor for a crystal structure search using Bayesian optimization. Physical Review Materials, 2020, 4, .	0.9	6
155	Dirac semimetal phase and switching of band inversion in XMg2Bi2 (Xâ€‰=â€‰Ba and Sr). Scientific Reports, 2021, 11, 21937.	1.6	6
156	Insight into anisotropic magnetocaloric effect of CrI<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Acta Materialia, 2022, 231, 117851.	3.8	6
157	Fermi surface and transport properties of YBa2Cu4O8. Journal of Physics and Chemistry of Solids, 1992, 53, 1525-1532.	1.9	5
158	Theoretical Study of the Exchange Interaction and the Exchange Force between Fe Films: Feasibility of Exchange Force Microscopy. Japanese Journal of Applied Physics, 1998, 37, 6575-6579.	0.8	5
159	Surface core-level shift of an oxygen-adsorbed W(110) surface. Surface Science, 1999, 438, 37-42.	0.8	5
160	First-Principle Studies on Elastic Properties and Spontaneous Polarizations of PbTiO3. Japanese Journal of Applied Physics, 2001, 40, 5806-5808.	0.8	5
161	CrySPY: a crystal structure prediction tool accelerated by machine learning. Science and Technology of Advanced Materials Methods, 2021, 1, 87-97.	0.4	5
162	Theoretical prediction of large anisotropic magnetocaloric effect in MnP. Computational Materials Science, 2021, 188, 110227.	1.4	5

#	Article	IF	Citations
163	Tavorite-like orthorhombic AVPO4F (A = Li, Na) for novel high-voltage cathodes in rechargeable batteries. Journal of Alloys and Compounds, 2021, 875, 159963.	2.8	5
164	Molecular orbital study of nitrogen chemisorption on tantalum (100) and (110) surfaces. Surface Science, 1981, 102, 443-462.	0.8	4
165	First-principles calculation of structural stability of alkali-atom adsorbed metal surfaces. Surface Science, 2001, 493, 99-105.	0.8	4
166	High-resolution resonant photoemission study of CeSi. Physica B: Condensed Matter, 2004, 351, 295-297.	1.3	4
167	The electronic structure of Ca-intercalated superconducting graphite CaC6. Physica C: Superconductivity and Its Applications, 2009, 469, 1041-1044.	0.6	4
168	Fermiological interpretation of FeTe _{1â^'x} Se _x thin crystal by quantum conductance oscillation. Europhysics Letters, 2013, 104, 37010.	0.7	4
169	Polar phase transitions and physical properties in fresnoite A2TiSi2O8 (A= Ba, Sr) by first principles calculations. Journal of Solid State Chemistry, 2016, 242, 136-142.	1.4	4
170	Symmetric and asymmetric exchange stiffnesses of transition-metal thin film interfaces in external electric field. Journal of Magnetism and Magnetic Materials, 2018, 457, 97-102.	1.0	4
171	Machine Learning Approach for Data Analysis of Magnetic Orbital Moments and Magnetocrystalline Anisotropy in Transition-Metal Thin Films on MgO(001). Journal of Electronic Materials, 2019, 48, 1319-1323.	1.0	4
172	Suppression of O-redox reactions by multivalent Cr in Li-excess <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mtext>Li</mml:mtext><mml:mn>2.4</mml:mn></mml:msub><mml:msub><mml:mi> (M, Mâ€™Â= Cr, Mn, and Ti) cathodes with layered and cation-disordered rock-salt structures. Electrochimica Acta, 2020, 354, 136630.	2.6	4
173	DFT-based Engineering of Dirac Surface States in Topological-insulator Multilayers. Journal of the Physical Society of Japan, 2020, 89, 094701.	0.7	4
174	Performance and reaction mechanisms of tin compounds as high-capacity negative electrodes of lithium and sodium ion batteries. Materials Advances, 2022, 3, 2793-2799.	2.6	4
175	Fermi surface and mass enhancement in the topological nodal-line semimetal NaAlSi. Physical Review B, 2022, 105, .	1.1	4
176	Theoretical study of STM in Cu(001)-(2Ã—1)â€“Li. Surface Science, 1999, 438, 26-30.	0.8	3
177	Comparisons of Piezoelectricities of Lead Zirconate Titanate for Various Phases by a First-Principles Method. Japanese Journal of Applied Physics, 2007, 46, 5199.	0.8	3
178	Bulk-sensitive spectroscopic studies on noncentrosymmetric superconducting system of Mgâ€“Irâ€“B. Physica C: Superconductivity and Its Applications, 2009, 469, 1034-1036.	0.6	3
179	Influences of Orientation on Magnetoelectric Coupling at La1â^'x Sr x MnO3/BaTiO3 Interface from Ab Initio Calculations. Journal of Electronic Materials, 2017, 46, 3808-3814.	1.0	3
180	Ta181 nuclear quadrupole resonance study of the noncentrosymmetric superconductor PbTaSe2. Physical Review B, 2020, 102, .	1.1	3

#	Article	IF	Citations
181	First-Principles Study on Structural Stability of Alkali and Alkali-Earth Coadsorbed on Cu(001) Surface. Journal of the Physical Society of Japan, 2002, 71, 880-887.	0.7	3
182	Modulation of Dirac electrons in epitaxial Bi2Se3 ultrathin films on van der Waals ferromagnet Cr2Si2Te6. Physical Review Materials, 2020, 4, .	0.9	3
183	Understanding doping effects on P2 <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Na</mml:mi><mml:mi>x</mml:mi></mml		

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199	Large magnetoresistance of a compensated metal Cu2Sb correlated with its Fermi surface topology. Physical Review Materials, 2021, 5, .	0.9	0
200	Theoretical Studies on Surface Electronics States. Super Structure of Alkali-atom Adsorbed Metal Surfaces-A First-principles Approach.. Hyomen Kagaku, 1998, 19, 167-172.	0.0	0
201	First-principles Study on Piezoelectricity and Spontaneous Polarization in Bi(Fe,Co)O₃. Journal of the Physical Society of Japan, 2021, 90, .	0.7	0
202	First-Principles Study on Cathode Properties of Li2MTiO4 and Na2MTiO4 (M = V, Cr, Mn, Fe, Co, Ni). Journal of the Physical Society of Japan, 2022, 91, .	0.7	0
203	Spin-Polarized Band Structure at MoTe₂/Bi₂Se₃ Interface Designed from First Principles. Journal of the Physical Society of Japan, 2022, 91, .	0.7	0
204	Significant effect of interfacial spin moments in ferromagnet-semiconductor heterojunctions on spin transport in a semiconductor. Physical Review B, 2022, 105, .	1.1	0
205	Electronic origin of phase stability in Mg--Zn--Y alloys with a long-period stacking order. Applied Physics Express, 0, , .	1.1	0