Teruyasu Mizoguchi

List of Publications by Year
in descending order

215 papers	6,801 citations	71097 41 h-index	79691 73 g-index
226 all docs	226 docs citations	226 times ranked	7667 citing authors

#	Article	IF	Citations
1	Giant thermoelectric Seebeck coefficient of a two-dimensional electron gas in SrTiO3. Nature Materials, 2007, 6, 129-134.	27.5	910
2	COMBO: An efficient Bayesian optimization library for materials science. Materials Discovery, 2016, 4, 18-21.	3.3	217
3	Atomic Structure of a CeO₂ Grain Boundary: The Role of Oxygen Vacancies. Nano Letters, 2010, 10, 4668-4672.	9.1	173
4	First-principles calculations of ELNES and XANES of selected wide-gap materials: Dependence on crystal structure and orientation. Physical Review B, 2004, 70, .	3.2	162
5	Oxygenâ€Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. Angewandte Chemie - International Edition, 2011, 50, 3053-3057.	13.8	127
6	Mechanism of incorporation of zinc into hydroxyapatite. Acta Biomaterialia, 2010, 6, 2289-2293.	8.3	122
7	Direct Imaging of Reconstructed Atoms on TiO ₂ (110) Surfaces. Science, 2008, 322, 570-573.	12.6	120
8	Coordination and interface analysis of atomic-layer-deposition Al2O3 on Si(001) using energy-loss near-edge structures. Applied Physics Letters, 2003, 83, 4306-4308.	3.3	112
9	XANES and ELNES in Ceramic Science. Journal of the American Ceramic Society, 2005, 88, 2013-2029.	3.8	111
10	Role of Pr Segregation in Acceptor-State Formation at ZnO Grain Boundaries. Physical Review Letters, 2006, 97, 106802.	7.8	109
11	Atomic-scale imaging of individual dopant atoms in a buried interface. Nature Materials, 2009, 8, 654-658.	27.5	109
12	Electronic Structure of Lithium Nickel Oxides by Electron Energy Loss Spectroscopy. Journal of Physical Chemistry B, 2005, 109, 10749-10755.	2.6	106
13	Yttrium doping effect on oxygen grain boundary diffusion in Î±-Al2O3. Acta Materialia, 2007, 55, 6627-6633.	7.9	101
14	Core-hole effects on theoretical electron-energy-loss near-edge structure and near-edge x-ray absorption fine structure of MgO. Physical Review B, 2000, 61, 2180-2187.	3.2	98
15	Atomic structure, electronic structure, and defect energetics in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>[</mml:mo><mml:mrow><mml:mn>001</mml:mn></mml:mrow><mml:mo>]</mml:mo></mml:mrow></mml:mrow></mml:math> boundaries of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:ms>. Physical Review B, 2008, 78, .	3.2	98
16	First-principles multielectron calculations of NiL2,3NEXAFS and ELNES forLiNiO2and related compounds. Physical Review B, 2005, 72, .	3.2	94
17	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:mi> 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, .	3.2	94
18	First-principles calculation of spectral features, chemical shift and absolute threshold of ELNES and XANES using a plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104204.	1.8	88

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19	Enhanced Seebeck coefficient of quantum-confined electrons in SrTiO3âˆ•SrTi0.8Nb0.2O3 superlattices. Applied Physics Letters, 2007, 91, .	3.3	85
20	Theoretical ELNES using one-particle and multi-particle calculations. Micron, 2010, 41, 695-709.	2.2	79
21	Identification of ultradilute dopants in ceramics. Nature Materials, 2003, 2, 541-545.	27.5	78
22	Interface Structures of Gold Nanoparticles on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>(110). Physical Review Letters, 2009, 102, 136105.	7.8	76
23	Prediction of interface structures and energies via virtual screening. Science Advances, 2016, 2, e1600746.	10.3	73
24	Assessment of Strain-Generated Oxygen Vacancies Using SrTiO₃ Bicrystals. Nano Letters, 2015, 15, 4129-4134.	9.1	69
25	Atomic structures of supersaturated ZnOâ€“Al2O3 solid solutions. Journal of Applied Physics, 2008, 103, 014309.	2.5	68
26	Measurement of vibrational spectrum of liquid using monochromated scanning transmission electron microscopyâ€“electron energy loss spectroscopy. Microscopy (Oxford, England), 2014, 63, 377-382.	1.5	66
27	High Elastic Moduli of a 54Al2O3-46Ta2O5 Glass Fabricated via Containerless Processing. Scientific Reports, 2015, 5, 15233.	3.3	66
28	First-principles calculation of defect energetics in cubic-BaTiO3 and a comparison with SrTiO3. Acta Materialia, 2007, 55, 6535-6540.	7.9	65
29	All-electron Bethe-Salpeter calculations for shallow-core x-ray absorption near-edge structures. Physical Review B, 2009, 79, .	3.2	65
30	Acceleration of stable interface structure searching using a kriging approach. Japanese Journal of Applied Physics, 2016, 55, 045502.	1.5	65
31	First-principles calculations of electron-energy-loss near-edge structure and near-edge x-ray-absorption fine structure of BN polytypes using model clusters. Physical Review B, 1999, 60, 4944-4951.	3.2	61
32	Defect energetics in SrTiO<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>symmetric tilt grain boundaries. Physical Review B, 2011, 83, .	3.2	58
33	Bonding nature of metal/oxide incoherent interfaces by first-principles calculations. Physical Review B, 2006, 74, .	3.2	55
34	Atomic structure of titania nanosheet with vacancies. Scientific Reports, 2013, 3, 2801.	3.3	53
35	Core-hole effect on dipolar and quadrupolar transitions ofSrTiO3andBaTiO3at TiKedge. Physical Review B, 2005, 71, .	3.2	50
36	First-principles multi-electron calculations for L2,3 ELNES/XANES of 3d transition metal monoxides. Ultramicroscopy, 2006, 106, 970-975.	1.9	50

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37	Electron energy loss near-edge structures of cubic Si3N4. Applied Physics Letters, 2001, 78, 2134-2136.	3.3	49
38	Sr vacancy segregation by heat treatment at SrTiO3 grain boundary. Applied Physics Letters, 2005, 87, 241920.	3.3	48
39	Growth and structure of PbVO3 thin films. Applied Physics Letters, 2007, 90, 062903.	3.3	47
40	Origins of Hole Doping and Relevant Optoelectronic Properties of Wide Gap p-Type Semiconductor, LaCuOSe. Journal of the American Chemical Society, 2010, 132, 15060-15067.	13.7	43
41	Mn L2,3-edge X-ray absorption spectroscopic studies on charge-discharge mechanism of Li2MnO3. Applied Physics Letters, 2014, 104, .	3.3	42
42	Data-driven approach for the prediction and interpretation of core-electron loss spectroscopy. Scientific Reports, 2018, 8, 13548.	3.3	42
43	Theoretical prediction of ELNES/XANES and chemical bondings of AlN polytypes. Micron, 2003, 34, 249-254.	2.2	41
44	Quantum Deep Field: Data-Driven Wave Function, Electron Density Generation, and Atomization Energy Prediction and Extrapolation with Machine Learning. Physical Review Letters, 2020, 125, 206401.	7.8	41
45	Distribution of solute atoms inÎ²- and spinelSi6âˆ’zAlzOzN8âˆ’zby AlK-edge x-ray absorption near-edge structure. Physical Review B, 2005, 71, .	3.2	40
46	Chemical bonding, interface strength, and oxygenKelectron-energy-loss near-edge structure of theCuâ•Al2O3interface. Physical Review B, 2006, 74, .	3.2	40
47	Electron-energy-loss near edge structures of six-fold-coordinated Zn in MgO. Ultramicroscopy, 2001, 86, 363-370.	1.9	38
48	The formation of a rock-salt type ZnO thin film by low-level alloying with MgO. Journal of Physics Condensed Matter, 2004, 16, 3801-3806.	1.8	38
49	Peak assignments of ELNES and XANES using overlap population diagrams. Ultramicroscopy, 2006, 106, 1120-1128.	1.9	38
50	Bayesian optimization for efficient determination of metal oxide grain boundary structures. Physica B: Condensed Matter, 2018, 532, 24-28.	2.7	38
51	The study of Al-L23 ELNES with resolution-enhancement software and first-principles calculation. Journal of Electron Microscopy, 2003, 52, 299-303.	0.9	35
52	Identification of native defects around grain boundary in Pr-doped ZnO bicrystal using electron energy loss spectroscopy and first-principles calculations. Applied Physics Letters, 2004, 84, 5311-5313.	3.3	35
53	Growth of Ruddlesden-Popper type faults in Sr-excess SrTiO3 homoepitaxial thin films by pulsed laser deposition. Applied Physics Letters, 2011, 99, .	3.3	35
54	Strontium vacancy clustering in Ti-excess SrTiO3 thin film. Applied Physics Letters, 2011, 99, .	3.3	35

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55	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.	3.1	34
56	Ceramic science of crystal defect cores. Journal of the Ceramic Society of Japan, 2022, 130, 648-667.	1.1	34
57	Atomic and electronic structure of [0001]/($$ar{1}ar{2}30$$) Î£7 symmetric tilt grain boundary in ZnO bicrystal with linear current-voltage characteristic. Journal of Materials Science, 2005, 40, 3059-3066.	3.7	32
58	First-principles study on incidence direction, individual site character, and atomic projection dependences of ELNES for perovskite compounds. Ultramicroscopy, 2006, 106, 92-104.	1.9	32
59	First-principles study of grain boundary sliding inÎ±â˜Al2O3. Physical Review B, 2007, 75, .	3.2	32
60	Critical thickness for giant thermoelectric Seebeck coefficient of 2DEG confined in SrTiO3/SrTi0.8Nb0.2O3 superlattices. Thin Solid Films, 2008, 516, 5916-5920.	1.8	32
61	Quantitative analyses of oxidation states for cubic SrMnO3 and orthorhombic SrMnO2.5 with electron energy loss spectroscopy. Journal of Applied Physics, 2010, 108, 124903.	2.5	32
62	Atomic structure and strain field of threading dislocations in CeO2 thin films on yttria-stabilized ZrO2. Applied Physics Letters, 2011, 98, 153104.	3.3	32
63	Arrangement of multiple structural units in a [0001]Î£49tilt grain boundary in ZnO. Physical Review B, 2005, 72, .	3.2	31
64	HRTEM and EELS characterization of atomic and electronic structures in CuÎ±-Al2O3 interfaces. Applied Surface Science, 2005, 241, 87-90.	6.1	30
65	First Principles Study on Intrinsic Vacancies in Cubic and Orthorhombic CaTiO₃. Materials Transactions, 2009, 50, 977-983.	1.2	30
66	First-principles study on migration mechanism in SrTiO3. Applied Physics Letters, 2011, 98, .	3.3	30
67	First-principles calculations of x-ray absorption near edge structure and energy loss near edge structure: present and future. Journal of Physics Condensed Matter, 2009, 21, 104201.	1.8	29
68	Structures of dissociated âŒ©11Â¯00âŒªdislocations and {11Â¯00} stacking faults of alumina (Î±-Al2O3). Acta Materialia, 2010, 58, 208-215.	7.9	27
69	Atomic-Scale Identification of Individual Lanthanide Dopants in Optical Glass Fiber. ACS Nano, 2013, 7, 5058-5063.	14.6	27
70	Transfer Learning to Accelerate Interface Structure Searches. Journal of the Physical Society of Japan, 2017, 86, 123601.	1.6	25
71	Basics and applications of ELNES calculations. Journal of Electron Microscopy, 2017, 66, 305-327.	0.9	25
72	Valence state ofTiin conductive nanowires in sapphire. Physical Review B, 2004, 70, .	3.2	24

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73	Al<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:m x-ray absorption spectra in III-V semiconductors: Many-body perturbation theory in comparison with experiment. Physical Review B, 2011, 83, .	3.2	24
74	Controlling Interface Intermixing and Properties of SrTiO₃â€Based Superlattices. Advanced Functional Materials, 2011, 21, 2258-2263.	14.9	24
75	Atomic-scale segregation behavior of Pr at a ZnO [0001]<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î£</mml:mi><mml:mn>49</mml:mn></mml:mrow></mml:math>tilt grain boundary. Physical Review B, 2009, 80, .	3.2	23
76	Characterization of vanadium in oil sands fluid petroleum coke using electron microscopy. Fuel, 2016, 178, 124-128.	6.4	23
77	Lattice expansion and local lattice distortion in Nb- and La-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> single crystals investigated by x-ray diffraction and first-principles calculations. Physical Review B, 2018, 98, .	3.2	23
78	Atomic structure of a Î£3 [110]/(111) grain boundary in CeO2. Applied Physics Letters, 2012, 100, .	3.3	22
79	Machine learning approaches for ELNES/XANES. Microscopy (Oxford, England), 2020, 69, 92-109.	1.5	22
80	Cation off-stoichiometric SrMnO3â^'Î´ thin film grown by pulsed laser deposition. Journal of Materials Science, 2011, 46, 4354-4360.	3.7	21
81	Removing the effects of elastic and thermal scattering from electron energy-loss spectroscopic data. Applied Physics Letters, 2012, 101, .	3.3	21
82	Effect of local coordination of Mn on Mn-L2,3 edge electron energy loss spectrum. Journal of Applied Physics, 2013, 114, .	2.5	21
83	A valence state evaluation of a positive electrode material in an Li-ion battery with first-principles K- and L-edge XANES spectral simulations and resonance photoelectron spectroscopy. Journal of Applied Physics, 2016, 120, .	2.5	21
84	Quantitative estimation of properties from core-loss spectrum via neural network. JPhys Materials, 2019, 2, 024003.	4.2	21
85	Formation of titanium-solute clusters in alumina: A first-principles study. Applied Physics Letters, 2004, 84, 4795-4797.	3.3	20
86	Theoretical Investigation of Al K-edge X-ray Absorption Spectra of Al, AlN and Al₂O₃. Materials Transactions, 2004, 45, 2031-2034.	1.2	20
87	Fabrication of electrically conductive nanowires using high-density dislocations in AlN thin films. Journal of Applied Physics, 2009, 106, .	2.5	20
88	Strong excitonic interactions in the oxygen K-edge of perovskite oxides. Ultramicroscopy, 2017, 178, 105-111.	1.9	20
89	Fast and Accurate Molecular Property Prediction: Learning Atomic Interactions and Potentials with Neural Networks. Journal of Physical Chemistry Letters, 2018, 9, 5733-5741.	4.6	20
90	Characterization of nanotextured AlN thin films by x-ray absorption near-edge structures. Applied Physics Letters, 2005, 86, 163113.	3.3	19

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91	Direct imaging of doped fluorine in LaFeAsO1â^'xFx superconductor by atomic scale spectroscopy. Applied Physics Letters, 2009, 95, .	3.3	19
92	First Principles Calculations of Vacancy Formation Energies in Σ13 Pyramidal Twin Grain Boundary of α-Al₂O₃. Materials Transactions, 2009, 50, 1019-1022.	1.2	19
93	An estimation of molecular dynamic behaviour in a liquid using core-loss spectroscopy. Scientific Reports, 2013, 3, 3503.	3.3	19
94	Fabrication of thin TEM sample of ionic liquid for high-resolution ELNES measurements. Ultramicroscopy, 2017, 178, 81-87.	1.9	19
95	Site dependence and peak assignment of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Y</mml:mi><mml:msub><mml:mi mathvariant="normal">Ba</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>7</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></	3.2	18
96	xmlns:mml="http://www.w3.. Physical Review B, 2008, 77, . Role of Dislocation Movement in the Electrical Conductance of Nanocontacts. Scientific Reports, 2012, 2, 623.	3.3	18
97	Simultaneous visualization of oxygen vacancies and the accompanying cation shifts in a perovskite oxide by combining annular imaging techniques. Applied Physics Letters, 2012, 100, .	3.3	18
98	Lithium-ion conducting La2/3â^'xLi3xTiO3 solid electrolyte thin films with stepped and terraced surfaces. Applied Physics Letters, 2012, 100, .	3.3	18
99	First-principles calculation of oxygen K-electron energy loss near edge structure of HfO₂. Journal of Physics Condensed Matter, 2009, 21, 104212.	1.8	17
100	Defect energetics in LaAlO3polymorphs: A first-principles study. Physical Review B, 2012, 86, .	3.2	17
101	Periodic Nanowire Array at the Crystal Interface. ACS Nano, 2013, 7, 6297-6302.	14.6	17
102	A new LiNbO3-type polar oxide with closed-shell cations: ZnPbO3. Journal of Applied Physics, 2015, 118, .	2.5	17
103	Local coordination state of rare earth in eutectic scintillators for neutron detector applications. Scientific Reports, 2015, 5, 13332.	3.3	17
104	Machine learning for structure determination and investigating the structure-property relationships of interfaces. JPhys Materials, 2019, 2, 034005.	4.2	17
105	Direct observations of Ca ordering in Ca0.33CoO2 thin films with different superstructures. Applied Physics Letters, 2008, 93, .	3.3	16
106	Overlap population diagram for ELNES and XANES: peak assignment and interpretation. Journal of Physics Condensed Matter, 2009, 21, 104215.	1.8	16
107	An experimental system combined with a micromachine and double-tilt TEM holder. Microelectronic Engineering, 2016, 164, 43-47.	2.4	16
108	Defect and electronic structures in TiSi2 thin films produced by co-sputtering Part 1: Defect analysis by transmission electron microscopy. Acta Materialia, 2001, 49, 83-92.	7.9	15

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109	X-ray absorption near-edge structures of disordered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mg</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:mi mathvariant="normal">Zn</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math>solid solutions. Physical Review B, 2007, 76, .	3.2	15
110	High-resolution transmission electron microscopy (HRTEM) observation of dislocation structures in AlN thin films. Journal of Materials Research, 2008, 23, 2188-2194.	2.6	15
111	Atomic and electronic structures of the SrVO3-LaAlO3 interface. Journal of Applied Physics, 2011, 110, 046104.	2.5	15
112	The atomic structure, band gap, and electrostatic potential at the (112)[11Â¯] twin grain boundary of CuInSe2. Applied Physics Letters, 2014, 104, .	3.3	15
113	Learning excited states from ground states by using an artificial neural network. Npj Computational Materials, 2020, 6, .	8.7	15
114	Zr segregation and associated Al vacancies in alumina grain boundaries. Journal of the Ceramic Society of Japan, 2011, 119, 840-844.	1.1	14
115	Characterization and atomic modeling of an asymmetric grain boundary. Physical Review B, 2011, 84, .	3.2	14
116	First principles pseudopotential calculation of electron energy loss near edge structures of lattice imperfections. Micron, 2012, 43, 37-42.	2.2	14
117	Atomic resolution chemical bond analysis of oxygen in La2CuO4. Journal of Applied Physics, 2013, 114, .	2.5	14
118	Effect of van der Waals interactions on the stability of SiC polytypes. Journal of Applied Physics, 2016, 119, .	2.5	14
119	Real-space analysis of diffusion behavior and activation energy of individual monatomic ions in a liquid. Science Advances, 2017, 3, e1701546.	10.3	14
120	Effective search for stable segregation configurations at grain boundaries with data-mining techniques. Physica B: Condensed Matter, 2018, 532, 9-14.	2.7	14
121	Vibrational Effects in X-ray Absorption Spectra of Two-Dimensional Layered Materials. Journal of Physical Chemistry C, 2019, 123, 9688-9692.	3.1	14
122	Real-Space Mapping of Oxygen Coordination in Phase-Separated Aluminosilicate Glass: Implication for Glass Stability. ACS Applied Nano Materials, 2020, 3, 5053-5060.	5.0	14
123	HAADF-STEM observations of aÎ£13 grain boundary in Î±-Al₂O₃from two orthogonal directions. Philosophical Magazine Letters, 2010, 90, 539-546.	1.2	13
124	First principles study on oxygen vacancy formation in rock salt-type oxides MO (M: Mg, Ca, Sr and Ba). Ceramics International, 2013, 39, S287-S292.	4.8	13
125	Searching the stable segregation configuration at the grain boundary by a Monte Carlo tree search. Journal of Chemical Physics, 2018, 148, 241741.	3.0	13
126	EQCM analysis of intercalation species into graphite positive electrodes for Al batteries. Journal of Alloys and Compounds, 2020, 846, 156469.	5.5	13

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127	Coreâ€“Exciton Interaction in Sodium L_{2,3} edge Structure Investigated Using the Betheâ€“Salpeter Equation. Journal of Physical Chemistry C, 2016, 120, 9036-9042.	3.1	12
128	First-principles calculations of Znâ€“K XANES in Ca-deficient hydroxyapatite. Journal of Physics Condensed Matter, 2010, 22, 384213.	1.8	11
129	Magnetic structures of FeTiO3-Fe2O3 solid solution thin films studied by soft X-ray magnetic circular dichroism and ab initio multiplet calculations. Applied Physics Letters, 2014, 104, .	3.3	11
130	Radial Distribution Function from X-ray Absorption near Edge Structure with an Artificial Neural Network. Journal of the Physical Society of Japan, 2020, 89, 103001.	1.6	11
131	Positron Annihilation Study of Formation of Mg Vacancy in MgO. Materials Science Forum, 2004, 445-446, 153-155.	0.3	10
132	Magnetic properties of ilmenite-hematite solid-solution thin films: Direct observation of antiphase boundaries and their correlation with magnetism. Physical Review B, 2009, 80, .	3.2	10
133	Cr diffusion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:msub><mml:mrow><mml:mtext>-Al</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mtext>O</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Secondary ion mass spectroscopy and first-principles study. Physical Review B, 2010, 82, .	3.2	10
134	Ab-initio multiplet calculation of oxygen vacancy effect on Ti-L2,3 electron energy loss near edge structures of BaTiO3. Applied Physics Letters, 2011, 99, 233109.	3.3	10
135	Nanowire of hexagonal gallium oxynitride: Direct observation of its stacking disorder and its long nanowire growth. Journal of the European Ceramic Society, 2012, 32, 1989-1993.	5.7	10
136	Atomic structure, energetics, and chemical bonding of Y doped Î£13 grain boundaries in Î±-Al₂O₃. Philosophical Magazine, 2013, 93, 1158-1171.	1.6	10
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.	1.5	10
138	First principles calculation of oxygen K edge absorption spectrum of acetic acid: Relationship between the spectrum and molecular dynamics. Chemical Physics Letters, 2016, 649, 92-96.	2.6	10
139	Identification of nanometer-scale compositional fluctuations in silicate glass using electron microscopy and spectroscopy. Scripta Materialia, 2018, 154, 197-201.	5.2	10
140	Quantum Deep Descriptor: Physically Informed Transfer Learning from Small Molecules to Polymers. Journal of Chemical Theory and Computation, 2021, 17, 7814-7821.	5.3	10
141	3D shape and orientation of nanoscale Pb inclusions at grain boundaries in Al observed by TEM and STEM tomography. Philosophical Magazine Letters, 2009, 89, 104-112.	1.2	9
142	Electrical current flow at conductive nanowires formed in GaN thin films by a dislocation template technique. Applied Physics Letters, 2010, 96, .	3.3	9
143	The effect of vacancies on the annular dark field image contrast of grain boundaries: A SrTiO3 case study. Ultramicroscopy, 2011, 111, 1531-1539.	1.9	9
144	Estimation of the molecular vibration of gases using electron microscopy. Scientific Reports, 2017, 7, 16434.	3.3	9

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145	Identifying lithium K edge anisotropy in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LiCo</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 98, .	3.2	9
146	Progress in nanoinformatics and informational materials science. MRS Bulletin, 2018, 43, 690-695.	3.5	9
147	Revealing Spatial Distribution of Al-Coordinated Species in a Phase-Separated Aluminosilicate Glass by STEM-EELS. Journal of Physical Chemistry Letters, 2020, 11, 9637-9642.	4.6	9
148	First principles calculation of ELNES by LCAO methods. Journal of Electron Microscopy, 2002, 51, S107-S112.	0.9	8
149	Structures of a Î£Â=Â9, [110]/{221} symmetrical tilt grain boundary in SrTiO3. Journal of Materials Science, 2011, 46, 4162-4168.	3.7	8
150	First principles calculation of dopant solution energy in HfO2 polymorphs. Journal of Applied Physics, 2012, 112, .	2.5	8
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