Masanori Kohyama

List of Publications by Year
in descending order

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236	8,008	46984	64755
papers	citations	47 h-index	79 g-index

237	237	237	7698
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Enhanced Electrocatalytic Activity of Pt Subnanoclusters on Graphene Nanosheet Surface. Nano Letters, 2009, 9, 2255-2259.	4.5	1,041
2	Visualizing Gas Molecules Interacting with Supported Nanoparticulate Catalysts at Reaction Conditions. Science, 2012, 335, 317-319.	6.0	395
3	Electronic Structure and Chemical Reactions at Metal-Alumina and Metal-Aluminum Nitride Interfaces. Journal of the American Ceramic Society, 1991, 74, 1163-1187.	1.9	147
4	Self-Interstitial Clustering in Crystalline Silicon. Physical Review Letters, 1997, 78, 4265-4268.	2.9	126
5	Analytical TEM study of Pt particle deposition in the proton-exchange membrane of a membrane-electrode-assembly. Journal of Power Sources, 2006, 159, 461-467.	4.0	126
6	Origin of intergranular embrittlement of Al alloys induced by Na and Ca segregation: Grain boundary weakening. Physical Review B, 2006, 73, .	1.1	122
7	Electronic structures of Au onTiO2(110)by first-principles calculations. Physical Review B, 2004, 69, .	1.1	119
8	Generation of Oxygen Vacancies at a Au/TiO₂ Perimeter Interface during CO Oxidation Detected by in Situ Electrical Conductance Measurement. Journal of the American Chemical Society, 2013, 135, 906-909.	6.6	118
9	Theoretical tensile strength of an Al grain boundary. Physical Review B, 2004, 69, .	1.1	116
10	Interstitial defects on {â€²113} in Si and Ge Line defect configuration incorporated with a self-interstitial atom chain. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1994, 70, 287-312.	0.7	111
11	Sub-nano-Pt cluster supported on graphene nanosheets for CO tolerant catalysts in polymer electrolyte fuel cells. Journal of Power Sources, 2011, 196, 110-115.	4.0	110
12	First-principles approaches to intrinsic strength and deformation of materials: perfect crystals, nano-structures, surfaces and interfaces. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 013001.	0.8	106
13	Electron Microscopy Study of Gold Nanoparticles Deposited on Transition Metal Oxides. Accounts of Chemical Research, 2013, 46, 1773-1782.	7.6	100
14	Electronic structures of Au supported on TiO2. Applied Catalysis A: General, 2005, 291, 45-54.	2.2	90
15	Computational studies of grain boundaries in covalent materials. Modelling and Simulation in Materials Science and Engineering, 2002, 10, R31-R59.	0.8	88
16	Weakening of an aluminum grain boundary induced by sulfur segregation: A first-principles computational tensile test. Physical Review B, 2007, 75, .	1.1	88
17	Ab initiocalculations of the Î²-SiC(001)/Al interface. Physical Review B, 1998, 57, 2334-2341.	1.1	87
18	Transmission electron microscopy observation of the structure of TiO2 nanotube and Au/TiO2 nanotube catalyst. Surface and Interface Analysis, 2005, 37, 265-269.	0.8	85

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19	Analytical TEM observation of Au nano-particles on cerium oxide. Catalysis Today, 2006, 117, 62-68.	2.2	84
20	Ab initiocalculations of electric-field-induced stress profiles for diamond/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>c</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi mathvariant="normal">B</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>(110) superlattices. Physical Review B, 2007, 76, .	1.1	84
21	Structures of Pt clusters on graphene by first-principles calculations. Surface Science, 2010, 604, 144-154.	0.8	82
22	Atomic structure and energy of the {113} planar interstitial defects in Si. Physical Review B, 1992, 46, 12305-12315.	1.1	75
23	TEM observation of gold nanoparticles deposited on cerium oxide. Journal of Materials Science, 2005, 40, 3101-3106.	1.7	75
24	Ab initiostudy of the tensile strength and fracture of coincidence tilt boundaries in cubic SiC:â€ƒPolar interfaces of the {122}Î£=9boundary. Physical Review B, 2002, 65, .	1.1	74
25	Real-Space Observation of Li Extractionâ^•Insertion in Li[sub 1.2]Mn[sub 0.4]Fe[sub 0.4]O[sub 2] Positive Electrode Material for Li-Ion Batteries. Electrochemical and Solid-State Letters, 2008, 11, A183.	2.2	74
26	The atomic and electronic structure of a (001) tilt grain boundary in Si. Journal of Physics C: Solid State Physics, 1988, 21, 3205-3215.	1.5	72
27	Tight-binding study of grain boundaries in Si: Energies and atomic structures of twist grain boundaries. Physical Review B, 1994, 49, 17102-17117.	1.1	72
28	A Study on the Mechanism for H₂ Dissociation on Au/TiO₂ Catalysts. Journal of Physical Chemistry C, 2014, 118, 1611-1617.	1.5	69
29	First-principles study of neutral oxygen vacancies in amorphous silica and germania. Physical Review B, 2004, 69, .	1.1	68
30	Reconstructed Structures of Symmetrical â€˜011â€‰ Tilt Grain Boundaries in Silicon. Physica Status Solidi (B): Basic Research, 1986, 138, 387-397.	0.7	66
31	Ab initiocalculations of the Î²-SiC(001)/Ti interface. Physical Review B, 2000, 61, 2672-2679.	1.1	65
32	Study of Surface Reaction of Spinel Li₄Ti₅O₁₂ during the First Lithium Insertion and Extraction Processes Using Atomic Force Microscopy and Analytical Transmission Electron Microscopy. Langmuir, 2012, 28, 12384-12392.	1.6	65
33	Ab InitioElectronic-Structure Calculations for Î±-(BEDT-TTF)2I3. Journal of the Physical Society of Japan, 2006, 75, 015005.	0.7	64
34	Tensile strength and fracture of a tilt grain boundary in cubic SiC: A first-principles study. Philosophical Magazine Letters, 1999, 79, 659-672.	0.5	63
35	Ab initiostudy on divacancy binding energies in aluminum and magnesium. Physical Review B, 2003, 68, .	1.1	62
36	Ab initiolocal stress and its application to Al (111) surfaces. Physical Review B, 2010, 81, .	1.1	62

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37	Characterization of two phase distribution in electrochemically-lithiated spinel Li4Ti5O12 secondary particles by electron energy-loss spectroscopy. Journal of Power Sources, 2013, 237, 26-32.	4.0	60
38	Reaction Mechanism of the Low-Temperature Waterâ€“Gas Shift Reaction on Au/TiO₂ Catalysts. Journal of Physical Chemistry C, 2017, 121, 12178-12187.	1.5	60
39	Theoretical study of grain boundaries in Si: Effects of structural disorder on the local electronic structure and the origin of band tails. Physical Review B, 1994, 50, 8502-8522.	1.1	59
40	Atomistic structure of the Cu(111)/Î±-Al2O3(0001) interface in terms of interatomic potentials fitted to ab initio results. Acta Materialia, 2004, 52, 1959-1970.	3.8	57
41	Growth mode and electronic structure of Au nano-clusters on NiO(001) and TiO2(110). Surface Science, 2006, 600, 1331-1338.	0.8	53
42	Ab initiostudy of symmetric tilt boundaries in ZnO. Physical Review B, 2001, 63, .	1.1	52
43	Ab initiostudy of symmetrical tilt grain boundaries in bcc Fe: structural units, magnetic moments, interfacial bonding, local energy and local stress. Journal of Physics Condensed Matter, 2013, 25, 135004.	0.7	52
44	Participation of Oxygen in Charge/Discharge Reactions in Li_{1.2}Mn_{0.4}Fe_{0.4}O₂: Evidence of Removal/Reinsertion of Oxide Ions. Journal of the Electrochemical Society, 2011, 158, A760-A768.	1.3	51
45	Electronic properties of Au nano-particles supported on stoichiometric and reduced TiO2(110) substrates. Surface Science, 2006, 600, 4430-4437.	0.8	50
46	Local barrier height of Au nanoparticles on a TiO2(1 1 0)-(1Ã—2) surface. Applied Surface Science, 2004, 222, 409-414.	3.1	49
47	Fe-rich and Mn-rich nanodomains in Li1.2Mn0.4Fe0.4O2 positive electrode materials for lithium-ion batteries. Applied Physics Letters, 2007, 91, .	1.5	49
48	Ab initiocalculations for SiC - Al interfaces: tests of electronic-minimization techniques. Modelling and Simulation in Materials Science and Engineering, 1996, 4, 397-408.	0.8	48
49	First-principles study of the tensile strength and failure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â€“</mml:mtext><mml:msub><mml:mi mathvariant="normal">Al</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mn>0001</mml:mn>		

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55	First-principles study on the tensile strength and fracture of the Al-terminated stoichiometric Î±-Al2O3(0001)/Cu(111) interface. Philosophical Magazine, 2005, 85, 2961-2976.	0.7	41
56	HAADFâ€STEM observation of Au nanoparticles on TiO₂. Surface and Interface Analysis, 2008, 40, 1760-1763.	0.8	41
57	Ab initio perspective of the âŒ©110âŒª symmetrical tilt grain boundaries in bcc Fe: application of local energy and local stress. Journal of Materials Science, 2014, 49, 3980-3995.	1.7	41
58	Structures and Energies of Symmetrical â€˜001â€‰ Tilt Grain Boundaries in Silicon. Physica Status Solidi (B): Basic Research, 1987, 141, 71-83.	0.7	40
59	Chemical bonding, interface strength, and oxygenKelectron-energy-loss near-edge structure of theCuâ•Al2O3interface. Physical Review B, 2006, 74, .	1.1	40
60	Ab initio study of EMIM-BF4 crystal interaction with a Li (100) surface as a model for ionic liquid/Li interfaces in Li-ion batteries. Journal of Chemical Physics, 2009, 131, 244705.	1.2	40
61	Electronic structure calculations of transition metal-alumina interfaces. Journal of Physics and Chemistry of Solids, 1992, 53, 345-354.	1.9	38
62	Ab initiostudy ofEMIM-BF4molecule adsorption on Li surfaces as a model for ionic liquid/Li interfaces in Li-ion batteries. Physical Review B, 2008, 78, .	1.1	38
63	Chemical bonding at the Al-terminated stoichiometric Î±-Al2O3(0001)/Cu(111) interface. Philosophical Magazine Letters, 2004, 84, 425-434.	0.5	37
64	Ab Initio Electronic Structure Calculation for Single-Component Molecular Conductor Au(tmdt)2 (tmdt = Trimethylenetetrathiafulvalenedithiolate). Journal of the Physical Society of Japan, 2005, 74, 843-846.	0.7	37
65	Si segregation at Fe grain boundaries analyzed byab initiolocal energy and local stress. Journal of Physics Condensed Matter, 2014, 26, 355005.	0.7	37
66	First-principles calculations of the self-interstitial clusterI4in Si. Physical Review B, 1999, 60, 8075-8080.	1.1	36
67	Theoretical strength and charge redistribution of fcc Ni in tension and shear. Journal of Physics Condensed Matter, 2008, 20, 335216.	0.7	36
68	Chemical misfit origin of solute strengthening in iron alloys. Acta Materialia, 2017, 131, 445-456.	3.8	36
69	First-principles analysis of the optical properties of structural disorder in<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:msub></mml:mrow></mml:math>. Physical Review B, 2008, 77, .	1.1	35
70	First-Principles Characterization of Atomic Structure of Al₂O₃(0001)/Cu Nano-Hetero Interface. Materials Transactions, 2004, 45, 1973-1977.	0.4	34
71	First-principles study of the effects of segregated Ga on an Al grain boundary. Journal of Physics Condensed Matter, 2006, 18, 5121-5128.	0.7	34
72	Direct O₂ Activation on Gold/Metal Oxide Catalysts through a Unique Double Linear Oï£¿Auï£¿O Structure. ChemCatChem, 2013, 5, 2217-2222.	1.8	34

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73	Tight-binding study of the {113} planar interstitial defects in Si. Physical Review B, 1995, 51, 13111-13116.	1.1	33
74	Ab initiopseudopotential calculation for TTF-TCNQ and TSeF-TCNQ. Physical Review B, 2000, 62, 7839-7844.	1.1	33
75	Generalized Stacking Fault Energy and Dislocation Properties for Various Slip Systems in Magnesium: a First-Principles Study. Materials Science Forum, 2003, 419-422, 225-230.	0.3	33
76	First-Principles Study of EMIM-FAFSA Molecule Adsorption on a Li(100) Surface as a Model for Li-Ion Battery Electrodes. Journal of Physical Chemistry C, 2012, 116, 8493-8509.	1.5	32
77	Theoretical Study of Atomic Oxygen on Gold Surface by HÃ¼ckel Theory and DFT Calculations. Journal of Physical Chemistry A, 2012, 116, 9568-9573.	1.1	32
78	The self-consistent tight-binding method: application to silicon and silicon carbide. Journal of Physics Condensed Matter, 1990, 2, 7791-7808.	0.7	30
79	A theoretical study of the atomic and electronic structure of a grain boundary in cubic SiC. Journal of Physics Condensed Matter, 1990, 2, 7809-7823.	0.7	30
80	HRTEM and EELS characterization of atomic and electronic structures in Cu/Î±-Al2O3 interfaces. Applied Surface Science, 2005, 241, 87-90.	3.1	30
81	TEM and HAADF-STEM study of the structure of Au nano-particles on CeO2. Journal of Materials Science, 2008, 43, 3917-3922.	1.7	30
82	Irreversible structural change of a spinel Li4Ti5O12 particle via Na insertion-extraction cycles of a sodium-ion battery. Electrochimica Acta, 2014, 148, 175-179.	2.6	30
83	Ab initio ELNES/XANES spectral calculation of polar and non-polar grain boundaries in Î²-SiC. Acta Materialia, 2004, 52, 3009-3018.	3.8	29
84	Effects of stoichiometry on electronic states of Au and Pt supported on TiO2(110). Journal of Materials Science, 2005, 40, 3075-3080.	1.7	29
85	Atomistic structure of a spinel Li4Ti5O12(111) surface elucidated by scanning tunneling microscopy and medium energy ion scattering spectrometry. Surface Science, 2014, 619, 5-9.	0.8	29
86	On the transferable SETB method for Si. Journal of Physics Condensed Matter, 1991, 3, 2193-2200.	0.7	28
87	Electron holographic 3-D nano-analysis of Au/TiO2 catalyst at interface. Journal of Electron Microscopy, 2003, 52, 21-26.	0.9	28
88	Analytical TEM study on structural changes of Au particles on cerium oxide using a heating holder. Catalysis Today, 2007, 122, 233-238.	2.2	28
89	First-principles computational tensile test on a Na-segregated Al grain boundary with an Si additive and an intergranular embrittlement suppression mechanism. Journal of Physics Condensed Matter, 2007, 19, 456225.	0.7	27
90	First-Principles Investigation of the Atomic and Electronic Structures of ?-Al2O3(0001)/Ni(111) Interfaces. Journal of the American Ceramic Society, 2007, 90, 2429-2440.	1.9	27

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91	First-principles study of Si and Mg segregation in grain boundaries in Al and Cu: application of local-energy decomposition. Journal of Materials Science, 2015, 50, 6864-6881.	1.7	27
92	Preparation of a spinel Li4Ti5O12 (111) surface from a rutile TiO2 single crystal. Applied Surface Science, 2012, 258, 3147-3151.	3.1	26
93	Ab initiolocal energy and local stress: application to tilt and twist grain boundaries in Cu and Al. Journal of Physics Condensed Matter, 2013, 25, 305006.	0.7	26
94	Theoretical study of polar interfaces of the (122) Sigma =9 grain boundary in cubic SiC. Journal of Physics Condensed Matter, 1991, 3, 7555-7573.	0.7	25
95	Structure and stability of Au rods on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> by first-principles calculations. Physical Review B, 2009, 80, .	1.1	25
96	Roles of Water and H₂ in CO Oxidation Reaction on Gold Catalysts. Journal of Physical Chemistry C, 2018, 122, 9523-9530.	1.5	25
97	First-principles characterization of the anisotropy of theoretical strength and the stressâ€“strain relation for a TiAl intermetallic compound. Journal of Physics Condensed Matter, 2009, 21, 175407.	0.7	24
98	Sequential HAADF-STEM observation of structural changes in Au nanoparticles supported on CeO2. Journal of Materials Science, 2011, 46, 4384-4391.	1.7	24
99	Atomic and electronic structures of Li4Ti5O12/Li7Ti5O12 (001) interfaces by first-principles calculations. Journal of Materials Science, 2014, 49, 4032-4037.	1.7	24
100	Relative stability ofP63/mandP63structures ofÎ²â^'Si3N4. Physical Review B, 2002, 65, .	1.1	23
101	Effects of Impurities on an Al Grain Boundary. Materials Transactions, 2003, 44, 337-343.	0.4	23
102	First-principles study of the adhesive and mechanical properties of the O-terminatedÎ±-Al2O3(0001)/Cu(111) interfaces. Philosophical Magazine, 2006, 86, 5123-5135.	0.7	23
103	Effects of Segregated Ga on an Al Grain Boundary: A First-Principles Computational Tensile Test. Materials Transactions, 2006, 47, 2678-2681.	0.4	23
104	First-principles study of twin grain boundaries in epitaxial BaSi2 on Si(111). Journal of Applied Physics, 2016, 120, .	1.1	22
105	Ab initio study of 3C-SiC/M (M = Ti or Al) nano-hetero interfaces. Applied Surface Science, 2003, 216, 471-477.	3.1	20
106	Spontaneous Li-Ion Transfer from Spinel Li₄Ti₅O₁₂Surfaces: Deterioration at Li₄Ti₅O₁₂/Electrolyte Interfaces Stored at Room Temperature. Journal of the Electrochemical Society, 2015, 162, A1272-A1275.	1.3	20
107	Mechanical properties of Fe-rich Si alloy from Hamiltonian. Npj Computational Materials, 2017, 3, .	3.5	20
108	Ab initio pseudopotential studies on an Al Î£ = 9 grain boundary: Effects of Na and Ca impurities. Philosophical Magazine Letters, 2001, 81, 757-766.	0.5	19

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109	Modeling interatomic interactions across Cu/Î±â€“Al2O3 interface. Computational Materials Science, 2006, 36, 281-291.	1.4	19
110	Formation and Disappearance of Spinel Nanograins in Li[sub 1.2â^'x]Mn[sub 0.4]Fe[sub 0.4]O[sub 2]â€,(0â‰¤xâ‰¤0.99) during Extraction and Insertion of Li Ions. Journal of the Electrochemical Society, 2009, 156, A839.	1.3	19
111	Origin of surface stress on late transition metal surfaces:Ab initiolocal stress and tight-binding model. Physical Review B, 2013, 87, .	1.1	19
112	<I>Ab Initio</I> Calculation on the Structure and Elastic Properties of a Magnesium-Lithium Alloy. Materials Transactions, 2001, 42, 1167-1171.	0.4	18
113	Coherency of copper/sapphire interface studied by atomistic simulation and geometrical analysis. Surface Science, 2003, 542, 45-55.	0.8	18
114	MPI parallelization of the first-principles pseudopotential method program with respect to each band. Modelling and Simulation in Materials Science and Engineering, 2004, 12, 945-957.	0.8	18
115	Preparation of a spinel LiMn2O4 single crystal film from a MnO wafer. Journal of Power Sources, 2013, 232, 7-11.	4.0	18
116	Electronic origin of grain boundary segregation of Al, Si, P, and S in bcc-Fe: combined analysis of ab initio local energy and crystal orbital Hamilton population. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 015001.	0.8	18
117	High Activity of Gold/Tin-Dioxide Catalysts for Low-Temperature CO Oxidation: Application of a Reducible Metal Oxide to a Catalyst Support. Catalysis Letters, 2014, 144, 2086-2090.	1.4	17
118	Impact of local atomic stress on oxygen segregation at tilt boundaries in silicon. Applied Physics Letters, 2017, 110, .	1.5	17
119	Tight-Binding Calculation of Grain Boundaries in Diamond. Materials Science Forum, 1996, 207-209, 261-264.	0.3	16
120	Influence of Interface Structure on Schottky Barrier Heights of α-Al₂O₃(0001)/Ni(111) interfaces: A First-Principles Study. Materials Transactions, 2006, 47, 2696-2700.	0.4	16
121	First-principles calculations of O-K ELNES/XANES of lithium titanate. Journal Physics D: Applied Physics, 2012, 45, 494004.	1.3	16
122	Ab initiolocal-energy and local-stress analysis of tensile behaviours of tilt grain boundaries in Al and Cu. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 015005.	0.8	16
123	First-principles study on the adhesion nature of the Î±-Al2O3(0001)/Ni(111) interface. Modelling and Simulation in Materials Science and Engineering, 2006, 14, S21-S28.	0.8	15
124	Simulation of growth process of Pt-particles - first-principles calculations. Journal of Physics: Conference Series, 2008, 100, 072044.	0.3	15
125	First-Principles Tensile Tests of Tilt and Twist Grain Boundaries in Al. Materials Transactions, 2012, 53, 140-146.	0.4	15
126	Full-PAW calculations of XANES/ELNES spectra of Ti-bearing oxide crystals and TiO-SiO glasses: Relation between pre-edge peaks and Ti coordination. Physical Review B, 2012, 85, .	1.1	15

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127	Imaging of a single atomic column in silicon grain boundary. Journal of Electron Microscopy, 2002, 51, 353-357.	0.9	14
128	Lithium analysis using reflection EELS for lithium compounds. Journal of Electron Spectroscopy and Related Phenomena, 2015, 203, 40-44.	0.8	14
129	Atomic forces in the selfâ€consistent tightâ€binding model. Physica Status Solidi (B): Basic Research, 1989, 152, 533-541.	0.7	13
130	Comparison of effects of sodium and silicon impurities on aluminium grain boundaries by first-principles calculation. Modelling and Simulation in Materials Science and Engineering, 2000, 8, 727-736.	0.8	13
131	Theoretical Studies of the Atomic and Electronic Structure of Nano-Hetero Metal/Inorganic Material Interfaces in Collaboration with Electron Microscopy Observations. Materials Transactions, 2007, 48, 675-683.	0.4	13
132	Infrared spectroscopic and theoretical studies on the formation of Au2NOâ^' and AunNO (n=2â€“5) in solid argon. Journal of Chemical Physics, 2009, 130, 134511.	1.2	13
133	Atomic oxygen adsorption on Au(1 0 0) and Au(1 1 1): Effects of coverage. Chemical Physics Letters, 2010, 492, 266-271.	1.2	13
134	A theoretical study of CO adsorption on gold by HÃ¼ckel theory and density functional theory calculations. Journal of Computational Chemistry, 2011, 32, 3276-3282.	1.5	13
135	Electron microscopy analysis of Ti-substituted Li2MnO3 positive electrode before and after carbothermal reduction. Journal of Power Sources, 2014, 254, 39-47.	4.0	13
136	Contribution of d electrons to surface stresses and their changes by layer relaxation for a series of 4 d transition metals. Surface Science, 2016, 644, 122-128.	0.8	13
137	Nanoscopic analysis of oxygen segregation at tilt boundaries in silicon ingots using atom probe tomography combined with TEM and ab initio calculations. Journal of Microscopy, 2017, 268, 230-238.	0.8	13
138	Combination of first-principles molecular dynamics and XANES simulations for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></m -electrolyte interfacial reactions in a lithium-ion battery. Physical Review B, 2017, 96, .	1.1	13
139	The atomic and electronic structure of the {211}/{111} facets in Si. Journal of Physics Condensed Matter, 1989, 1, 8251-8256.	0.7	12
140	Experimental and theoretical study of Î£=3 incoherent twin boundary in Î²-SiC. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2002, 82, 215-229.	0.7	12
141	First-principles pseudopotential study of an aluminium grain boundary containing sulphur atoms. Philosophical Magazine Letters, 2003, 83, 159-166.	0.5	12
142	Atomic structure of the Î£3 and Î£9 grain boundaries in CVD diamond film. Scripta Materialia, 2004, 51, 689-692.	2.6	12
143	Schottky-barrier heights of metal/alpha-SiC{0001} interfaces by first-principles calculations. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 2972-2976.	0.8	12
144	First-Principles Calculations of M₁₀/Graphene (M = Au, Pt) Systems —Atomic Structures and Hydrogen Adsorption—. Materials Transactions, 2008, 49, 2441-2444.	0.4	12

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145	Study of the interface between Na-rich and Li-rich phases in a Na-inserted spinel Li₄Ti₅O₁₂ crystal for an electrode of a sodium-ion battery. Physical Chemistry Chemical Physics, 2016, 18, 19888-19893.	1.3	12
146	Ab Initio Study of Grain Boundaries in SiC and Si. Materials Science Forum, 1999, 294-296, 231-234.	0.3	11
147	An efficient preconditioning scheme for plane-wave-based electronic structure calculations. Computational Materials Science, 1999, 14, 4-7.	1.4	11
148	<I>Ab-initio</I> Calculation of Si-K and Si-L ELNES Edges in an Extended Inactive Defect Model of Crystalline Silicon. Materials Transactions, 2002, 43, 1430-1434.	0.4	11
149	Atomic and Electronic Structures of Li_{0.44}MnO₂ Nanowires and Li₂MnO₃ Byproducts in the Formation Process of LiMn₂O₄ Nanowires. Journal of Physical Chemistry C, 2010, 114, 18358-18365.	1.5	11
150	Design of a Sodium-ion Cell with a Carbon-free Li₄Ti₅O₁₂ Negative Electrode. Electrochemistry, 2015, 83, 989-992.	0.6	11
151	Nanoscale controlled Li-insertion reaction induced by scanning electron-beam irradiation in a Li₄Ti₅O₁₂ electrode material for lithium-ion batteries. Physical Chemistry Chemical Physics, 2017, 19, 11581-11587.	1.3	11
152	Theoretical Study of Grain Boundaries in Silicon: Features of Atomic and Electronic Structures. Materials Science Forum, 1996, 207-209, 265-268.	0.3	10
153	Detection of inactive defects in crystalline silicon by high-resolution transmission-electron energy-loss spectroscopy. Physical Review B, 1998, 58, 10338-10342.	1.1	10
154	Ab initiopseudopotential calculation for (TMTSF)2ClO4. Journal of Physics Condensed Matter, 1999, 11, 2279-2283.	0.7	10
155	Ab Initio Study on the Structure of Mg-Li Alloys. Materials Science Forum, 2000, 350-351, 49-54.	0.3	10
156	<I>Ab initio</I> Studies on the Effects of Si and S Impurities on Al Grain Boundary. Materials Transactions, 2001, 42, 2238-2241.	0.4	10
157	Study of Interaction between Au and TiO₂(110) at Low Coverage. Materials Transactions, 2006, 47, 2663-2668.	0.4	10
158	Visualization of the distribution of anatase and rutile TiO₂ crystals in Au/TiO₂ powder catalysts by STEMâ€“EELS spectrum imaging. Surface and Interface Analysis, 2014, 46, 1249-1252.	0.8	10
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