Masanori Kohyama

List of Publications by Year in Descending Order

235 papers	7,162 citations	44 h-index	75 g-index
237 ext. papers	7,550 ext. citations	3.1 avg, IF	5.88 L-index

#	Paper	IF	Citations
235	Boundary plane-oriented grain boundary model generation. *Modelling and Simulation in Materials Science and Engineering*, **2022**, 30, 045005	2	2
234	A simplified methodology for the modeling of interfaces of elementary metals. *AIP Advances*, **2021**, 11, 115020	1.5	2
233	Atomic configurations and energies of Mg symmetric tilt grain boundaries: ab initio local analysis. *Modelling and Simulation in Materials Science and Engineering*, **2021**, 29, 085010	2	2
232	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	2	5
231	Roles of Water and H2 in CO Oxidation Reaction on Gold Catalysts. *Journal of Physical Chemistry C*, **2018**, 122, 9523-9530	3.8	17
230	Impact of local atomic stress on oxygen segregation at tilt boundaries in silicon. *Applied Physics Letters*, **2017**, 110, 062105	3.4	15
229	Chemical misfit origin of solute strengthening in iron alloys. *Acta Materialia*, **2017**, 131, 445-456	8.4	21
228	Mechanical properties of Fe-rich Si alloy from Hamiltonian. *Npj Computational Materials*, **2017**, 3,	10.9	15
227	Reaction Mechanism of the Low-Temperature Water□as Shift Reaction on Au/TiO2 Catalysts. *Journal of Physical Chemistry C*, **2017**, 121, 12178-12187	3.8	42
226	Nanoscale controlled Li-insertion reaction induced by scanning electron-beam irradiation in a LiTiO electrode material for lithium-ion batteries. *Physical Chemistry Chemical Physics*, **2017**, 19, 11581-11587	3.6	8
225	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	2	13
224	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	1.9	11
223	Mechanical properties of Fe rich Fe□Si alloys:ab initiolocal bulk-modulus viewpoint. *Materials Research Express*, **2017**, 4, 116518	1.7	6
222	Study of the Hydrate-Melt/LiTiO Interphase by Scanning Electron Microscopy-Based Spectroscopy. *Langmuir*, **2017**, 33, 13923-13928	4	3
221	Combination of first-principles molecular dynamics and XANES simulations for LiCoO2-electrolyte interfacial reactions in a lithium-ion battery. *Physical Review B*, **2017**, 96,	3.3	10
220	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	1.8	10
219	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, 19888-93	3.6	10

218	Stability of the LiMn2O4surface in a LiPF6-based non-aqueous electrolyte studied by in-situ atomic force microscopy. *Japanese Journal of Applied Physics*, **2016**, 55, 065801	1.4	4
217	Transmission electron microscopy investigation of the LiMn2O4/NaxMnO2 interface as a model study of a Na-ion battery electrode. *AIP Advances*, **2016**, 6, 115216	1.5	6
216	First-principles study of twin grain boundaries in epitaxial BaSi2 on Si(111). *Journal of Applied Physics*, **2016**, 120, 085311	2.5	21
215	A Simultaneous Solid Grinding Method for the Preparation of Gold Catalysts. *Catalysis Letters*, **2016** , 146, 2376-2380	2.8	2
214	Low-temperature CO oxidation properties and TEM/STEM observation of Au/Fe2O3 catalysts. *Journal of Catalysis*, **2015**, 324, 127-132	7.3	38
213	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	4.3	22
212	Understanding of the activity difference between nanogold and bulk gold by relativistic effects. *Journal of Energy Chemistry*, **2015**, 24, 485-489	12	5
211	Lithium analysis using reflection EELS for lithium compounds. *Journal of Electron Spectroscopy and Related Phenomena*, **2015**, 203, 40-44	1.7	12
210	Design of a Sodium-ion Cell with a Carbon-free Li4Ti5O12 Negative Electrode. *Electrochemistry*, **2015**, 83, 989-992	1.2	9
209	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	3.9	17
208	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	1.8	25
207	Atomic and electronic structures of Li4Ti5O12/Li7Ti5O12 (001) interfaces by first-principles calculations. *Journal of Materials Science*, **2014**, 49, 4032-4037	4.3	23
206	Ab initio perspective of the <110> symmetrical tilt grain boundaries in bcc Fe: application of local energy and local stress. *Journal of Materials Science*, **2014**, 49, 3980-3995	4.3	33
205	Two-phase separation in a lithiated spinel Li4Ti5O12 crystal as confirmed by electron energy-loss spectroscopy. *Journal of Power Sources*, **2014**, 257, 120-125	8.9	41
204	A Study on the Mechanism for H2 Dissociation on Au/TiO2 Catalysts. *Journal of Physical Chemistry C* , **2014**, 118, 1611-1617	3.8	54
203	Irreversible structural change of a spinel Li4Ti5O12 particle via Na insertion-extraction cycles of a sodium-ion battery. *Electrochimica Acta*, **2014**, 148, 175-179	6.7	27
202	Si segregation at Fe grain boundaries analyzed by ab initio local energy and local stress. *Journal of Physics Condensed Matter*, **2014**, 26, 355005	1.8	25
201	Structures and stabilities of gold oxide films on gold surfaces in O2 atmosphere. *Surface Science*, **2014**, 628, 41-49	1.8	3

200	Li-vapor induction growth of single-crystalline Li4Ti5O12 specimen for transmission electron microscopy. *Surface and Interface Analysis*, **2014**, 46, 1245-1248	1.5	10
199	Molecular electronic states in charge transfer complex studied by x-ray absorption spectroscopy. *Journal of Physics: Conference Series*, **2014**, 502, 012036	0.3	0
198	Visualization of the distribution of anatase and rutile TiO2 crystals in Au/TiO2 powder catalysts by STEM–EELS spectrum imaging. *Surface and Interface Analysis*, **2014**, 46, 1249-1252	1.5	5
197	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	2.8	14
196	Electron microscopy analysis of Ti-substituted Li2MnO3 positive electrode before and after carbothermal reduction. *Journal of Power Sources*, **2014**, 254, 39-47	8.9	11
195	Nanometer-thick V2O5 sheets on aluminum foil for an additive-free positive electrode of lithium-ion batteries. *Chemical Physics Letters*, **2014**, 592, 56-58	2.5	4
194	Atomic force microscopy on phase-control pulsed force mode in water: Imaging and force analysis on a rhodium-octaethylporphyrin layer on highly oriented pyrolytic graphite. *Applied Surface Science*, **2014**, 305, 111-116	6.7	2
193	First-principle calculations of C2H4 adsorption on Pd–Au (001) slab. *Surface Science*, **2013**, 612, 90-96	1.8	1
192	Ab initio study 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	1.8	43
191	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, 906-9	16.4	104
190	Preparation of a spinel LiMn2O4 single crystal film from a MnO wafer. *Journal of Power Sources*, **2013**, 232, 7-11	8.9	17
189	Hole doping by adsorption of oxygen on a Stone–Thrower–Wales defect in graphene. *Solid State Communications*, **2013**, 174, 10-15	1.6	6
188	Direct O2 Activation on Gold/Metal Oxide Catalysts through a Unique Double Linear O?Au?O Structure. *ChemCatChem*, **2013**, 5, 2217-2222	5.2	31
187	Electron microscopy study of gold nanoparticles deposited on transition metal oxides. *Accounts of Chemical Research*, **2013**, 46, 1773-82	24.3	86
186	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	8.9	49
185	The atomic and electronic structures of NiO(001)–Au(001) interfaces. *Journal of Chemical Physics*, **2013**, 139, 144705	3.9	7
184	Origin of surface stress on late transition metal surfaces: Ab initio local stress and tight-binding model. *Physical Review B*, **2013**, 87,	3.3	16
183	Ab initio local energy and local stress: application to tilt and twist grain boundaries in Cu and Al. *Journal of Physics Condensed Matter*, **2013**, 25, 305006	1.8	17

182	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	3.8	26
181	First-principles calculations of O-KELNES/XANES of lithium titanate. *Journal Physics D: Applied Physics*, **2012**, 45, 494004	3	13
180	Visualizing gas molecules interacting with supported nanoparticulate catalysts at reaction conditions. *Science*, **2012**, 335, 317-9	33.3	330
179	Theoretical study of atomic oxygen on gold surface by H□kel theory and DFT calculations. *Journal of Physical Chemistry A*, **2012**, 116, 9568-73	2.8	30
178	Preparation of a spinel Li4Ti5O12 (111) surface from a rutile TiO2 single crystal. *Applied Surface Science*, **2012**, 258, 3147-3151	6.7	24
177	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,	3.3	13
176	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, 12384-92	4	59
175	First-Principles Tensile Tests of Tilt and Twist Grain Boundaries in Al. *Materials Transactions*, **2012**, 53, 140-146	1.3	14
174	Sequential HAADF-STEM observation of structural changes in Au nanoparticles supported on CeO2. *Journal of Materials Science*, **2011**, 46, 4384-4391	4.3	23
173	Preface to the special issue on intergranular and interphase boundaries in materials. *Journal of Materials Science*, **2011**, 46, 4093-4094	4.3	2
172	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	8.9	98
171	A theoretical study of CO adsorption on gold by H□kel theory and density functional theory calculations. *Journal of Computational Chemistry*, **2011**, 32, 3276-82	3.5	11
170	Participation of Oxygen in Charge/Discharge Reactions in Li1.2Mn0.4Fe0.4O2: Evidence of Removal/Reinsertion of Oxide Ions. *Journal of the Electrochemical Society*, **2011**, 158, A760	3.9	48
169	TEM and STEM Study of the Au Nano-Particles Supported on Cerium Oxides. *Materials Science Forum*, **2010**, 654-656, 2362-2365	0.4	7
168	First-Principles Calculations of C2H4 Adsorption on Pd Surface Stacked on Fcc-Au. *Materials Science Forum*, **2010**, 654-656, 1666-1669	0.4	
167	Nanoparticle arrangement by DNA-programmed self-assembly for catalyst applications. *Journal of Applied Physics*, **2010**, 108, 094326	2.5	3
166	Atomic and Electronic Structures of Li0.44MnO2 Nanowires and Li2MnO3 Byproducts in the Formation Process of LiMn2O4 Nanowires. *Journal of Physical Chemistry C*, **2010**, 114, 18358-18365	3.8	11
165	Ab initio local stress and its application to Al (111) surfaces. *Physical Review B*, **2010**, 81,	3.3	53

164	Structures of Pt clusters on graphene by first-principles calculations. *Surface Science*, **2010**, 604, 144-154	1.8	76
163	Atomic oxygen adsorption on Au(1 0 0) and Au(1 1 1): Effects of coverage. *Chemical Physics Letters*, **2010**, 492, 266-271	2.5	12
162	Structure and stability of Au rods on TiO2(110) surfaces by first-principles calculations. *Physical Review B*, **2009**, 80,	3.3	24
161	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	3.9	31
160	Structure and dynamics of NiAl(110) studied by high-resolution ion scattering combined with density functional calculations. *Physical Review B*, **2009**, 80,	3.3	4
159	Formation and Disappearance of Spinel Nanograins in Li[sub 1.2]Mn[sub 0.4]Fe[sub 0.4]O[sub 2] (0≤x≤0.99) during Extraction and Insertion of Li Ions. *Journal of the Electrochemical Society*, **2009**, 156, A839	3.9	18
158	Investigating the effects of a Ga layer on an Al grain boundary by a first-principles computational tensile test. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 015003	2	5
157	Infrared spectroscopic and theoretical studies on the formation of Au2NO- and Au(n)NO (n = 2-5) in solid argon. *Journal of Chemical Physics*, **2009**, 130, 134511	3.9	12
156	First-principles characterization of the anisotropy of theoretical strength and the stress-strain relation for a TiAl intermetallic compound. *Journal of Physics Condensed Matter*, **2009**, 21, 175407	1.8	23
155	Enhanced electrocatalytic activity of Pt subnanoclusters on graphene nanosheet surface. *Nano Letters*, **2009**, 9, 2255-9	11.5	977
154	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	2	100
153	First-Principles Study of the Stability and Interfacial Bonding of Tilt and Twist Grain Boundaries in Al and Cu. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2009**, 73, 559-565	0.4	
152	Frontiers of Computational Materials Science and Engineering(1). *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2009**, 73, 549	0.4	
151	Coexistence of layered and cubic rocksalt structures with a common oxygen sublattice in Li1.2Mn0.4Fe0.4O2 particles: A transmission electron microscopy study. *Journal of Applied Physics*, **2008**, 103, 104911	2.5	36
150	First-principles analysis of optical absorption edge in pure and fluorine-doped SiO2 glass. *Computational Materials Science*, **2008**, 44, 61-66	3.2	3
149	Reactions of gold atoms with nitrous oxide in excess argon: a matrix infrared spectroscopic and theoretical study. *Journal of Physical Chemistry A*, **2008**, 112, 13495-9	2.8	5
148	Theoretical strength and charge redistribution of fcc Ni in tension and shear. *Journal of Physics Condensed Matter*, **2008**, 20, 335216	1.8	34
147	First-Principles Calculations of Pd/Au(100) Interfaces with Adsorbates. *Solid State Phenomena*, **2008**, 139, 47-52	0.4	7

146	First-Principles Study of Ceramic Interfaces: Structures and Electronic and Mechanical Properties. *Key Engineering Materials*, **2008**, 403, 205-206	0.4	
145	First-Principles Calculations of the Atomic and Electronic Structures in Au-Pd Slab Interfaces. *Solid State Phenomena*, **2008**, 139, 29-34	0.4	5
144	Real-Space Observation of Li Extraction□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		67
143	Effects of Supports on Hydrogen Adsorption on Pt Clusters. *Solid State Phenomena*, **2008**, 139, 41-46	0.4	5
142	Simulation of growth process of Pt-particles - first-principles calculations. *Journal of Physics: Conference Series*, **2008**, 100, 072044	0.3	9
141	First-principles analysis of the optical properties of structural disorder in SiO2 glass. *Physical Review B*, **2008**, 77,	3.3	29
140	Ab initio study of EMIM-BF4 molecule adsorption on Li surfaces as a model for ionic liquid/Li interfaces in Li-ion batteries. *Physical Review B*, **2008**, 78,	3.3	37
139	Phase-field model for deposition process of platinum nanoparticles on carbon substrate. *Journal of Physics: Conference Series*, **2008**, 100, 072042	0.3	3
138	Analytical TEM study of the core-shell structure of Au-Pd nano-particles prepared by sonochemical technique. *Journal of Physics: Conference Series*, **2008**, 100, 012014	0.3	2
137	First-Principles Calculations of M10/Graphene (M = Au, Pt) Systems —Atomic Structures and Hydrogen Adsorption—. *Materials Transactions*, **2008**, 49, 2441-2444	1.3	11
136	TEM and HAADF-STEM study of the structure of Au nano-particles on CeO2. *Journal of Materials Science*, **2008**, 43, 3917-3922	4.3	28
135	HAADF-STEM observation of Au nanoparticles on TiO2. *Surface and Interface Analysis*, **2008**, 40, 1760-1763	1.3	35
134	CO adsorption on a LaNi5 hydrogen storage alloy surface: a theoretical investigation. *ChemPhysChem*, **2008**, 9, 1564-9	3.2	3
133	Analytical TEM observation of Au□Pd nanoparticles prepared by sonochemical method. *Catalysis Today*, **2008**, 131, 90-97	5.3	41
132	Weakening of an aluminum grain boundary induced by sulfur segregation: A first-principles computational tensile test. *Physical Review B*, **2007**, 75,	3.3	81
131	Analytical TEM study on structural changes of Au particles on cerium oxide using a heating holder. *Catalysis Today*, **2007**, 122, 233-238	5.3	26
130	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		11
129	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	3.8	20

128	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	1.8	24
127	First-principles study of the tensile strength and failure of Al2O3(0001)Ni(111) interfaces. *Physical Review B*, **2007**, 76,	3.3	41
126	Ab initio calculations of electric-field-induced stress profiles for diamond/cBN (110) superlattices. *Physical Review B*, **2007**, 76,	3.3	75
125	Fe-rich and Mn-rich nanodomains in Li1.2Mn0.4Fe0.4O2 positive electrode materials for lithium-ion batteries. *Applied Physics Letters*, **2007**, 91, 054103	3.4	46
124	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	1.3	13
123	Gap states due to stretched bonds at the (112) Σ3 boundary in diamond. *Journal of Physics Condensed Matter*, **2007**, 19, 026223	1.8	6
122	Electronic properties of Au nano-particles supported on stoichiometric and reduced TiO2(1 1 0) substrates. *Surface Science*, **2006**, 600, 4430-4437	1.8	50
121	Analytical TEM observation of Au nano-particles on cerium oxide. *Catalysis Today*, **2006**, 117, 62-68	5.3	78
120	Effects of Segregated Ga on an Al Grain Boundary: A First-Principles Computational Tensile Test. *Materials Transactions*, **2006**, 47, 2678-2681	1.3	23
119	First-principles study of the effects of segregated Ga on an Al grain boundary. *Journal of Physics Condensed Matter*, **2006**, 18, 5121-5128	1.8	32
118	Origin of intergranular embrittlement of Al alloys induced by Na and Ca segregation: Grain boundary weakening. *Physical Review B*, **2006**, 73,	3.3	112
117	Chemical bonding, interface strength, and oxygen K electron-energy-loss near-edge structure of the CuAl2O3 interface. *Physical Review B*, **2006**, 74,	3.3	36
116	First-principles study of the adhesive and mechanical properties of the O-terminated Al2O3(0001)/Cu(111) interfaces. *Philosophical Magazine*, **2006**, 86, 5123-5135	1.6	19
115	First-principles study on the adhesion nature of the Al2O3(0001)/Ni(111) interface. *Modelling and Simulation in Materials Science and Engineering*, **2006**, 14, S21-S28	2	13
114	Modeling interatomic interactions across Cu/Al2O3 interface. *Computational Materials Science*, **2006**, 36, 281-291	3.2	16
113	Ab InitioElectronic-Structure Calculations for (BEDT-TTF)2I3. *Journal of the Physical Society of Japan*, **2006**, 75, 015005	1.5	60
112	Electronic Structures of Ag and Au Adsorbed on TiO2(110) Surfaces by First-Principles Calculations. *Materials Transactions*, **2006**, 47, 2669-2673	1.3	8
111	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	1.3	15

110	Study of Interaction between Au and TiO2(110) at Low Coverage. *Materials Transactions*, **2006**, 47, 2663-2668	1.3	10
109	First-Principles Study of Molecule/Al Interfaces. *Materials Transactions*, **2006**, 47, 2701-2705	1.3	1
108	First-Principles Calculations of Schottky Barrier Heights of Monolayer Metal/6H-SiC{0001} Interfaces. *Materials Transactions*, **2006**, 47, 2690-2695	1.3	9
107	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	8.9	112
106	Growth mode and electronic structure of Au nano-clusters on NiO(001) and TiO2(110). *Surface Science*, **2006**, 600, 1331-1338	1.8	47
105	First-principles study on the tensile strength and fracture of the Al-terminated stoichiometric □Al2O3(0001)/Cu(111) interface. *Philosophical Magazine*, **2005**, 85, 2961-2976	1.6	38
104	ELNES Analysis of Local Electronic Structures at Cu/Al2O3 (0001) Interface. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2005**, 69, 86-89	0.4	2
103	Quasicontinuum Analysis of Alumina/Copper Interface. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2005**, 69, 194-197	0.4	2
102	Large Scale Atomistic Simulation of Cu/Al2O3 Interface via Quasicontinuum Analysis. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2005**, 69, 90-95	0.4	4
101	Atomic structure of Si-rich 6H-SiC(0001□)-2□ surface. *Physical Review B*, **2005**, 71,	3.3	7
100	HRTEM and EELS characterization of atomic and electronic structures in Cu/□Al2O3 interfaces. *Applied Surface Science*, **2005**, 241, 87-90	6.7	26
99	Electronic structures of Au supported on TiO2. *Applied Catalysis A: General*, **2005**, 291, 45-54	5.1	80
98	Effects of stoichiometry on electronic states of Au and Pt supported on TiO2(110). *Journal of Materials Science*, **2005**, 40, 3075-3080	4.3	28
97	TEM observation of gold nanoparticles deposited on cerium oxide. *Journal of Materials Science*, **2005**, 40, 3101-3106	4.3	69
96	Transmission electron microscopy observation of the structure of TiO2 nanotube and Au/TiO2 nanotube catalyst. *Surface and Interface Analysis*, **2005**, 37, 265-269	1.5	79
95	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	1.5	37
94	First-Principles Calculations of Metal/Oxide Interfaces: Effects of Interface Stoichiometry. *Materials Science Forum*, **2005**, 502, 27-32	0.4	1
93	Atomic and Electronic Structures of Cu/Sapphire Interfaces by HRTEM and EELS Analyses. *Materials Science Forum*, **2005**, 475-479, 3859-3862	0.4	2

92	TEM observations of Au and Ir particles supported on CeO2. *Microscopy (Oxford, England)*, **2005**, 54 Suppl 1, i81-5	1.3	5
91	Local Barrier Height of Ir/TiO2Model Catalysts. *Japanese Journal of Applied Physics*, **2004**, 43, 4595-4598	1.4	5
90	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	2	18
89	Electronic structures of Au on TiO2(110) by first-principles calculations. *Physical Review B*, **2004**, 69,	3.3	114
88	First-principles study of neutral oxygen vacancies in amorphous silica and germania. *Physical Review B*, **2004**, 69,	3.3	60
87	E? center in Ge-doped SiO2 glass. *Physical Review B*, **2004**, 70,	3.3	7
86	Ab initio electronic structure study for TTF-TCNQ under uniaxial compression. *Physical Review B*, **2004**, 69,	3.3	8
85	Chemical bonding at the Al-terminated stoichiometric □Al2O3(0001)/Cu(111) interface. *Philosophical Magazine Letters*, **2004**, 84, 425-434	1	34
84	Atomic structure of the □3 and □9 grain boundaries in CVD diamond film. *Scripta Materialia*, **2004**, 51, 689-692	5.6	12
83	Atomistic structure of the Cu(111)/□Al2O3(0001) interface in terms of interatomic potentials fitted to ab initio results. *Acta Materialia*, **2004**, 52, 1959-1970	8.4	50
82	Ab initio ELNES/XANES spectral calculation of polar and non-polar grain boundaries in □SiC. *Acta Materialia*, **2004**, 52, 3009-3018	8.4	28
81	Local barrier height of Au nanoparticles on a TiO2(1 1 0)-(1□2) surface. *Applied Surface Science*, **2004**, 222, 409-414	6.7	44
80	Theoretical tensile strength of an Al grain boundary. *Physical Review B*, **2004**, 69,	3.3	106
79	A Second-Variational Prediction Operator for Fast Convergence in Self-Consistent Electronic-Structure Calculations. *Materials Transactions*, **2004**, 45, 1422-1428	1.3	7
78	First-Principles Characterization of Atomic Structure of Al2O3(0001)/Cu Nano-Hetero Interface. *Materials Transactions*, **2004**, 45, 1973-1977	1.3	32
77	First-Principles Study of a {122} Σ = 9 Boundary in Cubic SiC: Relative Stability between Zigzag and Straight Models and Comparison with Electron Microscopy Observation. *Materials Transactions*, **2004**, 45, 1461-1464	1.3	
76	Electron holographic 3-D nano-analysis of Au/TiO2 catalyst at interface. *Journal of Electron Microscopy*, **2003**, 52, 21-6		28
75	Effects of Impurities on an Al Grain Boundary. *Materials Transactions*, **2003**, 44, 337-343	1.3	22

74	Coherency of copper/sapphire interface studied by atomistic simulation and geometrical analysis. *Surface Science*, **2003**, 542, 45-55	1.8	14
73	Ab initio study of 3C-SiC/M (M = Ti or Al) nano-hetero interfaces. *Applied Surface Science*, **2003**, 216, 471-477	0.7	19
72	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	0.4	31
71	Theoretical Study of the Atomic and Electronic Structure of Grain Boundaries in SiC. *Solid State Phenomena*, **2003**, 93, 387-392	0.4	2
70	Atomic Size Effects on Al, Ca and Sc in Mg Solid Solutions from First-Principles Calculations. *Materials Science Forum*, **2003**, 426-432, 599-604	0.4	7
69	First-Principles Calculation of 3C-SiC(111)/Al Nano-Hetero Polar Interfaces. *Solid State Phenomena*, **2003**, 93, 393-398	0.4	2
68	Formation of Extended Defects in Polycrystalline SiGe by Electron Irradiation. *Solid State Phenomena*, **2003**, 93, 361-366	0.4	
67	Ab initio study on divacancy binding energies in aluminum and magnesium. *Physical Review B*, **2003**, 68,	3.3	60
66	Calculation of positron states in C60. *Physical Review B*, **2003**, 67,	3.3	5
65	First-principles pseudopotential study of an aluminium grain boundary containing sulphur atoms. *Philosophical Magazine Letters*, **2003**, 83, 159-166	1	12
64	Computational studies of grain boundaries in covalent materials. *Modelling and Simulation in Materials Science and Engineering*, **2002**, 10, R31-R59	2	83
63	Ab initio electronic structure calculation for □TDAE□C60. *Physical Review B*, **2002**, 65,	3.3	3
62	Relative stability of P63/m and P63 structures of □i3N4. *Physical Review B*, **2002**, 65,	3.3	22
61	Ab initio study of the tensile strength and fracture of coincidence tilt boundaries in cubic SiC: Polar interfaces of the {122} □9 boundary. *Physical Review B*, **2002**, 65,	3.3	72
60	Experimental and theoretical study of □3 incoherent twin boundary in □SiC. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **2002**, 82, 215-229		8
59	Atomic and electronic structure analysis of □= 3 incoherent twin boundaries in □SiC. *Journal of Electron Microscopy*, **2002**, 51, S265-S270		4
58	Ab-initio Calculation of Si-K and Si-L ELNES Edges in an Extended Inactive Defect Model of Crystalline Silicon. *Materials Transactions*, **2002**, 43, 1430-1434	1.3	10
57	Imaging of a single atomic column in silicon grain boundary. *Journal of Electron Microscopy*, **2002**, 51, 353-7		13

56	Ab initio Studies on the Effects of Si and S Impurities on Al Grain Boundary. *Materials Transactions*, **2001**, 42, 2238-2241	1.3	10
55	Ab Initio Calculation on the Structure and Elastic Properties of a Magnesium-Lithium Alloy. *Materials Transactions*, **2001**, 42, 1167-1171	1.3	18
54	Positron 2D-ACAR Study of the Quasi-One-Dimensional Organic Superconductor (TMTSF)2ClO4. *Materials Science Forum*, **2001**, 363-365, 552-554	0.4	
53	Ab initio study of symmetric tilt boundaries in ZnO. *Physical Review B*, **2001**, 63,	3.3	46
52	Ground-state structure of □3N4 by first-principles calculations. *Physical Review B*, **2001**, 64,	3.3	3
51	Ab initio pseudopotential studies on an Al □ 9 grain boundary: Effects of Na and Ca impurities. *Philosophical Magazine Letters*, **2001**, 81, 757-766	1	19
50	Ab initio calculation of positron distribution, ACAR and lifetime in TTF-TCNQ. *Radiation Physics and Chemistry*, **2000**, 58, 437-441	2.5	4
49	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	2	13
48	Ab initio pseudopotential calculation for TTF-TCNQ and TSeF-TCNQ. *Physical Review B*, **2000**, 62, 7839-7844	3.3	31
47	Ab initio calculations of the □SiC(001)/Ti interface. *Physical Review B*, **2000**, 61, 2672-2679	3.3	61
46	Ab Initio Study on the Structure of Mg-Li Alloys. *Materials Science Forum*, **2000**, 350-351, 49-54	0.4	10
45	Electron momentum density of TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane) studied by Compton scattering. *Journal of Physics Condensed Matter*, **1999**, 11, 9025-9032	1.8	2
44	Semiempirical Band Calculation of Pd-Adsorbed SnO2Surface. *Japanese Journal of Applied Physics*, **1999**, 38, 4993-4996	1.4	3
43	Ab initiopseudopotential calculation for (TMTSF)2ClO4. *Journal of Physics Condensed Matter*, **1999**, 11, 2279-2283	1.8	8
42	Electron-positron momentum density in (TMTSF)2ClO4. *Physical Review B*, **1999**, 60, R3747-R3750	3.3	4
41	First-principles calculations of the self-interstitial cluster I4 in Si. *Physical Review B*, **1999**, 60, 8075-8080	3.3	34
40	Ab initio Pseudopotential Band Calculation of Organic Conductors. *Journal of Low Temperature Physics*, **1999**, 117, 1753-1757	1.3	5
39	Tensile strength and fracture of a tilt grain boundary in cubic SiC: A first-principles study. *Philosophical Magazine Letters*, **1999**, 79, 659-672	1	61

38	An efficient preconditioning scheme for plane-wave-based electronic structure calculations. *Computational Materials Science*, **1999**, 14, 4-7	3.2	10
37	Ab-initio Calculations of Sodium Segregation in Aluminum Grain Boundaries. *Materials Transactions, JIM*, **1999**, 40, 1193-1197		7
36	Acceleration of Self-Consistent Electronic-Structure Calculations: Storage-Saving and Multiple-Secant Implementation of the Broyden Method. *Materials Transactions, JIM*, **1999**, 40, 1186-1192		5
35	Ab Initio Study of Grain Boundaries in SiC and Si. *Materials Science Forum*, **1998**, 294-296, 231-234	0.4	7
34	Ab Initio Calculations of SiC/Metal Interfaces. *Materials Science Forum*, **1998**, 294-296, 95-98	0.4	
33	The Variety of Structures of the Σ3 Incoherent Twin Boundary in β-SiC. *Materials Science Forum*, **1998**, 294-296, 187-190	0.4	7
32	Ab initio calculations of the β-SiC(001)/Al interface. *Physical Review B*, **1998**, 57, 2334-2341	3.3	81
31	Detection of inactive defects in crystalline silicon by high-resolution transmission-electron energy-loss spectroscopy. *Physical Review B*, **1998**, 58, 10338-10342	3.3	10
30	Ab Initio Tensile Tests of Grain Boundaries in SiC. *Materials Science Forum*, **1998**, 294-296, 657-660	0.4	2
29	Dielectric properties of extended defects in silicon studied by high-resolution transmission EELS. *Journal of Electron Microscopy*, **1998**, 47, 311-317		8
28	Self-Interstitial Clustering in Crystalline Silicon. *Physical Review Letters*, **1997**, 78, 4265-4268	7.4	112
27	High Resolution EELS Study of Extended Defects in Silicon. *Materials Science Forum*, **1997**, 258-263, 547-552	0.4	
26	Theoretical studies of grain boundaries in covalent materials. *Materials Chemistry and Physics*, **1997**, 50, 159-165	4.4	8
25	Tight-Binding Calculation of Grain Boundaries in Diamond. *Materials Science Forum*, **1996**, 207-209, 261-264	0.4	12
24	Ab Initio Calculations for SiC-Al Interfaces. *Materials Science Forum*, **1996**, 207-209, 269-272	0.4	
23	Theoretical Study of Grain Boundaries in Silicon: Features of Atomic and Electronic Structures. *Materials Science Forum*, **1996**, 207-209, 265-268	0.4	7
22	Ab initiocalculations for SiC - Al interfaces: tests of electronic-minimization techniques. *Modelling and Simulation in Materials Science and Engineering*, **1996**, 4, 397-408	2	44
21	Tight-binding study of the {113} planar interstitial defects in Si. *Physical Review B*, **1995**, 51, 13111-13116	3.3	33

20	Electronic structure of beta -SiC surfaces. *Journal of Physics Condensed Matter*, **1995**, 7, 1069-1099	1.8	3
19	Interstitial defects on {?113} 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		101
18	Tight-binding study of grain boundaries in Si: Energies and atomic structures of twist grain boundaries. *Physical Review B*, **1994**, 49, 17102-17117	3.3	65
17	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	3.3	51
16	Energies and Atomic Structures of Grain Boundaries in Diamond: Comparison With Grain Boundaries in Silicon. *Materials Research Society Symposia Proceedings*, **1994**, 339, 681		3
15	Tight-Binding Study of the 211 Σ3 Grain Boundary in Cubic Silicon-Carbide. *Materials Research Society Symposia Proceedings*, **1994**, 339, 9		3
14	Effects of Structural Disorder on the Electronic Properties of Silicon: Tight-Binding Calculations of Grain Boundaries. *Materials Research Society Symposia Proceedings*, **1993**, 297, 177		2
13	Atomic structure and energy of the {113} planar interstitial defects in Si. *Physical Review B*, **1992**, 46, 12305-12315	3.3	74
12	Electronic structure calculations of transition metal-alumina interfaces. *Journal of Physics and Chemistry of Solids*, **1992**, 53, 345-354	3.9	33
11	Electronic Structure and Chemical Reactions at Metal/Alumina and Metal/Aluminum Nitride Interfaces. *Journal of the American Ceramic Society*, **1991**, 74, 1163-1187	3.8	123
10	On the transferable SETB method for Si. *Journal of Physics Condensed Matter*, **1991**, 3, 2193-2200	1.8	24
9	Theoretical study of polar interfaces of the (122) Sigma =9 grain boundary in cubic SiC. *Journal of Physics Condensed Matter*, **1991**, 3, 7555-7573	1.8	22
8	The self-consistent tight-binding method: application to silicon and silicon carbide. *Journal of Physics Condensed Matter*, **1990**, 2, 7791-7808	1.8	24
7	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	1.8	27
6	The atomic and electronic structure of the {211}/{111} facets in Si. *Journal of Physics Condensed Matter*, **1989**, 1, 8251-8256	1.8	11
5	Atomic forces in the self-consistent tight-binding model. *Physica Status Solidi (B): Basic Research*, **1989**, 152, 533-541	1.3	13
4	The atomic and electronic structure of a (001) tilt grain boundary in Si. *Journal of Physics C: Solid State Physics*, **1988**, 21, 3205-3215		66
3	The atomic and electronic structure of the Σ3 (211) twin boundary in Si. *Journal of Physics C: Solid State Physics*, **1988**, 21, L695-L700		41

2	Structures and Energies of Symmetrical <001> Tilt Grain Boundaries in Silicon. *Physica Status Solidi (B): Basic Research*, **1987**, 141, 71-83	1.3	35
1	Reconstructed Structures of Symmetrical <011> Tilt Grain Boundaries in Silicon. *Physica Status Solidi (B): Basic Research*, **1986**, 138, 387-397	1.3	61