Yoshitada Morikawa

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

276 papers	9,324 citations	52 h-index	88 g-index
295 ext. papers	10,085 ext. citations	3.5 avg, IF	5.96 L-index

#	Paper	IF	Citations
276	Effect of impurities from deposition precursors on the electronic properties of Si/SiO2 interfaces. *Journal of Applied Physics*, **2022**, 131, 055306	2.5	
275	Growing 3D-nanostructured carbon allotropes from CO2 at room temperature under the dynamic CO2 electrochemical reduction environment. *Carbon*, **2022**, 187, 241-255	10.4	0
274	Dry Reforming of Methane on Cobalt Catalysts: DFT-Based Insights into Carbon Deposition Versus Removal. *Journal of Physical Chemistry C*, **2021**, 125, 21902-21913	3.8	1
273	Role of Intermolecular Interactions in the Catalytic Reaction of Formic Acid on Cu(111). *Small*, **2021**, 17, e2008010	11	2
272	Activation free energies for formation and dissociation of N□N, C□□, and C□H bonds in a Na□Ca melt. *Computational Materials Science*, **2021**, 194, 110366	3.2	0
271	Chemical stability of hydrogen boride nanosheets in water. *Communications Materials*, **2021**, 2,	6	2
270	Oxidative etching mechanism of the diamond (100) surface. *Carbon*, **2021**, 174, 36-51	10.4	2
269	Density functional theory study on a nitrogen-rich carbon nitride material CN as photocatalyst for CO reduction to C1 and C2 products. *Journal of Colloid and Interface Science*, **2021**, 585, 740-749	9.3	15
268	Mechanistic insight into oxygen vacancy migration in SrFeO from DFT+U simulations. *Physical Chemistry Chemical Physics*, **2021**, 23, 18628-18639	3.6	1
267	A flat-lying dimer as a key intermediate in NO reduction on Cu(100). *Physical Chemistry Chemical Physics*, **2021**, 23, 16880-16887	3.6	2
266	Adsorption of toxic gases on borophene: surface deformation links to chemisorptions.. *RSC Advances*, **2021**, 11, 18279-18287	3.7	6
265	High-Speed Etching of Silicon Carbide Wafer Using High-Pressure SF6 Plasma. *ECS Journal of Solid State Science and Technology*, **2021**, 10, 014005	2	1
264	Alkaline earth atom doping-induced changes in the electronic and magnetic properties of graphene: a density functional theory study.. *RSC Advances*, **2021**, 11, 6268-6283	3.7	4
263	Multi-scale Simulation of Equilibrium Step Fluctuations on Cu(111) Surfaces. *ACS Omega*, **2021**, 6, 5183-5196	3.7	1
262	Diffusion of excessively adsorbed hydrogen atoms on hydrogen terminated Si(100)(2□1) surface. *AIP Advances*, **2021**, 11, 085318	1.5	
261	Isotope effect of methane adsorbed on fcc metal (1 1 1) surfaces. *Chemical Physics Letters*, **2021**, 780, 138943	2.5	0
260	Optimal deformation procedure for hybrid adaptive x-ray mirror based on mechanical and piezo-driven bending system.. *Review of Scientific Instruments*, **2021**, 92, 123706	1.7	1

259	High-throughput deterministic plasma etching using array-type plasma generator system.. *Review of Scientific Instruments*, **2021**, 92, 125107	1.7	
258	Absolute surface energies of oxygen-adsorbed GaN surfaces. *Journal of Crystal Growth*, **2020**, 549, 125868	1.8	5
257	An abrasive-free chemical polishing method assisted by nickel catalyst generated by in situ electrochemical plating. *Review of Scientific Instruments*, **2020**, 91, 045108	1.7	2
256	Atomic and molecular adsorption on single platinum atom at the graphene edge: A density functional theory study. *Journal of Chemical Physics*, **2020**, 152, 104707	3.9	4
255	Blue moon ensemble simulation of aquation free energy profiles applied to mono and bifunctional platinum anticancer drugs. *Journal of Computational Chemistry*, **2020**, 41, 1973-1984	3.5	4
254	Insight into Trimeric Formation of Nitric Oxide on Cu(111): A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2020**, 124, 2968-2977	3.8	13
253	Analyses of three-dimensional atomic arrangements of impurities doped in Si relating to electrical activity by spectro-photoelectron holography. *Japanese Journal of Applied Physics*, **2020**, 59, 010503	1.4	3
252	Correlation between mobility and the hydrogen bonding network of water at an electrified-graphite electrode using molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2020**, 22, 1767-1773	3.6	5
251	Ionic-Liquid-Originated Carrier Trapping Dynamics at the Interface in Electric Double-Layer Organic FET Revealed by Operando Interfacial Analyses. *Journal of Physical Chemistry C*, **2020**, 124, 2543-2552	3.8	9
250	Identifying Atomic-Level Correlation between Geometric and Electronic Structure at a Metal–Organic Interface. *Journal of Physical Chemistry C*, **2020**, 124, 17696-17701	3.8	2
249	Enhanced CO tolerance of Pt clusters supported on graphene with lattice vacancies. *Physical Review B*, **2020**, 102,	3.3	8
248	Oxygen vacancy induced insulator-metal transition in LaNiO3 thin films. *Physical Review B*, **2020**, 102,	3.3	3
247	Manipulable Metal Catalyst for Nanographene Synthesis. *Nano Letters*, **2020**, 20, 8339-8345	11.5	5
246	Development of Co Supported on $CoAl_2O_4$ Spinel Catalysts from Exsolution of Amorphous $CoAl_2O_4$ Oxides for Carbon Dioxide Reforming of Methane. *ChemCatChem*, **2019**, 11, 5593-5605	5.2	17
245	Platinum single-atom adsorption on graphene: a density functional theory study. *Nanoscale Advances*, **2019**, 1, 1165-1174	5.1	12
244	Vibration-driven reaction of CO on Cu surfaces via Eley-Rideal-type mechanism. *Nature Chemistry*, **2019**, 11, 722-729	17.6	38
243	Catalyzed chemical polishing of SiO glasses in pure water. *Review of Scientific Instruments*, **2019**, 90, 045115	1.7	6
242	Van der Waals density functional study of formic acid adsorption and decomposition on Cu(111). *Journal of Chemical Physics*, **2019**, 150, 154707	3.9	11

241	Experimental and computational studies on ruthenium(ii) bis-diimine complexes of N,N'-chelate ligands: the origin of changes in absorption spectra upon oxidation and reduction. *Physical Chemistry Chemical Physics*, **2019**, 21, 7973-7988	3.6	9
240	Improvements in graphene growth on 4H-SiC(0001) using plasma induced surface oxidation. *Journal of Applied Physics*, **2019**, 126, 065301	2.5	
239	First-principles theoretical study on carrier doping effects induced by Zn vacancies in Mn-doped in ZnSnAs2. *Japanese Journal of Applied Physics*, **2019**, 58, 110601	1.4	0
238	X-ray optics for advanced ultrafast pump-probe X-ray experiments at SACLA. *Journal of Synchrotron Radiation*, **2019**, 26, 333-338	2.4	15
237	High-Efficiency Planarization of SiC Wafers by Water-CARE (Catalyst-Referred Etching) Employing Photoelectrochemical Oxidation. *Materials Science Forum*, **2019**, 963, 525-529	0.4	1
236	A micro channel-cut crystal X-ray monochromator for a self-seeded hard X-ray free-electron laser. *Journal of Synchrotron Radiation*, **2019**, 26, 1496-1502	2.4	6
235	Platinum-catalyzed hydrolysis etching of SiC in water: A density functional theory study. *Japanese Journal of Applied Physics*, **2018**, 57, 055703	1.4	5
234	Structural and dynamic properties of 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide/mica and graphite interfaces revealed by molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2018**, 20, 6668-6676	3.6	21
233	Mechanistic Analysis of Oxygen Vacancy Formation and Ionic Transport in Sr3Fe2O7□*Journal of Physical Chemistry C*, **2018**, 122, 4172-4181	3.8	12
232	First-principles study of ZnSnAs2-based dilute magnetic semiconductors. *Japanese Journal of Applied Physics*, **2018**, 57, 020306	1.4	11
231	Microscopic properties of ionic liquid/organic semiconductor interfaces revealed by molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2018**, 20, 13075-13083	3.6	11
230	A New Pentacene Polymorph Induced by Interaction with a Bi(0001) Substrate. *Journal of Physical Chemistry C*, **2018**, 122, 6240-6245	3.8	4
229	Potential dependent changes in the structural and dynamical properties of 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide on graphite electrodes revealed by molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2018**, 20, 19408-19415	3.6	8
228	Enhancement of CO adsorption on oxygen-functionalized epitaxial graphene surface under near-ambient conditions. *Physical Chemistry Chemical Physics*, **2018**, 20, 19532-19538	3.6	13
227	Diffusion mechanism of Na ion-polaron complex in potential cathode materials NaVOPO and VOPO for rechargeable sodium-ion batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 23625-23634	3.6	17
226	Computational Study on Atomic Structures, Electronic Properties, and Chemical Reactions at Surfaces and Interfaces and in Biomaterials. *Journal of the Physical Society of Japan*, **2018**, 87, 061013	1.5	1
225	Performance of a hard X-ray split-and-delay optical system with a wavefront division. *Journal of Synchrotron Radiation*, **2018**, 25, 20-25	2.4	18
224	Characteristics and Mechanism of Catalyst-Referred Etching Method: Application to 4H-SiC. *International Journal of Automation Technology*, **2018**, 12, 154-159	0.8	6

223	First-principles study of polar, nonpolar, and semipolar GaN surfaces during oxide vapor phase epitaxy growth. *Japanese Journal of Applied Physics*, **2018**, 57, 115504	1.4	1
222	Effects of Surface Termination and Layer Thickness on Electronic Structures of LaNiO3 Thin Films. *Journal of the Physical Society of Japan*, **2018**, 87, 114704	1.5	2
221	Hydrogen Bond-Induced Nitric Oxide Dissociation on Cu(110). *Journal of Physical Chemistry C*, **2018**, 122, 11814-11824	3.8	6
220	Adsorption of CO2 on Graphene: A Combined TPD, XPS, and vdW-DF Study. *Journal of Physical Chemistry C*, **2017**, 121, 2807-2814	3.8	52
219	Chemical etching of silicon carbide in pure water by using platinum catalyst. *Applied Physics Letters*, **2017**, 110, 201601	3.4	15
218	Electronic states and growth modes of Zn atoms deposited on Cu(111) studied by XPS, UPS and DFT. *Surface Science*, **2017**, 663, 1-10	1.8	15
217	First-principles study of the surface phase diagrams of GaN(0001) and (000$\bar{1}$) under oxide vapor phase epitaxy growth conditions. *Physica Status Solidi (B): Basic Research*, **2017**, 254, 1600706	1.3	2
216	First-Principles Molecular Dynamics Analysis of Ligand-Free Suzuki-Miyaura Cross-Coupling in Water Solvent: Oxidative Addition Step. *Journal of Physical Chemistry B*, **2017**, 121, 164-173	3.4	6
215	Image potential states from the van der Waals density functional. *Journal of Chemical Physics*, **2017**, 147, 044708	3.9	4
214	Augmented pH-sensitivity absorbance of a ruthenium(ii) bis(bipyridine) complex with elongation of the conjugated ligands: an experimental and theoretical investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 25734-25745	3.6	5
213	First-Principles Molecular Dynamics Analysis of Ligand-Free Suzuki–Miyaura Cross-Coupling in Water: Transmetalation and Reductive Elimination. *Journal of Physical Chemistry C*, **2017**, 121, 19904-19914	3.8	8
212	CO adsorption on the copper surfaces: van der Waals density functional and TPD studies. *Journal of Chemical Physics*, **2017**, 147, 094702	3.9	33
211	Desorption dynamics of CO from formate decomposition on Cu(111). *Chemical Communications*, **2017**, 53, 9222-9225	5.8	16
210	Computational investigations of electronic structure modifications of ferrocene-terminated self-assembled monolayers: effects of electron donating/withdrawing functional groups attached on the ferrocene moiety. *Physical Chemistry Chemical Physics*, **2017**, 19, 32715-32722	3.6	5
209	Individual Atomic Imaging of Multiple Dopant Sites in As-Doped Si Using Spectro-Photoelectron Holography. *Nano Letters*, **2017**, 17, 7533-7538	11.5	37
208	Hybrid image potential states in molecular overlayers on graphene. *Physical Review Materials*, **2017**, 1,	3.2	12
207	Characterization of temporal coherence of hard X-ray free-electron laser pulses with single-shot interferograms. *IUCrJ*, **2017**, 4, 728-733	4.7	21
206	Dynamic fracture of tantalum under extreme tensile stress. *Science Advances*, **2017**, 3, e1602705	14.3	30

205	High-efficiency planarization method combining mechanical polishing and atmospheric-pressure plasma etching for hard-to-machine semiconductor substrates. *Mechanical Engineering Journal*, **2016**, 3, 15-00527-15-00527	0.5	
204	Self-consistent van der Waals density functional study of benzene adsorption on Si(100). *Physical Review B*, **2016**, 93,	3.3	32
203	Photoelectron Holographic Atomic Arrangement Imaging of Cleaved Bimetal-intercalated Graphite Superconductor Surface. *Scientific Reports*, **2016**, 6, 36258	4.9	18
202	Theoretical Study on Electronic Structure of Bathocuproine: Renormalization of the Band Gap in the Crystalline State and the Large Exciton Binding Energy. *Journal of the Chinese Chemical Society*, **2016**, 63, 513-520	1.5	2
201	Mechanism for enhanced single-crystal GaN growth in the C-assisted Na-flux method. *Applied Physics Express*, **2016**, 9, 015601	2.4	8
200	Nearly diffraction-limited X-ray focusing with variable-numerical-aperture focusing optical system based on four deformable mirrors. *Scientific Reports*, **2016**, 6, 24801	4.9	28
199	Development of speckle-free channel-cut crystal optics using plasma chemical vaporization machining for coherent x-ray applications. *Review of Scientific Instruments*, **2016**, 87, 063118	1.7	10
198	Density Functional Theory Investigations of Ferrocene-Terminated Self-Assembled Monolayers: Electronic State Changes Induced by Electric Dipole Field of Coadsorbed Species. *Journal of Physical Chemistry C*, **2016**, 120, 8684-8692	3.8	4
197	Simulation and Experimental Study of Wavefront Measurement Accuracy of the Pencil-Beam Method. *Synchrotron Radiation News*, **2016**, 29, 32-36	0.6	6
196	Ab initio molecular dynamics of solvation effects on reactivity at electrified interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E4937-45	11.5	50
195	Hard X-ray nanofocusing using adaptive focusing optics based on piezoelectric deformable mirrors. *Review of Scientific Instruments*, **2015**, 86, 043102	1.7	19
194	Electronic structure of the 4 □4 silicene monolayer on semi-infinite Ag(111). *New Journal of Physics*, **2015**, 17, 015013	2.9	20
193	Improvement of I-V Characteristics of Schottky Barrier Diode by 4H-SiC Surface Planarization. *Materials Science Forum*, **2015**, 821-823, 567-570	0.4	3
192	Development of ion beam figuring system with electrostatic deflection for ultraprecise X-ray reflective optics. *Review of Scientific Instruments*, **2015**, 86, 093103	1.7	8
191	Study on the mechanism of platinum-assisted hydrofluoric acid etching of SiC using density functional theory calculations. *Applied Physics Letters*, **2015**, 107, 201601	3.4	6
190	Catalyst-Assisted Electroless Flattening of Ge Surfaces in Dissolved-O2-Containing Water. *ChemElectroChem*, **2015**, 2, 1656-1659	4.3	5
189	First-principles investigation of the GaN growth process in carbon-added Na-flux method. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 1084-1088	1.3	6
188	Search for a Self-Regenerating Perovskite Catalyst with Ab Initio Thermodynamics II: Cu-Doped Layered Perovskites with K2NiF4 Structure. *Catalysis Letters*, **2014**, 144, 736-743	2.8	6

187	Dissociative adsorption of CO2 on flat, stepped, and kinked Cu surfaces. *Journal of Chemical Physics* , **2014**, 141, 034702	3.9	50
186	Generation of 10(20) W cm(-2) hard X-ray laser pulses with two-stage reflective focusing system. *Nature Communications*, **2014**, 5, 3539	17.4	105
185	Theoretical investigation of the band structure of picene single crystals within theGWapproximation. *Japanese Journal of Applied Physics*, **2014**, 53, 05FY02	1.4	13
184	Aggregation of carbon atoms at SiO2/SiC(0 0 0 1) interface by plasma oxidation toward formation of pit-free graphene. *Carbon*, **2014**, 80, 440-445	10.4	4
183	Cooperative H2 Activation at Ag Cluster/Al2O3(110) Dual Perimeter Sites: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2014**, 118, 7996-8006	3.8	28
182	Enhancement of photoluminescence efficiency from GaN(0001) by surface treatments. *Japanese Journal of Applied Physics*, **2014**, 53, 021001	1.4	9
181	Planarization of 4H-SiC(0001) by catalyst-referred etching using pure water etchant **2014**,		2
180	4H-SiC Planarization Using Catalyst-Referred Etching with Pure Water. *Materials Science Forum*, **2014**, 778-780, 722-725	0.4	3
179	Investigation of the Barrier Heights for Dissociative Adsorption of HF on SiC Surfaces in the Catalyst-Referred Etching Process. *Materials Science Forum*, **2014**, 778-780, 726-729	0.4	1
178	Intermolecular interaction as the origin of red shifts in absorption spectra of zinc-phthalocyanine from first-principles. *Journal of Physical Chemistry A*, **2013**, 117, 11246-53	2.8	33
177	First-principles theoretical study of hydrolysis of stepped and kinked Ga-terminated GaN surfaces. *Nanoscale Research Letters*, **2013**, 8, 232	5	9
176	First-principles investigation on the segregation of Pd at LaFe1-xPdxO3-y surfaces. *Nanoscale Research Letters*, **2013**, 8, 203	5	15
175	Planarization of SiC and GaN Wafers Using Polishing Technique Utilizing Catalyst Surface Reaction. *ECS Journal of Solid State Science and Technology*, **2013**, 2, N3028-N3035	2	19
174	Focusing of X-ray free-electron laser pulses with reflective optics. *Nature Photonics*, **2013**, 7, 43-47	33.9	195
173	HOMO band dispersion of crystalline rubrene: Effects of self-energy corrections within the GW approximation. *Physical Review B*, **2013**, 88,	3.3	34
172	Understanding the MetalMolecule Interface from First Principles **2013**, 51-89		9
171	Search for a Self-Regenerating Perovskite Catalyst Using ab Initio Thermodynamics Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 1278-1286	3.8	23
170	Study of Terminated Species on 4H-SiC (0001) Surfaces Planarized by Catalyst-Referred Etching. *Materials Science Forum*, **2013**, 740-742, 510-513	0.4	2

169	Study on Reactive Species in Catalyst-Referred Etching of 4H□SiC using Platinum and Hydrofluoric Acid. *Materials Science Forum*, **2013**, 740-742, 847-850	0.4	4
168	Structural Analysis of Carbon-Added Na□Ga Melts in Na Flux GaN Growth by First-Principles Calculation. *Japanese Journal of Applied Physics*, **2013**, 52, 08JA04	1.4	5
167	Atomically Smooth Gallium Nitride Surfaces Prepared by Chemical Etching with Platinum Catalyst in Water. *Journal of the Electrochemical Society*, **2012**, 159, H417-H420	3.9	26
166	First-principles theoretical study of organic/metal interfaces: Vacuum level shifts and interface dipoles. *Current Applied Physics*, **2012**, 12, S2-S9	2.6	14
165	Density functional theory on the comparison of the Pd segregation behavior at LaO- and FeO2-terminated surfaces of LaFe1□PdxO3□. *Current Applied Physics*, **2012**, 12, S105-S109	2.6	5
164	Chemisorption-induced gap states at organic-metal interfaces: benzenethiol and benzeneselenol on metal surfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 4101-8	3.6	8
163	Structural and chemical characteristics of atomically smooth GaN surfaces prepared by abrasive-free polishing with Pt catalyst. *Journal of Crystal Growth*, **2012**, 349, 83-88	1.6	26
162	Local electronic properties at organic-metal interfaces: thiophene derivatives on Pt(111). *Physical Chemistry Chemical Physics*, **2012**, 14, 15412-20	3.6	8
161	Adsorption of hydrogen fluoride on SiC surfaces: A density functional theory study. *Current Applied Physics*, **2012**, 12, S42-S46	2.6	13
160	The charged interface between Pt and water: First principles molecular dynamics simulations. *AIP Advances*, **2012**, 2, 032182	1.5	15
159	Smoothing of Single Crystalline SiC and GaN by Catalyst Referred Etching. *Journal of the Japan Society for Precision Engineering*, **2012**, 78, 947-951	0.1	1
158	Surface Observation of 4H-SiC (0001) Planarized by Catalyst-Referred Etching. *Key Engineering Materials*, **2012**, 516, 452-456	0.4	
157	High-Resolution TEM Observation of 4H-SiC (0001) Surface Planarized by Catalyst-Referred Etching. *Materials Science Forum*, **2012**, 717-720, 873-876	0.4	5
156	First-Principles Analysis of Dissociative Absorption of HF Molecule at SiC Surface Step Edge. *Materials Science Forum*, **2012**, 717-720, 581-584	0.4	4
155	First-Principles Study of Reaction Process of SiC and HF Molecules in Catalyst-Referred Etching. *Key Engineering Materials*, **2012**, 523-524, 173-177	0.4	2
154	3.?/Pt?????????????????????. *Electrochemistry*, **2012**, 80, 932-937	1.2	
153	New Polishing Technique of Semiconductor SiC Substrate : Development of Polishing Technique Utilizing Catalyst Surface Reaction. *Journal of the Society of Mechanical Engineers*, **2012**, 115, 767-771	0	1
152	Improvement of Removal Rate in Abrasive-Free Planarization of 4H-SiC Substrates Using Catalytic Platinum and Hydrofluoric Acid. *Japanese Journal of Applied Physics*, **2012**, 51, 046501	1.4	10

151	A density functional theory study of self-regenerating catalysts LaFe(1-x)M(x)O(3-y) (M = Pd, Rh, Pt). *Journal of the American Chemical Society*, **2011**, 133, 18506-9	16.4	71
150	First-principles Theoretical Study of Organic-metal Interfaces. *Hyomen Kagaku*, **2011**, 32, 9-14		
149	TEM Observation of 8 Deg Off-Axis 4H-SiC (0001) Surfaces Planarized by Catalyst-Referred Etching. *Materials Science Forum*, **2011**, 679-680, 489-492	0.4	6
148	Evaluation of Schottky barrier diodes fabricated directly on processed 4H-SiC(0001) surfaces. *Journal of Nanoscience and Nanotechnology*, **2011**, 11, 2809-13	1.3	1
147	Dependence of process characteristics on atomic-step density in catalyst-referred etching of 4H-SiC(0001) surface. *Journal of Nanoscience and Nanotechnology*, **2011**, 11, 2928-30	1.3	24
146	Influence of gallium additives on surface roughness for photoelectrochemical planarization of GaN. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2011**, 8, 2223-2225		3
145	Density Functional Theoretical Study of Perfluoropentacene/Noble Metal Interfaces with van der Waals Corrections: Adsorption States and Vacuum Level Shifts. *Journal of Physical Chemistry C*, **2011**, 115, 5767-5772	3.8	22
144	Density-functional theoretical study of fluorination effect on organic/metal interfaces. *Organic Electronics*, **2011**, 12, 295-299	3.5	12
143	Adsorption of benzene on noble metal surfaces studied by density functional theory with Van der Waals correction. *Journal of Nanoscience and Nanotechnology*, **2011**, 11, 2836-43	1.3	9
142	Adsorption of Alq3 on Mg(001) surface: Role of chemical bonding, molecular distortion, and van der Waals interaction. *Physical Review B*, **2011**, 83,	3.3	6
141	A density-functional theory study of water on clean and hydrogen preadsorbed Rh(111) surfaces. *Journal of Chemical Physics*, **2011**, 134, 154701	3.9	12
140	Mechanism of atomic-scale passivation and flattening of semiconductor surfaces by wet-chemical preparations. *Journal of Physics Condensed Matter*, **2011**, 23, 394202	1.8	5
139	State-selective dissociation of a single water molecule on an ultrathin MgO film. *Nature Materials*, **2010**, 9, 442-7	27	146
138	Breaking the 10 nm barrier in hard-X-ray focusing. *Nature Physics*, **2010**, 6, 122-125	16.2	413
137	Interaction of water with a metal surface: Importance of van der Waals forces. *Physical Review B*, **2010**, 81,	3.3	55
136	Symmetric hydrogen bond in a water-hydroxyl complex on Cu(110). *Physical Review B*, **2010**, 81,	3.3	37
135	Crystal Machining Using Atmospheric Pressure Plasma **2010**, 313-330		
134	Spin- and energy-dependent tunneling through a single molecule with intramolecular spatial resolution. *Physical Review Letters*, **2010**, 105, 047204	7.4	240

133	C60 Adsorbed on Platinum Surface: A Good Mediator of Metal Wave Function. *Journal of Physical Chemistry C*, **2010**, 114, 3504-3506	3.8	19
132	Density functional theoretical study of pentacene/noble metal interfaces with van der Waals corrections: vacuum level shifts and electronic structures. *Journal of Chemical Physics*, **2010**, 132, 134703	3.9	114
131	Chemisorption-induced gap state at organic-metal interface: Benzenethiol on Pt(111). *Physical Chemistry Chemical Physics*, **2010**, 12, 10914-8	3.6	7
130	Adsorption of n-butane on Cu(100), Cu(111), Au(111), and Pt(111): Van der Waals density-functional study. *Physical Review B*, **2010**, 82,	3.3	48
129	Origin of Surface-Band Dispersion at the Pentacene/Cu Interface. *Applied Physics Express*, **2010**, 3, 025701	2.4	9
128	Ultra-precision Figured 4H-SiC(0001) Surfaces. *Hyomen Kagaku*, **2010**, 31, 466-473		
127	Electronic structure of hydrogen-terminated silicon surfaces [H-Si(111)] studied by two-photon photoemission. *Applied Physics A: Materials Science and Processing*, **2010**, 98, 735-743	2.6	8
126	Structures of Pt clusters on graphene by first-principles calculations. *Surface Science*, **2010**, 604, 144-154	1.8	76
125	A novel mechanism for spectator CO-mediated reaction with unique cis-(NO)2 dimer on a Co2+-dimer/Al2O3(110) model catalyst: Density functional theory calculations. *Catalysis Today*, **2010**, 154, 118-126	5.3	1
124	Termination dependence of surface stacking at 4H-SiC(0001): Density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	21
123	Green's function method for elimination of the spurious multipole interaction in the surface/interface slab model. *Physical Review B*, **2009**, 80,	3.3	60
122	The relationship between formate adsorption energy and electronic properties: A first principles density functional theory study. *Science in China Series B: Chemistry*, **2009**, 52, 1427-1433		8
121	A Study on a Surface Preparation Method for Single-Crystal SiC Using an Fe Catalyst. *Journal of Electronic Materials*, **2009**, 38, 159-163	1.9	24
120	First-principles study of the pentacene/Cu(111) interface: Adsorption states and vacuum level shifts. *Journal of Electron Spectroscopy and Related Phenomena*, **2009**, 174, 78-84	1.7	43
119	First-principles study of benzene on noble metal surfaces: Adsorption states and vacuum level shifts. *Surface Science*, **2009**, 603, 2912-2922	1.8	79
118	Theoretical investigation of the electronic structure of the Alq(3)/Mg interface. *Journal of Physics Condensed Matter*, **2009**, 21, 064247	1.8	12
117	Tunneling dynamics of a hydroxyl group adsorbed on Cu(110). *Physical Review B*, **2009**, 79,	3.3	58
116	Electron emission spectra of thermal collisions of He metastable atoms with Au(111) and Pt(111) surfaces: Evidence for Penning ionization. *Physical Review A*, **2009**, 80,	2.6	3

115	??*Electrochemistry*, **2009**, 77, 241-247	1.2	3
114	Damage-Free Planarization of 2-Inch 4H-SiC Wafer Using Pt Catalyst Plate and HF Solution. *Materials Science Forum*, **2008**, 600-603, 835-838	0.4	11
113	Role of molecular orbitals near the fermi level in the excitation of vibrational modes of a single molecule at a scanning tunneling microscope junction. *Physical Review Letters*, **2008**, 100, 136104	7.4	65
112	Density-Functional Analysis of Hydrogen on Pt(111): Electric Field, Solvent, and Coverage Effects. *Journal of Physical Chemistry C*, **2008**, 112, 10889-10898	3.8	68
111	Defect-Free Planarization of 4H□SiC(0001) Substrate Using Reference Plate. *Japanese Journal of Applied Physics*, **2008**, 47, 104-107	1.4	14
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