Yoshitada Morikawa

List of Publications by Citations

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	CO chemisorption at metal surfaces and overlayers. *Physical Review Letters*, **1996**, 76, 2141-2144	7.4	1135
275	Breaking the 10 nm barrier in hard-X-ray focusing. *Nature Physics*, **2010**, 6, 122-125	16.2	413
274	Adsorption state of dimethyl disulfide on Au(111): Evidence for adsorption as thiolate at the bridge site. *Journal of Chemical Physics*, **2001**, 114, 7615-7621	3.9	271
273	Spin- and energy-dependent tunneling through a single molecule with intramolecular spatial resolution. *Physical Review Letters*, **2010**, 105, 047204	7.4	240
272	Theoretical study of hydrogenation process of formate on clean and Zn deposited Cu(1 1 1) surfaces. *Applied Surface Science*, **2001**, 169-170, 11-15	6.7	198
271	Focusing of X-ray free-electron laser pulses with reflective optics. *Nature Photonics*, **2013**, 7, 43-47	33.9	195
270	Theoretical study of n-alkane adsorption on metal surfaces. *Physical Review B*, **2004**, 69,	3.3	178
269	Efficient focusing of hard x rays to 25nm by a total reflection mirror. *Applied Physics Letters*, **2007**, 90, 051903	3.4	173
268	Jahn-Teller distortion and magnetic structures in LaMnO3. *Physical Review B*, **1997**, 56, 12154-12160	3.3	152
267	State-selective dissociation of a single water molecule on an ultrathin MgO film. *Nature Materials*, **2010**, 9, 442-7	27	146
266	Density functional theory investigation of benzenethiol adsorption on Au(111). *Journal of Chemical Physics*, **2004**, 120, 6705-11	3.9	128
265	Optimized structures and electronic properties of alkali-metal (Na, K) -adsorbed Si(001) surfaces. *Physical Review B*, **1992**, 45, 3469-3484	3.3	125
264	Microstitching interferometry for x-ray reflective optics. *Review of Scientific Instruments*, **2003**, 74, 2894-2898	2.7	117
263	Electrode Dynamics from First Principles. *Journal of the Physical Society of Japan*, **2008**, 77, 024802	1.5	116
262	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
261	Electronic structures of Au on TiO2(110) by first-principles calculations. *Physical Review B*, **2004**, 69,	3.3	114
260	Structure of the water/platinum interface--a first principles simulation under bias potential. *Physical Chemistry Chemical Physics*, **2008**, 10, 3609-12	3.6	108

259	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
258	Adsorption geometries and vibrational modes of C2H2 on the Si(001) surface. *Physical Review B*, **2001**, 63,	3.3	104
257	Density Functional Calculations of N2Adsorption and Dissociation on a Ru(0001) Surface. *Journal of Catalysis*, **1997**, 169, 85-92	7.3	97
256	Origin of the stability of Ge(105) on si: a new structure model and surface strain relaxation. *Physical Review Letters*, **2002**, 88, 176101	7.4	94
255	Relative angle determinable stitching interferometry for hard x-ray reflective optics. *Review of Scientific Instruments*, **2005**, 76, 045102	1.7	93
254	First-principles molecular dynamics simulation of biased electrode/solution interface. *Surface Science*, **2007**, 601, 5237-5240	1.8	92
253	Novel abrasive-free planarization of 4H-SiC (0001) using catalyst. *Journal of Electronic Materials*, **2006**, 35, L11-L14	1.9	91
252	Order-disorder phase transition on the Si(001) surface: Critical role of dimer defects. *Physical Review B*, **1994**, 49, 14774-14777	3.3	89
251	Direct observation of hydrogen-bond exchange within a single water dimer. *Physical Review Letters*, **2008**, 100, 166101	7.4	88
250	Oxygen vacancy promoting catalytic dehydration of formic acid on TiO2(110) by in situ scanning tunneling microscopic observation. *Journal of Physical Chemistry B*, **2005**, 109, 18831-8	3.4	87
249	Fabrication of elliptical mirror at nanometer-level accuracy for hard x-ray focusing by numerically controlled plasma chemical vaporization machining. *Review of Scientific Instruments*, **2003**, 74, 4549-4553	1.7	87
248	First-principles theoretical study of alkylthiolate adsorption on Au(). *Surface Science*, **2002**, 507-510, 46-50	1.8	87
247	CO adsorption and dissociation on Pt(111) and Ni(111) surfaces. *Surface Science*, **1997**, 386, 67-72	1.8	85
246	Kinetic mechanism of methanol decomposition on Ni(111) surface: a theoretical study. *Journal of Physical Chemistry B*, **2005**, 109, 12431-42	3.4	84
245	First-principles study of benzene on noble metal surfaces: Adsorption states and vacuum level shifts. *Surface Science*, **2009**, 603, 2912-2922	1.8	79
244	First-principles molecular dynamics study of acetylene adsorption on the Si(001) surface. *Surface Science*, **1995**, 341, L1091-L1095	1.8	79
243	Structures of Pt clusters on graphene by first-principles calculations. *Surface Science*, **2010**, 604, 144-154	1.8	76
242	Imaging of all dangling bonds and their potential on the Ge/Si105 surface by noncontact atomic force microscopy. *Physical Review Letters*, **2004**, 93, 266102	7.4	75

241	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
240	Cluster and periodic DFT calculations of adsorption and activation of CO2 on the Cu(hkl) surfaces. *Surface Science*, **2004**, 570, 205-217	1.8	70
239	A density-functional study of the atomic structures and vibrational spectra of NO/Pt(111). *Surface Science*, **2002**, 514, 394-403	1.8	70
238	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
237	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
236	Atomic-scale flattening of SiC surfaces by electroless chemical etching in HF solution with Pt catalyst. *Applied Physics Letters*, **2007**, 90, 202106	3.4	65
235	Further lowering of work function by oxygen adsorption on the K/Si(001) surface. *Physical Review B* , **1995**, 51, 14802-14805	3.3	65
234	Why is formate synthesis insensitive to copper surface structures?. *Journal of Physical Chemistry B*, **2006**, 110, 9-11	3.4	63
233	Comparison of localized basis and plane-wave basis for density-functional calculations of organic molecules on metals. *Physical Review B*, **2007**, 75,	3.3	62
232	First-principles theoretical study of metallic states of DCNQI-(Cu,Ag) systems: Simplicity and variety in complex systems. *Physical Review Letters*, **1995**, 74, 5104-5107	7.4	61
231	Green function method for elimination of the spurious multipole interaction in the surface/interface slab model. *Physical Review B*, **2009**, 80,	3.3	60
230	Fabrication of elliptically figured mirror for focusing hard x rays to size less than 50nm. *Review of Scientific Instruments*, **2005**, 76, 063708	1.7	59
229	First-Principles Theoretical Study and Scanning Tunneling Microscopic Observation of Dehydration Process of Formic Acid on a TiO2(110) Surface *Journal of Physical Chemistry B*, **2004**, 108, 14446-14451	3.4	59
228	Tunneling dynamics of a hydroxyl group adsorbed on Cu(110). *Physical Review B*, **2009**, 79,	3.3	58
227	Interaction of water with a metal surface: Importance of van der Waals forces. *Physical Review B*, **2010**, 81,	3.3	55
226	Comparative study of dehydrogenation of methanol at Pt(1 1 1)/water and Pt(1 1 1)/vacuum interfaces. *Chemical Physics Letters*, **2003**, 377, 236-242	2.5	54
225	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
224	Dissociative adsorption of CO2 on flat, stepped, and kinked Cu surfaces. *Journal of Chemical Physics* , **2014**, 141, 034702	3.9	50

223	At-wavelength figure metrology of hard x-ray focusing mirrors. *Review of Scientific Instruments*, **2006**, 77, 063712	1.7	50
222	Theoretical support to the double-layer model for potassium adsorption on the Si(001) surface. *Physical Review B*, **1991**, 44, 3459-3462	3.3	50
221	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
220	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
219	First-principles theoretical study of Alq3Al interfaces: origin of the interfacial dipole. *Journal of Chemical Physics*, **2008**, 128, 244704	3.9	48
218	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
217	Ab initio study of surface structural changes during methanol synthesis over Zn/Cu(111). *Chemical Physics Letters*, **1999**, 304, 91-97	2.5	43
216	Methylthiolate induced vacancy formation on Au(111): a density functional theoretical study. *Surface Science*, **2002**, 514, 389-393	1.8	41
215	First-principles molecular dynamics study of alkali-metal adsorption on a Si(001) surface. *Surface Science*, **1993**, 283, 377-382	1.8	41
214	Vibration-driven reaction of CO on Cu surfaces via Eley-Rideal-type mechanism. *Nature Chemistry*, **2019**, 11, 722-729	17.6	38
213	Individual Atomic Imaging of Multiple Dopant Sites in As-Doped Si Using Spectro-Photoelectron Holography. *Nano Letters*, **2017**, 17, 7533-7538	11.5	37
212	Symmetric hydrogen bond in a water-hydroxyl complex on Cu(110). *Physical Review B*, **2010**, 81,	3.3	37
211	Switchover of Reaction Mechanism for the Catalytic Decomposition of HCOOH on a TiO2(110) Surface. *Journal of Physical Chemistry C*, **2007**, 111, 16379-16386	3.8	37
210	Important role of molecular permanent dipoles of the Alq3/Al interface studied from first-principles. *Chemical Physics Letters*, **2006**, 420, 523-528	2.5	37
209	Thinning of silicon-on-insulator wafers by numerically controlled plasma chemical vaporization machining. *Review of Scientific Instruments*, **2004**, 75, 942-946	1.7	36
208	HOMO band dispersion of crystalline rubrene: Effects of self-energy corrections within the GW approximation. *Physical Review B*, **2013**, 88,	3.3	34
207	Direct determination of the wave field of an x-ray nanobeam. *Physical Review A*, **2008**, 77,	2.6	34
206	Catalyst-referred etching of 4H?SiC substrate utilizing hydroxyl radicals generated from hydrogen peroxide molecules. *Surface and Interface Analysis*, **2008**, 40, 998-1001	1.5	34

205	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
204	CO adsorption on the copper surfaces: van der Waals density functional and TPD studies. *Journal of Chemical Physics*, **2017**, 147, 094702	3.9	33
203	Self-consistent van der Waals density functional study of benzene adsorption on Si(100). *Physical Review B*, **2016**, 93,	3.3	32
202	A theoretical study of surface-structural sensitivity of the reverse water-gas shift reaction over Cu(hkl) surfaces. *Surface Science*, **2003**, 543, 118-130	1.8	32
201	Rebonded SB step model of Ge/Si()12: A first-principles theoretical study. *Surface Science*, **2002**, 513, L445-L450	1.8	30
200	Dynamic fracture of tantalum under extreme tensile stress. *Science Advances*, **2017**, 3, e1602705	14.3	30
199	Structure and binding energies of unsaturated hydrocarbons on Si(001) and Ge(001). *Journal of Chemical Physics*, **2006**, 124, 024716	3.9	29
198	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
197	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
196	Structural phase transition on Si(001) and Ge(001) surfaces. *Phase Transitions*, **1995**, 53, 143-163	1.3	28
195	Coverage-dependent core-level binding-energy shifts of alkali-metal atoms on metal surfaces. *Physical Review B*, **1993**, 47, 4014-4017	3.3	28
194	Angle-resolved photoemission from Nd2-xCexCuO4(001): A dispersive bandlike Fermi-liquid state of Cu 3d character near the Fermi level. *Physical Review B*, **1990**, 42, 4189-4195	3.3	28
193	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
192	A Comparison of N2 and CO Adsorption on Ru(001). *Zeitschrift Fur Physikalische Chemie*, **1997**, 198, 113-122	3.1	27
191	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
190	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
189	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
188	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

187	First principles study of thermal decomposition of alkyl□gallium and tertiary butylarsine. *Journal of Chemical Physics*, **2000**, 112, 9549-9556	3.9	24
186	Search for a Self-Regenerating Perovskite Catalyst Using ab Initio Thermodynamics Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 1278-1286	3.8	23
185	Highly accurate differential deposition for X-ray reflective optics. *Surface and Interface Analysis*, **2008**, 40, 1019-1022	1.5	23
184	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
183	Adsorption states of methylthiolate on the Au(111) surface. *Journal of Physics Condensed Matter*, **2007**, 19, 365245	1.8	22
182	Stability of homochiral and heterochiral phases of glycinate on Cu(001): a first principles theoretical study. *Surface Science*, **2004**, 553, L63-L67	1.8	22
181	Coverage-dependent core level photoemission investigations of Na/Cu(111) and Na/Ni(111). *Surface Science*, **1993**, 290, 69-79	1.8	22
180	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
179	Termination dependence of surface stacking at 4H-SiC(0001)□□: Density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	21
178	Characterization of temporal coherence of hard X-ray free-electron laser pulses with single-shot interferograms. *IUCrJ*, **2017**, 4, 728-733	4.7	21
177	Electronic structure of the 4 □4 silicene monolayer on semi-infinite Ag(111). *New Journal of Physics*, **2015**, 17, 015013	2.9	20
176	First-principles molecular dynamics study of CO adsorption on the Si(001) surface. *Chemical Physics Letters*, **1998**, 287, 131-136	2.5	20
175	Density functional theoretical calculations for a Co2/gamma-Al2O3 model catalyst: structures of the gamma-Al2O3 bulk and surface and attachment sites for Co2+ ions. *Journal of Physical Chemistry B*, **2006**, 110, 4929-36	3.4	20
174	Hard X-ray nanofocusing using adaptive focusing optics based on piezoelectric deformable mirrors. *Review of Scientific Instruments*, **2015**, 86, 043102	1.7	19
173	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
172	C60 Adsorbed on Platinum Surface: A Good Mediator of Metal Wave Function. *Journal of Physical Chemistry C*, **2010**, 114, 3504-3506	3.8	19
171	Two-dimensional self-assembled structures of adenine molecules: modeling and simulation. *Surface Science*, **2004**, 556, 109-120	1.8	19
170	Chemisorption and thermal decomposition of benzene on palladium(110): high-resolution electron energy loss spectroscopy, low-energy electron diffraction, and thermal desorption studies. *The Journal of Physical Chemistry*, **1991**, 95, 7415-7422		19

169	Water Monomer and Dimer on Cu(110) Studied Using a Scanning Tunneling Microscope. *E-Journal of Surface Science and Nanotechnology*, **2008**, 6, 296-300	0.7	19
168	Photoelectron Holographic Atomic Arrangement Imaging of Cleaved Bimetal-intercalated Graphite Superconductor Surface. *Scientific Reports*, **2016**, 6, 36258	4.9	18
167	Spatial electron distribution of CO adsorbed on Ni(100) and Ni(111) surfaces probed by metastable impact electron spectroscopy. *Journal of Chemical Physics*, **2001**, 114, 8546-8554	3.9	18
166	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
165	Development of Co Supported on CoAl Spinel Catalysts from Exsolution of Amorphous CoAl Oxides for Carbon Dioxide Reforming of Methane. *ChemCatChem*, **2019**, 11, 5593-5605	5.2	17
164	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
163	Fabrication of ultrathin and highly uniform silicon on insulator by numerically controlled plasma chemical vaporization machining. *Review of Scientific Instruments*, **2007**, 78, 086102	1.7	17
162	Desorption dynamics of CO from formate decomposition on Cu(111). *Chemical Communications*, **2017**, 53, 9222-9225	5.8	16
161	Chemical etching of silicon carbide in pure water by using platinum catalyst. *Applied Physics Letters*, **2017**, 110, 201601	3.4	15
160	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
159	First-principles investigation on the segregation of Pd at LaFe1-xPdxO3-y surfaces. *Nanoscale Research Letters*, **2013**, 8, 203	5	15
158	The charged interface between Pt and water: First principles molecular dynamics simulations. *AIP Advances*, **2012**, 2, 032182	1.5	15
157	Local Electronic Properties Induced at the MoleculeMetal Interface. *Journal of Physical Chemistry C*, **2007**, 111, 11747-11750	3.8	15
156	Theoretical Investigation on the Electronic Structure of the Tris-(8-hydroxyquinolinato) Aluminum/Aluminum Interface. *Japanese Journal of Applied Physics*, **2006**, 45, 413-416	1.4	15
155	Improvement of the thickness distribution of a quartz crystal wafer by numerically controlled plasma chemical vaporization machining. *Review of Scientific Instruments*, **2005**, 76, 096103	1.7	15
154	X-ray optics for advanced ultrafast pump-probe X-ray experiments at SACLA. *Journal of Synchrotron Radiation*, **2019**, 26, 333-338	2.4	15
153	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
152	First-principles theoretical study of organic/metal interfaces: Vacuum level shifts and interface dipoles. *Current Applied Physics*, **2012**, 12, S2-S9	2.6	14

151	Defect-Free Planarization of 4H□SiC(0001) Substrate Using Reference Plate. *Japanese Journal of Applied Physics*, **2008**, 47, 104-107	1.4	14
150	A first-principles study on nitrogen solubility in Na flux toward theoretical search for a novel flux for bulk GaN growth. *Journal of Crystal Growth*, **2007**, 303, 34-36	1.6	14
149	Investigation of the Surface Removal Process of Silicon Carbide in Elastic Emission Machining. *Journal of Electronic Materials*, **2007**, 36, 92-97	1.9	14
148	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
147	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
146	Theoretical investigation of the band structure of picene single crystals within theGWapproximation. *Japanese Journal of Applied Physics*, **2014**, 53, 05FY02	1.4	13
145	Adsorption of hydrogen fluoride on SiC surfaces: A density functional theory study. *Current Applied Physics*, **2012**, 12, S42-S46	2.6	13
144	The local electronic properties and formation process of titanium silicide nanostructures on Si(001)-(2 □1). *Journal of Physics Condensed Matter*, **2008**, 20, 485006	1.8	13
143	Adsorption structure of benzenethiol on Au(1 1 1): first-principles study. *Applied Surface Science*, **2004**, 237, 434-439	6.7	13
142	Platinum single-atom adsorption on graphene: a density functional theory study. *Nanoscale Advances*, **2019**, 1, 1165-1174	5.1	12
141	Mechanistic Analysis of Oxygen Vacancy Formation and Ionic Transport in Sr3Fe2O7□*Journal of Physical Chemistry C*, **2018**, 122, 4172-4181	3.8	12
140	Density-functional theoretical study of fluorination effect on organic/metal interfaces. *Organic Electronics*, **2011**, 12, 295-299	3.5	12
139	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
138	Theoretical investigation of the electronic structure of the Alq(3)/Mg interface. *Journal of Physics Condensed Matter*, **2009**, 21, 064247	1.8	12
137	Stitching interferometric metrology for steeply curved x-ray mirrors. *Surface and Interface Analysis*, **2008**, 40, 1023-1027	1.5	12
136	Structural and vibrational properties of alkali-metal overlayers on metals. *Surface Science*, **1993**, 291, 87-92	1.8	12
135	Angle-resolved photoemission from epitaxial Nd2-xCexCu O4 (001) films. *Solid State Communications*, **1990**, 74, 609-611	1.6	12
134	Hybrid image potential states in molecular overlayers on graphene. *Physical Review Materials*, **2017**, 1,	3.2	12

133	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
132	First-principles study of ZnSnAs2-based dilute magnetic semiconductors. *Japanese Journal of Applied Physics*, **2018**, 57, 020306	1.4	11
131	Microscopic properties of ionic liquid/organic semiconductor interfaces revealed by molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2018**, 20, 13075-13083	3.6	11
130	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
129	A new aspect of heterogeneous catalysis: Highly reactive cis-(NO)2 dimer and Eley□Rideal mechanism for NO□CO reaction on a Co-dimer/□alumina catalyst. *Chemical Physics Letters*, **2007**, 443, 66-70	2.5	11
128	First-principles molecular dynamics study of Al/Alq3 interfaces. *Science and Technology of Advanced Materials*, **2007**, 8, 191-195	7.1	10
127	Study of Interaction between Au and TiO2(110) at Low Coverage. *Materials Transactions*, **2006**, 47, 2663-2668	1.3	10
126	Stability and electronic structure of Ge(105)1□2: a first-principles theoretical study. *Surface Science*, **2005**, 576, 61-66	1.8	10
125	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
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123	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
122	Enhancement of photoluminescence efficiency from GaN(0001) by surface treatments. *Japanese Journal of Applied Physics*, **2014**, 53, 021001	1.4	9
121	First-principles theoretical study of hydrolysis of stepped and kinked Ga-terminated GaN surfaces. *Nanoscale Research Letters*, **2013**, 8, 232	5	9
120	Understanding the Metal□Molecule Interface from First Principles **2013**, 51-89		9
119	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
118	Origin of Surface-Band Dispersion at the Pentacene/Cu Interface. *Applied Physics Express*, **2010**, 3, 025701	2.4	9
117	Simulation of growth process of Pt-particles - first-principles calculations. *Journal of Physics: Conference Series*, **2008**, 100, 072044	0.3	9
116	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

115	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
114	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
113	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
112	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
111	Local electronic properties at organic-metal interfaces: thiophene derivatives on Pt(111). *Physical Chemistry Chemical Physics*, **2012**, 14, 15412-20	3.6	8
110	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
109	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
108	Theoretical study of vacuum level shift at the C6H6/Al(111) interface. *Surface and Interface Analysis* , **2008**, 40, 1059-1062	1.5	8
107	Electronic Structures of Ag and Au Adsorbed on TiO2(110) Surfaces by First-Principles Calculations. *Materials Transactions*, **2006**, 47, 2669-2673	1.3	8
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