Atsushi Oshiyama

List of Publications by Year in Descending Order

138 papers	8,709 citations	42 h-index	92 g-index
141 ext. papers	9,072 ext. citations	3.6 avg, IF	5.94 L-index

#	Paper	IF	Citations
138	Exploration of a large-scale reconstructed structure on GaN(0001) surface by Bayesian optimization. *Applied Physics Letters*, **2022**, 120, 021602	3.4	3
137	Defect-free interface between amorphous (Al2O3)1−x(SiO2)x and GaN(0001) revealed by first-principles simulated annealing technique. *Applied Physics Letters*, **2021**, 119, 011602	3.4	2
136	Order-N orbital-free density-functional calculations with machine learning of functional derivatives for semiconductors and metals. *Physical Review Research*, **2021**, 3,	3.9	3
135	Density functional calculations for structures and energetics of atomic steps and their implication for surface morphology on Si-face SiC polar surfaces. *Physical Review B*, **2020**, 101,	3.3	5
134	Screw dislocation that converts p-type GaN to n-type: Microscopic study on Mg condensation and leakage current in p− diodes. *Applied Physics Letters*, **2020**, 117, 012105	3.4	12
133	Microscopic Identification of Surface Steps on SiC by Density-Functional Calculations. *Materials Science Forum*, **2020**, 1004, 145-152	0.4	1
132	Structural determination of phosphosilicate glass based on first-principles molecular dynamics calculation. *Japanese Journal of Applied Physics*, **2019**, 58, 011001	1.4	
131	First-principle study of ammonia decomposition and nitrogen incorporation on the GaN surface in metal organic vapor phase epitaxy. *Journal of Crystal Growth*, **2019**, 507, 421-424	1.6	4
130	Structural stability and energy levels of carbon-related defects in amorphous SiO2 and its interface with SiC. *Japanese Journal of Applied Physics*, **2018**, 57, 125701	1.4	9
129	Microscopic mechanism of carbon annihilation upon SiC oxidation due to phosphorus treatment: Density functional calculations combined with ion mass spectrometry. *Applied Physics Express*, **2018**, 11, 121301	2.4	1
128	Reaction Pathway of Surface-Catalyzed Ammonia Decomposition and Nitrogen Incorporation in Epitaxial Growth of Gallium Nitride. *Journal of Physical Chemistry C*, **2018**, 122, 24665-24671	3.8	5
127	Microscopic Mechanisms of Initial Formation Process of Graphene on SiC(0001) Surfaces: Selective Si Desorption from Step Edges. *Journal of Physical Chemistry C*, **2017**, 121, 5041-5049	3.8	6
126	First-Principles Calculations That Clarify Energetics and Reactions of Oxygen Adsorption and Carbon Desorption on 4H-SiC (112 0) Surface. *Journal of Physical Chemistry C*, **2017**, 121, 3920-3928	3.8	7
125	A Novel Intrinsic Interface State Controlled by Atomic Stacking Sequence at Interfaces of SiC/SiO. *Nano Letters*, **2017**, 17, 6458-6463	11.5	28
124	Indirect phase transition of TiC, ZrC, and HfC crystal structures. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 1177-1185	1.3	7
123	Large-scale real-space density-functional calculations: Moir−induced electron localization in graphene. *Journal of Applied Physics*, **2015**, 117, 112811	2.5	6
122	Electron doping through lithium intercalation to interstitial channels in tetrahedrally bonded SiC. *Journal of Applied Physics*, **2015**, 118, 175704	2.5	7

121	Origin of Repulsive Interactions between Bunched Steps on Vicinal Solid Surfaces. *E-Journal of Surface Science and Nanotechnology*, **2015**, 13, 231-234	0.7	1
120	Surface energy of Si(110)- and 3C-SiC(111)-terminated surfaces. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 1408-1415	1.3	14
119	Interstitial channels that control band gaps and effective masses in tetrahedrally bonded semiconductors. *Physical Review Letters*, **2014**, 112, 136403	7.4	26
118	Atom-Scale Reaction Pathways and Free-Energy Landscapes in Oxygen Plasma Etching of Graphene. *Journal of Physical Chemistry Letters*, **2013**, 4, 1592-6	6.4	27
117	Floating electron states in covalent semiconductors. *Physical Review Letters*, **2012**, 108, 246404	7.4	38
116	Si nanowire FET and its modeling. *Science China Information Sciences*, **2011**, 54, 1004-1011	3.4	13
115	A Simple scheme for estimating the pKa values of 5-substituted uracils. *Chemical Physics Letters*, **2011**, 502, 248-252	2.5	30
114	Energy compensation mechanism for charge-separated protonation states in aspartate-histidine amino acid residue pairs. *Journal of Physical Chemistry B*, **2010**, 114, 6567-78	3.4	6
113	A massively-parallel electronic-structure calculations based on real-space density functional theory. *Journal of Computational Physics*, **2010**, 229, 2339-2363	4.1	92
112	Large-Scale First-Principles Electronic Structure Calculations for Nano-Meter Size Si Quantum Dots. *E-Journal of Surface Science and Nanotechnology*, **2010**, 8, 48-51	0.7	3
111	First principles studies on In-related nitride semiconductors. *Journal of Crystal Growth*, **2009**, 311, 2772-2775	1.7	26
110	Significant change in electronic structures of heme upon reduction by strong Coulomb repulsion between Fe d electrons. *Journal of Physical Chemistry B*, **2009**, 113, 6866-72	3.4	5
109	Increased stability of C60 encapsulated in double walled carbon nanotubes. *Chemical Physics Letters*, **2008**, 455, 88-92	2.5	4
108	Possible mechanism of proton transfer through peptide groups in the H-pathway of the bovine cytochrome c oxidase. *Journal of the American Chemical Society*, **2007**, 129, 9663-73	16.4	57
107	Formation of titanium-carbide in a nanospace of C78 fullerenes. *Chemical Physics Letters*, **2007**, 438, 274-278	2.5	8
106	Quantum effects in a cylindrical carbon-nanotube capacitor. *Journal of Physics Condensed Matter*, **2007**, 19, 365218	1.8	4
105	First-principles molecular dynamics study of proton transfer mechanism in bovine cytochrome c oxidase. *Journal of Physics Condensed Matter*, **2007**, 19, 365220	1.8	7
104	Atomic and electronic structures of carbon nanotubes on Si(001) stepped surfaces. *Physical Review Letters*, **2006**, 96, 105505	7.4	29

103	Enol-to-keto tautomerism of peptide groups. *Journal of Physical Chemistry B*, **2006**, 110, 4443-50	3.4	21
102	Enhanced Si and B diffusion in semiconductor-grade SiO2 and the effect of strain on diffusion. *Thin Solid Films*, **2006**, 508, 270-275	2.2	5
101	Double-Metal-Ion/Single-Metal-Ion Mechanisms of the Cleavage Reaction of Ribozymes: First-Principles Molecular Dynamics Simulations of a Fully Hydrated Model System. *Journal of Chemical Theory and Computation*, **2005**, 1, 925-34	6.4	45
100	New electron states that float on semiconductor and metal surfaces. *Surface Science*, **2005**, 585, L177-L182	1.8	6
99	Free energy molecular dynamics simulations of pulsed-laser-irradiated SiO2: Si–Si bond formation in a matrix of SiO2. *Applied Physics Letters*, **2005**, 86, 201910	3.4	16
98	Electronic structure of semiconducting nanotubes adsorbed on metal surfaces. *Physical Review Letters*, **2005**, 95, 206804	7.4	45
97	E′CENTERS IN SILICON DIOXIDE: FIRST-PRINCIPLES MOLECULAR DYNAMICS STUDIES. *Modern Physics Letters B*, **2004**, 18, 707-724	1.6	12
96	A new alternative model of type-C defects on Si() surfaces. *Surface Science*, **2004**, 554, 272-279	1.8	45
95	Electronic structure of stacked C60 shuttlecocks. *Chemical Physics Letters*, **2004**, 399, 157-161	2.5	19
94	Electronic Structures of Polyglycine and Active Sites of Cytochrome c Oxidase. *Journal of the Physical Society of Japan*, **2004**, 73, 3198-3208	1.5	6
93	Scanning tunneling microscopy images of argon monolayer on a monolayer graphite surface. *Chemical Physics Letters*, **2003**, 371, 528-533	2.5	11
92	Theoretical study on stable structures and diffusion mechanisms of B in SiO2. *Applied Surface Science*, **2003**, 216, 490-496	6.7	3
91	Energetics and electronic structure of C70-peapods and one-dimensional chains of C70. *New Journal of Physics*, **2003**, 5, 122-122	2.9	21
90	Nanometer-Scale Ferromagnet: Carbon Nanotubes with Finite Length. *Journal of the Physical Society of Japan*, **2003**, 72, 1510-1515	1.5	80
89	Curvature-induced metallization of double-walled semiconducting zigzag carbon nanotubes. *Physical Review Letters*, **2003**, 91, 216801	7.4	65
88	E′centers in alpha quartz in the absence of oxygen vacancies: a first-principles molecular-dynamics study. *Physical Review Letters*, **2003**, 91, 206401	7.4	27
87	First-principle study on GaN epitaxy on lattice-matched ZrB2 substrates. *Applied Physics Letters*, **2003**, 83, 2560-2562	3.4	13
86	Prediction of electronic properties of carbon-based nanostructures. *Physica B: Condensed Matter*, **2002**, 323, 21-29	2.8	18

85	Electronic and geometric structures of multi-walled BN nanotubes. *Physica B: Condensed Matter*, **2002**, 323, 224-226	2.8	12
84	First-Principles Study of Hydrogen Incorporation in Multivacancy in Silicon. *Journal of the Physical Society of Japan*, **2001**, 70, 1627-1634	1.5	13
83	Pressure and Orientation Effects on the Electronic Structure of Carbon Nanotube Bundles. *Journal of the Physical Society of Japan*, **2001**, 70, 2345-2352	1.5	16
82	Atomic and electronic structures of N-incorporated Si oxides. *Physical Review Letters*, **2001**, 86, 3574-7	7.4	21
81	Energetics and electronic structures of encapsulated C60 in a carbon nanotube. *Physical Review Letters*, **2001**, 86, 3835-8	7.4	359
80	Magnetic ordering in hexagonally bonded sheets with first-row elements. *Physical Review Letters*, **2001**, 87, 146803	7.4	339
79	Open Edge Growth Mechanisms of Single Wall Carbon Nanotubes. *Journal of the Physical Society of Japan*, **2001**, 70, 1995-2011	1.5	11
78	Border states in heterosheets with hexagonal symmetry. *Physical Review B*, **2000**, 62, 9896-9899	3.3	64
77	Okada, Saito, and Oshiyama Reply:. *Physical Review Letters*, **2000**, 85, 5672-5672	7.4	2
76	Nearly free electron states in carbon nanotube bundles. *Physical Review B*, **2000**, 62, 7634-7638	3.3	75
75	Magnetic ordering of Ga wires on Si(100) surfaces. *Physical Review B*, **2000**, 62, R13286-R13289	3.3	6
74	First-principles study of intrinsic defects in yttrium oxysulfide. *Physical Review B*, **1999**, 60, 1707-1715	3.3	25
73	Chemical differences in surface diffusion: Si and Ge adatoms at the DB step on the hydrogenated Si(100) surface. *Physical Review B*, **1999**, 60, R11269-R11272	3.3	7
72	Energetics and kinetics for Si□Ge intermixing on Ge-adsorbed hydrogenated Si(100) surfaces. *Surface Science*, **1999**, 436, L666-L670	1.8	4
71	New Metallic Crystalline Carbon: Three Dimensionally Polymerized C60 Fullerite. *Physical Review Letters*, **1999**, 83, 1986-1989	7.4	111
70	First-principles band-structure calculation of yttrium oxysulfide. *Physical Review B*, **1998**, 57, 8939-8944	3.3	43
69	Structural Stability and Adatom Diffusion at Steps on Hydrogenated Si(100) Surfaces. *Physical Review Letters*, **1998**, 81, 5366-5369	7.4	56
68	Hole-Injection-Induced Structural Transformation of Oxygen Vacancy in □Quartz. *Japanese Journal of Applied Physics*, **1998**, 37, L232-L234	1.4	57

67	Diffusion mechanisms of a Si adatom on H-terminated Si(100) surfaces. *Physical Review B*, **1998**, 58, 12958-12963	3.3	27
66	Atomic structure and phonons in the π-bonded chain of the clean diamond (111) surface. *Physical Review B*, **1998**, 57, R9412-R9415	3.3	9
65	Atomic and Electronic Structures of Deformed Graphite Sheets. *Journal of the Physical Society of Japan*, **1998**, 67, 3976-3984	1.5	7
64	Magic Numbers of Multivacancy in Crystalline Si: Tight-Binding Studies for the Stability of the Multivacancy. *Journal of the Physical Society of Japan*, **1998**, 67, 4110-4116	1.5	22
63	Adsorption and Diffusion of Si Adatom on Hydrogenated Si(100) Surfaces. *Physical Review Letters*, **1997**, 79, 4425-4428	7.4	66
62	Microscopic surface structures and macroscopic thin-film morphology. *Thin Solid Films*, **1996**, 272, 364-374	2.2	1
61	Lifetimes of positrons trapped at Si vacancies. *Physical Review B*, **1996**, 53, 7810-7814	3.3	76
60	Covalency, elasticity and electron correlation in Si vacancies. *Applied Surface Science*, **1995**, 85, 239-245	6.7	29
59	Role of Ge surface segregation in Si/Ge interfacial ordering: Interface formation on a monohydride surface. *Physical Review B*, **1995**, 51, 14786-14789	3.3	14
58	Structures of steps and appearances of {311} facets on Si(100) surfaces. *Physical Review Letters*, **1995**, 74, 130-133	7.4	95
57	Structures and reactions of missing dimers in epitaxial growth of Ge on Si(100). *Physical Review B*, **1995**, 52, 8337-8343	3.3	12
56	Saito and Oshiyama reply. *Physical Review Letters*, **1995**, 74, 4354	7.4	13
55	Electronic structure of Si46 and Na2Ba6Si46. *Physical Review B*, **1995**, 51, 2628-2631	3.3	147
54	Resonant bonds in symmetry-lowering distortion around a Si divacancy. *Physical Review Letters*, **1994**, 73, 866-869	7.4	42
53	Design of C60-graphite cointercalation compounds. *Physical Review B*, **1994**, 49, 17413-17419	3.3	34
52	Reaction pathway for Sb-dimer rotation in conversion of Sb4 precursors on Si(001). *Physical Review B*, **1994**, 50, 8942-8945	3.3	15
51	Diffusion and dimer exchange in surfactant-mediated epitaxial growth. *Physical Review Letters*, **1994**, 72, 3190-3193	7.4	74
50	Scanning-tunneling-microscopy images of Ge adsorbed on an As-covered Si(001) surface. *Physical Review B*, **1994**, 50, 14631-14634	3.3	15

49	Electronic and Geometric Structures of Fullerenes and Metallofullerenes. *Japanese Journal of Applied Physics*, **1993**, 32, 1438-1443	1.4	16
48	Chemical trends and s-p hybridization in the DX center in GaAs. *Physical Review B*, **1993**, 48, 11804-11809	3.3	2
47	Sr6C60 and Ba6C60: Semimetallic fullerides. *Physical Review Letters*, **1993**, 71, 121-124	7.4	66
46	Dimer exchange mechanism for substitutional As adsorption on Si(100). *Physical Review Letters*, **1993**, 71, 585-588	7.4	42
45	Energetics and local vibrations of the DX center in GaAs. *Physical Review B*, **1993**, 47, 13205-13214	3.3	21
44	Electronic structure of alkali and alkaline-earth doped solid C60. *Journal of Physics and Chemistry of Solids*, **1993**, 54, 1759-1765	3.9	20
43	Electronic and geometric structures of fullerenes. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1993**, 19, 105-110	3.1	16
42	Electronic structure of fullerenes and fullerides: artificial atoms and their solids. *Nanotechnology*, **1992**, 3, 167-172	3.4	1
41	Vacancy in Si: Successful description within the local-density approximation. *Physical Review Letters*, **1992**, 68, 1858-1861	7.4	209
40	Validity of the broken-bond model for the DX center in GaAs. *Physical Review B*, **1992**, 45, 13745-13748	3.3	15
39	Microscopic mechanism of atomic diffusion in Si under pressure. *Physical Review B*, **1992**, 46, 12335-12341	3.3	53
38	Real-space-partitioned separable pseudopotential. *Physical Review B*, **1992**, 46, 2606-2609	3.3	31
37	Electronic structures of solid BC59. *Physical Review B*, **1992**, 46, 1749-1753	3.3	47
36	Linear dependence of superconducting transition temperature on Fermi-level density-of-states in alkali-doped C60. *Solid State Communications*, **1992**, 82, 41-45	1.6	103
35	Halogen doping in solid C60. *Solid State Communications*, **1992**, 82, 437-441	1.6	26
34	Electronic structure of calcium-doped C60. *Solid State Communications*, **1992**, 83, 107-110	1.6	66
33	Electronic structure of fullerides. *Journal of Physics and Chemistry of Solids*, **1992**, 53, 1689-1697	3.9	9
32	Electronic structures of C60 fullerides and related materials. *Journal of Physics and Chemistry of Solids*, **1992**, 53, 1457-1471	3.9	80

31	New one-dimensional conductors: Graphitic microtubules. *Physical Review Letters*, **1992**, 68, 1579-1581	7.4	2930
30	Fermi Surfaces of Alkali-Metal-Doped C60Solid. *Japanese Journal of Applied Physics*, **1991**, 30, L2036-L2038	1.4	20
29	Electronic and geometric structures of C70. *Physical Review B*, **1991**, 44, 11532-11535	3.3	107
28	Effect of anisotropic Coulomb field on Si 2p core levels in oxidized silicon. *Physical Review B*, **1991**, 44, 5931-5934	3.3	23
27	Ionic metal KxC60: Cohesion and energy bands. *Physical Review B*, **1991**, 44, 11536-11539	3.3	99
26	Anisotropic momentum distribution of positron-annihilation radiation in semiconductors. *Physical Review B*, **1991**, 44, 10601-10609	3.3	45
25	Energetics in the initial stage of oxidation of silicon. *Physical Review B*, **1991**, 43, 9287-9290	3.3	37
24	X-Ray Emission Spectrum of Solid C60. *Journal of the Physical Society of Japan*, **1991**, 60, 2518-2521	1.5	31
23	Cohesive mechanism and energy bands of solid C60. *Physical Review Letters*, **1991**, 66, 2637-2640	7.4	930
22	Metastable atomic configurations for oxygen adsorption on Si (100) surfaces. *Solid State Communications*, **1990**, 74, 343-346	1.6	17
21	Atomic and electronic structures of oxygen on Si(100) surfaces: Metastable adsorption sites. *Physical Review B*, **1990**, 41, 12680-12686	3.3	99
20	Atomic and electronic structures of an interface between silicon and beta -cristobalite. *Physical Review B*, **1990**, 41, 12637-12640	3.3	46
19	Sequential Lattice Relaxation Model within the Double Configuration Coordinate for theDXCenter in AlGaAs. *Japanese Journal of Applied Physics*, **1990**, 29, L530-L533	1.4	4
18	Electronic structure of the silicon divacancy. *Physical Review B*, **1990**, 42, 11869-11874	3.3	18
17	Electronic structure and band gap of (GaP)1(InP)1(111) superlattice. *Superlattices and Microstructures*, **1989**, 5, 171-173	2.8	6
16	Spin-polarized electronic structures of La2CuO4. *Solid State Communications*, **1988**, 66, 629-632	1.6	46
15	Spin-polarized electronic structure of Cr impurities in ZnS. *Physical Review B*, **1988**, 37, 1395-1398	3.3	8
14	Stable atomic geometries of oxygen microclusters in silicon. *Physical Review B*, **1988**, 38, 10711-10717	3.3	45

13	Electronic structure of a modulation-doped spherical semiconductor heterostructure with mesoscopic dimensions. *Physical Review B*, **1988**, 38, 3733-3740	3.3	11
12	First-Principles Pseudopotential Total-Energy Calculations for Elemental, Compound and Alloy Semiconductors. *Journal of the Physical Society of Japan*, **1987**, 56, 2104-2112	1.5	45
11	Stability and electronic structure of ultrathin-layer superlattices: (GaAs)n/(AlAs)n. *Physical Review B* , **1987**, 36, 6156-6159	3.3	28
10	Electronic structure of the superatom: A quasiatomic system based on a semiconductor heterostructure. *Physical Review Letters*, **1986**, 57, 2560-2563	7.4	55
9	DX center: Crossover of deep and shallow states in Si-doped AlxGa1-xAs. *Physical Review B*, **1986**, 33, 4320-4323	3.3	59
8	Self-Consistent Band Structures of First-Stage Alkali-Metal Graphite Intercalation Compounds. *Journal of the Physical Society of Japan*, **1986**, 55, 4341-4348	1.5	9
7	Microscopic theory of impurity-defect reactions and impurity diffusion in silicon. *Physical Review Letters*, **1985**, 54, 360-363	7.4	134
6	Theory of electronically stimulated defect migration in semiconductors. *Physical Review B*, **1984**, 30, 2260-2262	3.3	31
5	Electronic Structure of Quasi-One-Dimensional Transition Metal Chalcogenide Nb3X4. *Journal of the Physical Society of Japan*, **1983**, 52, 587-596	1.5	39
4	Energy bands and Fermi surfaces of quasi-one-dimensional transition metal chalcogenides Nb3X4. *Solid State Communications*, **1982**, 43, 607-612	1.6	40
3	Electronic structure of (SN)xand its intercalate (SNBry)x. *Journal of Physics C: Solid State Physics*, **1981**, 14, 5091-5107		15
2	Theory of electrical resistivity in an interacting two-carrier system: application to (SN)Xand (SNBry)X. *Journal of Physics C: Solid State Physics*, **1981**, 14, 5109-5125		3
1	Electrical Resistivity due to Electron-Electron Scattering in Quasi-One-Dimensional Metals. *Journal of the Physical Society of Japan*, **1978**, 45, 1136-1146	1.5	31