Atsushi Oshiyama

List of Publications by Year
in descending order

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141 papers	9,541 citations	61945 43 h-index	37183 96 g-index
141 all docs	141 docs citations	141 times ranked	5499 citing authors

#	Article	IF	Citations
1	New one-dimensional conductors: Graphitic microtubules. Physical Review Letters, 1992, 68, 1579-1581.	2.9	3,267
2	Cohesive mechanism and energy bands of solidC60. Physical Review Letters, 1991, 66, 2637-2640.	2.9	995
3	Energetics and Electronic Structures of EncapsulatedC60in a Carbon Nanotube. Physical Review Letters, 2001, 86, 3835-3838.	2.9	378
4	Magnetic Ordering in Hexagonally Bonded Sheets with First-Row Elements. Physical Review Letters, 2001, 87, 146803.	2.9	369
5	Vacancy in Si: Successful description within the local-density approximation. Physical Review Letters, 1992, 68, 1858-1861.	2.9	220
6	Electronic structure ofSi46andNa2Ba6Si46. Physical Review B, 1995, 51, 2628-2631.	1.1	153
7	Microscopic Theory of Impurity-Defect Reactions and Impurity Diffusion in Silicon. Physical Review Letters, 1985, 54, 360-363.	2.9	146
8	New Metallic Crystalline Carbon: Three Dimensionally PolymerizedC60Fullerite. Physical Review Letters, 1999, 83, 1986-1989.	2.9	117
9	Electronic and geometric structures ofC70. Physical Review B, 1991, 44, 11532-11535.	1.1	114
10	A massively-parallel electronic-structure calculations based on real-space density functional theory. Journal of Computational Physics, 2010, 229, 2339-2363.	1.9	114
11	Linear dependence of superconducting transition temperature on Fermi-level density-of-states in alkali-doped C60. Solid State Communications, 1992, 82, 41-45.	0.9	108
12	Structures of Steps and Appearances of {311} Facets on Si(100) Surfaces. Physical Review Letters, 1995, 74, 130-133.	2.9	107
13	Ionic metalKxC60: Cohesion and energy bands. Physical Review B, 1991, 44, 11536-11539.	1.1	102
14	Atomic and electronic structures of oxygen on Si(100) surfaces: Metastable adsorption sites. Physical Review B, 1990, 41, 12680-12686.	1.1	100
15	Electronic structures of C60 fullerides and related materials. Journal of Physics and Chemistry of Solids, 1992, 53, 1457-1471.	1.9	86
16	Nanometer-Scale Ferromagnet: Carbon Nanotubes with Finite Length. Journal of the Physical Society of Japan, 2003, 72, 1510-1515.	0.7	82
17	Nearly free electron states in carbon nanotube bundles. Physical Review B, 2000, 62, 7634-7638.	1.1	81
18	Diffusion and dimer exchange in surfactant-mediated epitaxial growth. Physical Review Letters, 1994, 72, 3190-3193.	2.9	77

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19	Lifetimes of positrons trapped at Si vacancies. Physical Review B, 1996, 53, 7810-7814.	1.1	76
20	Curvature-Induced Metallization of Double-Walled Semiconducting Zigzag Carbon Nanotubes. Physical Review Letters, 2003, 91, 216801.	2.9	74
21	Sr6C60andBa6C60: Semimetallic fullerides. Physical Review Letters, 1993, 71, 121-124.	2.9	73
22	Electronic structure of calcium-doped C60. Solid State Communications, 1992, 83, 107-110.	0.9	72
23	Adsorption and Diffusion of Si Adatom on Hydrogenated Si(100) Surfaces. Physical Review Letters, 1997, 79, 4425-4428.	2.9	70
24	Border states in heterosheets with hexagonal symmetry. Physical Review B, 2000, 62, 9896-9899.	1.1	70
25	Electronic Structure of the Superatom: A Quasiatomic System Based on a Semiconductor Heterostructure. Physical Review Letters, 1986, 57, 2560-2563.	2.9	65
26	Hole-Injection-Induced Structural Transformation of Oxygen Vacancy in Î±-Quartz. Japanese Journal of Applied Physics, 1998, 37, L232-L234.	0.8	65
27	Structural Stability and Adatom Diffusion at Steps on Hydrogenated Si(100) Surfaces. Physical Review Letters, 1998, 81, 5366-5369.	2.9	64
28	DXcenter: Crossover of deep and shallow states in Si-dopedAlxGa1âˆ’xAs. Physical Review B, 1986, 33, 4320-4323.	1.1	61
29	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, 9663-9673.	6.6	61
30	Microscopic mechanism of atomic diffusion in Si under pressure. Physical Review B, 1992, 46, 12335-12341.	1.1	56
31	Atomic and electronic structures of an interface between silicon and Î²-cristobalite. Physical Review B, 1990, 41, 12637-12640.	1.1	50
32	Electronic structures of solidBC59. Physical Review B, 1992, 46, 1749-1753.	1.1	50
33	Floating Electron States in Covalent Semiconductors. Physical Review Letters, 2012, 108, 246404.	2.9	50
34	Stable atomic geometries of oxygen microclusters in silicon. Physical Review B, 1988, 38, 10711-10717.	1.1	47
35	First-principles band-structure calculation of yttrium oxysulfide. Physical Review B, 1998, 57, 8939-8944.	1.1	47
36	Electronic Structure of Semiconducting Nanotubes Adsorbed on Metal Surfaces. Physical Review Letters, 2005, 95, 206804.	2.9	47

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37	Double-Metal-Ion/Single-Metal-Ion Mechanisms of the Cleavage Reaction of Ribozymes:Â First-Principles Molecular Dynamics Simulations of a Fully Hydrated Model System. Journal of Chemical Theory and Computation, 2005, 1, 925-934.	2.3	47
38	Spin-polarized electronic structures of La2CuO4. Solid State Communications, 1988, 66, 629-632.	0.9	46
39	Dimer exchange mechanism for substitutional As adsorption on Si(100). Physical Review Letters, 1993, 71, 585-588.	2.9	46
40	Resonant Bonds in Symmetry-Lowering Distortion around a Si Divacancy. Physical Review Letters, 1994, 73, 866-869.	2.9	46
41	A new alternative model of type-C defects on Si() surfaces. Surface Science, 2004, 554, 272-279.	0.8	46
42	First-Principles Pseudopotential Total-Energy Calculations for Elemental, Compound and Alloy Semiconductors. Journal of the Physical Society of Japan, 1987, 56, 2104-2112.	0.7	45
43	Anisotropic momentum distribution of positron-annihilation radiation in semiconductors. Physical Review B, 1991, 44, 10601-10609.	1.1	45
44	Energy bands and Fermi surfaces of quasi-one-dimensional transition metal chalcogenides Nb3X4. Solid State Communications, 1982, 43, 607-612.	0.9	44
45	Electronic Structure of Quasi-One-Dimensional Transition Metal Chalcogenide Nb3X4. Journal of the Physical Society of Japan, 1983, 52, 587-596.	0.7	43
46	Energetics in the initial stage of oxidation of silicon. Physical Review B, 1991, 43, 9287-9290.	1.1	39
47	Design ofC60-graphite cointercalation compounds. Physical Review B, 1994, 49, 17413-17419.	1.1	36
48	A Novel Intrinsic Interface State Controlled by Atomic Stacking Sequence at Interfaces of SiC/SiO₂. Nano Letters, 2017, 17, 6458-6463.	4.5	36
49	Electrical Resistivity due to Electron-Electron Scattering in Quasi-One-Dimensional Metals. Journal of the Physical Society of Japan, 1978, 45, 1136-1146.	0.7	34
50	Theory of electronically stimulated defect migration in semiconductors. Physical Review B, 1984, 30, 2260-2262.	1.1	33
51	X-Ray Emission Spectrum of Solid C60. Journal of the Physical Society of Japan, 1991, 60, 2518-2521.	0.7	33
52	A Simple scheme for estimating the pKa values of 5-substituted uracils. Chemical Physics Letters, 2011, 502, 248-252.	1.2	32
53	Real-space-partitioned separable pseudopotential. Physical Review B, 1992, 46, 2606-2609.	1.1	31
54	Covalency, elasticity and electron correlation in Si vacancies. Applied Surface Science, 1995, 85, 239-245.	3.1	31

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55	Atom-Scale Reaction Pathways and Free-Energy Landscapes in Oxygen Plasma Etching of Graphene. Journal of Physical Chemistry Letters, 2013, 4, 1592-1596.	2.1	31
56	Stability and electronic structure of ultrathin-layer superlattices: (GaAs)n/(AlAs)n. Physical Review B, 1987, 36, 6156-6159.	1.1	30
57	Atomic and Electronic Structures of Carbon Nanotubes on Si(001) Stepped Surfaces. Physical Review Letters, 2006, 96, 105505.	2.9	29
58	Interstitial Channels that Control Band Gaps and Effective Masses in Tetrahedrally Bonded Semiconductors. Physical Review Letters, 2014, 112, 136403.	2.9	29
59	First-principles study of intrinsic defects in yttrium oxysulfide. Physical Review B, 1999, 60, 1707-1715.	1.1	28
60	Halogen doping in solid C60. Solid State Communications, 1992, 82, 437-441.	0.9	27
61	Diffusion mechanisms of a Si adatom on H-terminated Si(100) surfaces. Physical Review B, 1998, 58, 12958-12963.	1.1	27
62	Eâ€²Centers inÎ±Quartz in the Absence of Oxygen Vacancies: A First-Principles Molecular-Dynamics Study. Physical Review Letters, 2003, 91, 206401.	2.9	27
63	First principles studies on In-related nitride semiconductors. Journal of Crystal Growth, 2009, 311, 2772-2775.	0.7	27
64	Effect of anisotropic Coulomb field on Si 2pcore levels in oxidized silicon. Physical Review B, 1991, 44, 5931-5934.	1.1	24
65	Enol-to-keto Tautomerism of Peptide Groups. Journal of Physical Chemistry B, 2006, 110, 4443-4450.	1.2	24
66	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.	0.7	23
67	Energetics and local vibrations of theDXcenter in GaAs. Physical Review B, 1993, 47, 13205-13214.	1.1	22
68	Energetics and electronic structure of C70-peapods and one-dimensional chains of C70. New Journal of Physics, 2003, 5, 122-122.	1.2	22
69	Screw dislocation that converts p-type GaN to n-type: Microscopic study on Mg condensation and leakage current in pâ€“n diodes. Applied Physics Letters, 2020, 117, 012105.	1.5	22
70	Atomic and Electronic Structures of N-Incorporated Si Oxides. Physical Review Letters, 2001, 86, 3574-3577.	2.9	21
71	Electronic structure of stacked C60 shuttlecocks. Chemical Physics Letters, 2004, 399, 157-161.	1.2	21
72	Electronic structure of the silicon divacancy. Physical Review B, 1990, 42, 11869-11874.	1.1	20

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73	Fermi Surfaces of Alkali-Metal-Doped C60Solid. Japanese Journal of Applied Physics, 1991, 30, L2036-L2038.	0.8	20
74	Electronic structure of alkali and alkaline-earth doped solid C60. Journal of Physics and Chemistry of Solids, 1993, 54, 1759-1765.	1.9	20
75	Prediction of electronic properties of carbon-based nanostructures. Physica B: Condensed Matter, 2002, 323, 21-29.	1.3	20
76	Electronic and geometric structures of fullerenes. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1993, 19, 105-110.	1.7	19
77	Si nanowire FET and its modeling. Science China Information Sciences, 2011, 54, 1004-1011.	2.7	19
78	Metastable atomic configurations for oxygen adsorption on Si (100) surfaces. Solid State Communications, 1990, 74, 343-346.	0.9	18
79	Pressure and Orientation Effects on the Electronic Structure of Carbon Nanotube Bundles. Journal of the Physical Society of Japan, 2001, 70, 2345-2352.	0.7	18
80	Free energy molecular dynamics simulations of pulsed-laser-irradiated SiO2: Siâ€“Si bond formation in a matrix of SiO2. Applied Physics Letters, 2005, 86, 201910.	1.5	18
81	Surface energy of Si(110)- and 3C-SiC(111)-terminated surfaces. Physica Status Solidi (B): Basic Research, 2014, 251, 1408-1415.	0.7	18
82	Electronic and Geometric Structures of Fullerenes and Metallofullerenes. Japanese Journal of Applied Physics, 1993, 32, 1438-1443.	0.8	17
83	Electronic structure of (SN)xand its intercalate (SNBry)x. Journal of Physics C: Solid State Physics, 1981, 14, 5091-5107.	1.5	16
84	Validity of the broken-bond model for theDXcenter in GaAs. Physical Review B, 1992, 45, 13745-13748.	1.1	16
85	Order- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>N</mml:mi></mml:math> orbital-free density-functional calculations with machine learning of functional derivatives for semiconductors and metals. Physical Review Research, 2021, 3, .	1.3	16
86	Reaction pathway for Sb-dimer rotation in conversion ofSb4precursors on Si(001). Physical Review B, 1994, 50, 8942-8945.	1.1	15
87	Scanning-tunneling-microscopy images of Ge adsorbed on an As-covered Si(001) surface. Physical Review B, 1994, 50, 14631-14634.	1.1	15
88	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.	0.8	15
89	Role of Ge surface segregation in Si/Ge interfacial ordering: Interface formation on a monohydride surface. Physical Review B, 1995, 51, 14786-14789.	1.1	14
90	Structures and reactions of missing dimers in epitaxial growth of Ge on Si(100). Physical Review B, 1995, 52, 8337-8343.	1.1	14

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91	Saito and Oshiyama Reply:. Physical Review Letters, 1995, 74, 4354-4354.	2.9	14
92	First-Principles Study of Hydrogen Incorporation in Multivacancy in Silicon. Journal of the Physical Society of Japan, 2001, 70, 1627-1634.	0.7	14
93	Electronic and geometric structures of multi-walled BN nanotubes. Physica B: Condensed Matter, 2002, 323, 224-226.	1.3	13
94	First-principle study on GaN epitaxy on lattice-matched ZrB2 substrates. Applied Physics Letters, 2003, 83, 2560-2562.	1.5	13
95	E' CENTERS IN SILICON DIOXIDE: FIRST-PRINCIPLES MOLECULAR DYNAMICS STUDIES. Modern Physics Letters B, 2004, 18, 707-724.	1.0	13
96	Open Edge Growth Mechanisms of Single Wall Carbon Nanotubes. Journal of the Physical Society of Japan, 2001, 70, 1995-2011.	0.7	12
97	Electron doping through lithium intercalation to interstitial channels in tetrahedrally bonded SiC. Journal of Applied Physics, 2015, 118, .	1.1	12
98	Indirect phase transition of TiC, ZrC, and HfC crystal structures. Physica Status Solidi (B): Basic Research, 2016, 253, 1177-1185.	0.7	12
99	Spin-polarized electronic structure of Cr impurities in ZnS. Physical Review B, 1988, 37, 1395-1398.	1.1	11
100	Electronic structure of a modulation-doped spherical semiconductor heterostructure with mesoscopic dimensions. Physical Review B, 1988, 38, 3733-3740.	1.1	11
101	Scanning tunneling microscopy images of argon monolayer on a monolayer graphite surface. Chemical Physics Letters, 2003, 371, 528-533.	1.2	11
102	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, .	1.1	11
103	Electronic structure of fullerides. Journal of Physics and Chemistry of Solids, 1992, 53, 1689-1697.	1.9	10
104	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.	1.5	10
105	Atomic structure and phonons in the Ï€-bonded chain of the clean diamond (111) surface. Physical Review B, 1998, 57, R9412-R9415.	1.1	9
106	Formation of titanium-carbide in a nanospace of C78 fullerenes. Chemical Physics Letters, 2007, 438, 274-278.	1.2	9
107	Self-Consistent Band Structures of First-Stage Alkali-Metal Graphite Intercalation Compounds. Journal of the Physical Society of Japan, 1986, 55, 4341-4348.	0.7	9
108	Atomic and Electronic Structures of Deformed Graphite Sheets. Journal of the Physical Society of Japan, 1998, 67, 3976-3984.	0.7	8

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109	New electron states that float on semiconductor and metal surfaces. Surface Science, 2005, 585, L177-L182.	0.8	8
110	First-principles molecular dynamics study of proton transfer mechanism in bovine cytochromecoxidase. Journal of Physics Condensed Matter, 2007, 19, 365220.	0.7	8
111	Large-scale real-space density-functional calculations: MoirÃ©-induced electron localization in graphene. Journal of Applied Physics, 2015, 117, 112811.	1.1	8
112	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.	1.5	8
113	First-Principles Calculations That Clarify Energetics and Reactions of Oxygen Adsorption and Carbon Desorption on 4H-SiC (112ì...0) Surface. Journal of Physical Chemistry C, 2017, 121, 3920-3928.	1.5	8
114	Chemical differences in surface diffusion:â€ƒSi and Ge adatoms at theDBstep on the hydrogenated Si(100) surface. Physical Review B, 1999, 60, R11269-R11272.	1.1	7
115	Significant Change in Electronic Structures of Heme Upon Reduction by Strong Coulomb Repulsion between Fe d Electrons. Journal of Physical Chemistry B, 2009, 113, 6866-6872.	1.2	7
116	Energy Compensation Mechanism for Charge-Separated Protonation States in Aspartateâ˜Histidine Amino Acid Residue Pairs. Journal of Physical Chemistry B, 2010, 114, 6567-6578.	1.2	7
117	Exploration of a large-scale reconstructed structure on GaN(0001) surface by Bayesian optimization. Applied Physics Letters, 2022, 120, 021602.	1.5	7
118	Electronic structure and band gap of (GaP)1(InP)1(111) superlattice. Superlattices and Microstructures, 1989, 5, 171-173.	1.4	6
119	Magnetic ordering of Ga wires on Si(100) surfaces. Physical Review B, 2000, 62, R13286-R13289.	1.1	6
120	Theoretical study on stable structures and diffusion mechanisms of B in SiO2. Applied Surface Science, 2003, 216, 490-496.	3.1	6
121	Electronic Structures of Polyglycine and Active Sites of Cytochrome c Oxidase. Journal of the Physical Society of Japan, 2004, 73, 3198-3208.	0.7	6
122	Enhanced Si and B diffusion in semiconductor-grade SiO2 and the effect of strain on diffusion. Thin Solid Films, 2006, 508, 270-275.	0.8	6
123	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.	0.7	6
124	Quantum effects in a cylindrical carbon-nanotube capacitor. Journal of Physics Condensed Matter, 2007, 19, 365218.	0.7	5
125	A two-dimensional liquid-like phase on Ga-rich GaN (0001) surfaces evidenced by first principles molecular dynamics. Japanese Journal of Applied Physics, 2020, 59, SGGK04.	0.8	5
126	Sequential Lattice Relaxation Model within the Double Configuration Coordinate for theDXCenter in AlGaAs. Japanese Journal of Applied Physics, 1990, 29, L530-L533.	0.8	4

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127	Energetics and kinetics for Siâ€“Ge intermixing on Ge-adsorbed hydrogenated Si(100) surfaces. Surface Science, 1999, 436, L666-L670.	0.8	4
128	Increased stability of C60 encapsulated in double walled carbon nanotubes. Chemical Physics Letters, 2008, 455, 88-92.	1.2	4
129	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.	1.5	3
130	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.	0.1	3
131	Electronic structure of fullerenes and fullerides: artificial atoms and their solids. Nanotechnology, 1992, 3, 167-172.	1.3	2
132	Chemical trends ands-phybridization in theDXcenter in GaAs. Physical Review B, 1993, 48, 11804-11809.	1.1	2
133	Okada, Saito, and Oshiyama Reply:. Physical Review Letters, 2000, 85, 5672-5672.	2.9	2
134	Origin of Repulsive Interactions between Bunched Steps on Vicinal Solid Surfaces. E-Journal of Surface Science and Nanotechnology, 2015, 13, 231-234.	0.1	2
135	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.	1.1	2
136	Microscopic Identification of Surface Steps on SiC by Density-Functional Calculations. Materials Science Forum, 0, 1004, 145-152.	0.3	2
137	Defect-free interface between amorphous (Al2O3)1â^'x(SiO2)x and GaN(0001) revealed by first-principles simulated annealing technique. Applied Physics Letters, 2021, 119, .	1.5	2
138	Microscopic surface structures and macroscopic thin-film morphology. Thin Solid Films, 1996, 272, 364-374.	0.8	1
139	Role of the Ionicity in Defect Formation in Hf-Based Dielectrics. ECS Transactions, 2007, 11, 199-211.	0.3	1
140	Structural determination of phosphosilicate glass based on first-principles molecular dynamics calculation. Japanese Journal of Applied Physics, 2019, 58, 011001.	0.8	1
141	LSD Calculation of Electronic Structure of HighTcSuperconductor: Laâ€“Srâ€“Cuâ€“O Systems. Japanese Journal of Applied Physics, 1987, 26, 983.	0.8	1