Osamu Sugino

List of Publications by Year
in descending order

125 papers	5,078 citations	147566 31 h-index	88477 70 g-index
128 all docs	128 docs citations	128 times ranked	4267 citing authors

#	Article	IF	Citations
1	First-principles calculations of charged surfaces and interfaces: A plane-wave nonrepeated slab approach. Physical Review B, 2006, 73, .	1.1	616
2	First-principles study on energetics ofc-BN(001) reconstructed surfaces. Physical Review B, 1996, 54, 5586-5603.	1.1	460
3	Dirac Fermions in Borophene. Physical Review Letters, 2017, 118, 096401.	2.9	353
4	Ab InitioMolecular Dynamics Study of First-Order Phase Transitions: Melting of Silicon. Physical Review Letters, 1995, 74, 1823-1826.	2.9	246
5	Graphitic ribbons without hydrogen-termination: Electronic structures and stabilities. Physical Review B, 2000, 62, R16349-R16352.	1.1	236
6	Density-functional approach to electron dynamics: Stable simulation under a self-consistent field. Physical Review B, 1999, 59, 2579-2586.	1.1	221
7	Vacancy in Si: Successful description within the local-density approximation. Physical Review Letters, 1992, 68, 1858-1861.	2.9	220
8	Experimental realization of two-dimensional Dirac nodal line fermions in monolayer Cu2Si. Nature Communications, 2017, 8, 1007.	5.8	219
9	First-Principles Molecular Dynamics at a Constant Electrode Potential. Physical Review Letters, 2012, 109, 266101.	2.9	165
10	Electrode Dynamics from First Principles. Journal of the Physical Society of Japan, 2008, 77, 024802.	0.7	133
11	Structure of the water/platinum interfaceâ€“â€“a first principles simulation under bias potential. Physical Chemistry Chemical Physics, 2008, 10, 3609.	1.3	124
12	Completing density functional theory by machine learning hidden messages from molecules. Npj Computational Materials, 2020, 6, .	3.5	121
13	First-principles molecular dynamics simulation of biased electrode/solution interface. Surface Science, 2007, 601, 5237-5240.	0.8	96
14	Nonadiabatic couplings from time-dependent density functional theory: Formulation in the Casida formalism and practical scheme within modified linear response. Journal of Chemical Physics, 2007, 127, 064103.	1.2	91
15	Discovery of 2D Anisotropic Dirac Cones. Advanced Materials, 2018, 30, 1704025.	11.1	91
16	Greenâ€™s function method for elimination of the spurious multipole interaction in the surface/interface slab model. Physical Review B, 2009, 80, .	1.1	72
17	Comparative study of dehydrogenation of methanol at Pt(111)/water and Pt(111)/vacuum interfaces. Chemical Physics Letters, 2003, 377, 236-242.	1.2	58
18	Microscopic mechanism of atomic diffusion in Si under pressure. Physical Review B, 1992, 46, 12335-12341.	1.1	56

#	Article	IF	Citations
19	First-principles study on energetics of cBN(001) reconstructed surfaces. Surface Science, 1995, 341, L1037-L1041.	0.8	52
20	Improved modeling of electrified interfaces using the effective screening medium method. Physical Review B, 2013, 88, .	1.1	49
21	All-electronGW+Bethe-Salpeter calculations on small molecules. Physical Review B, 2015, 91, .	1.1	49
22	First-principles thermodynamic description of hydrogen electroadsorption on the Pt(111) surface. Surface Science, 2014, 625, 104-111.	0.8	41
23	Nanotube and nanohorn nucleation from graphitic patches: Tight-binding molecular-dynamics simulations. Physical Review B, 2002, 66, .	1.1	40
24	Nonadiabatic couplings from time-dependent density functional theory. II. Successes and challenges of the pseudopotential approximation. Journal of Chemical Physics, 2008, 128, 154111.	1.2	39
25	Nonadiabatic couplings from the Kohn-Sham derivative matrix: Formulation by time-dependent density-functional theory and evaluation in the pseudopotential framework. Physical Review A, 2010, 82, .	1.0	38
26	Advances and challenges for experiment and theory for multi-electron multi-proton transfer at electrified solidâ€“liquid interfaces. Physical Chemistry Chemical Physics, 2020, 22, 19401-19442.	1.3	38
27	Modified linear response for time-dependent density-functional theory: Application to Rydberg and charge-transfer excitations. Physical Review A, 2006, 74, .	1.0	37
28	Hyper-Volcano Surface for Oxygen Reduction Reactions over Noble Metals. Journal of Physical Chemistry C, 2010, 114, 4473-4478.	1.5	37
29	Pressure dependence of the magnetic ground states in MnP. Physical Review B, 2016, 93, .	1.1	36
30	Real-space-partitioned separable pseudopotential. Physical Review B, 1992, 46, 2606-2609.	1.1	31
31	Covalency, elasticity and electron correlation in Si vacancies. Applied Surface Science, 1995, 85, 239-245.	3.1	31
32	Efficient n-type doping of diamond using surfactant-mediated epitaxial growth. Applied Physics Letters, 2000, 76, 976-978.	1.5	30
33	All-electron calculation of nonadiabatic couplings from time-dependent density functional theory: Probing with the Hartreeâ€“Fock exact exchange. Journal of Chemical Physics, 2009, 131, 114101.	1.2	30
34	A time-dependent density-functional approach to nonadiabatic electron-nucleus dynamics: formulation and photochemical application. Physical Chemistry Chemical Physics, 2009, 11, 4570.	1.3	30
35	DFT calculation of vibrational frequency of hydrogen atoms on Pt electrodes: Analysis of the electric field dependence of the Ptâ€“H stretching frequency. Chemical Physics Letters, 2007, 437, 170-175.	1.2	28
36	General Sum Rule for Chiral Index of Coalescing Ultrathin Nanotubes. Physical Review Letters, 2002, 89, 085901.	2.9	26

#	Article	IF	Citations
37	Electronic structures of oxygen-deficient Ta2O5. AIP Advances, 2013, 3, .	0.6	26
38	Localized-orbital Hartree-Fock description of alkali-metal clusters. Physical Review Letters, 1990, 65, 2696-2699.	2.9	25
39	Unusual Ti adsorption on Si(001) and subsequent activation of Si ejection. Physical Review B, 1998, 58, 3549-3552.	1.1	25
40	Dopant arrangements in Y-doped BaZrO3 under processing conditions and their impact on proton conduction: a large-scale first-principles thermodynamics study. Journal of Materials Chemistry A, 2020, 8, 12674-12686.	5.2	25
41	Structural and electronic properties of metal-silicide/silicon interfaces: A first-principles study. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2001, 19, 1180.	1.6	24
42	Hydrogen adsorption on Pt(111) revisited from random phase approximation. Journal of Chemical Physics, 2018, 149, 164702.	1.2	24
43	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
44	Ab initiostudy of incorporation ofO2molecules intoSi(001)surfaces: Oxidation bySiejection. Physical Review B, 2004, 70, .	1.1	23
45	Energetics and local vibrations of theDXcenter in GaAs. Physical Review B, 1993, 47, 13205-13214.	1.1	22
46	Band gap of Î²-PtO2 from first-principles. AIP Advances, 2012, 2, 022172.	0.6	22
47	First-Principles Investigation on Structural and Optical Properties of M⁺@C₆₀ (Where M = H, Li, Na, and K). Journal of Physical Chemistry C, 2013, 117, 15362-15368.	1.5	22
48	Average excitation energies from time-dependent density functional response theory. Journal of Chemical Physics, 2007, 126, 074112.	1.2	21
49	Machine-learning-based exchange correlation functional with physical asymptotic constraints. Physical Review Research, 2022, 4, .	1.3	21
50	Electronic structure of the silicon divacancy. Physical Review B, 1990, 42, 11869-11874.	1.1	20
51	First-principles electron-ion dynamics of excited systems: H-terminated Si(111) surfaces. Physical Review B, 2000, 62, 2039-2044.	1.1	20
52	Second-order nonadiabatic couplings from time-dependent density functional theory: Evaluation in the immediate vicinity of Jahn-Teller/Renner-Teller intersections. Journal of Chemical Physics, 2011, 135, 074101.	1.2	20
53	First-principles investigation of polarization and ion conduction mechanisms in hydroxyapatite. Physical Chemistry Chemical Physics, 2018, 20, 8744-8752.	1.3	20
54	Scaling Relation of Oxygen Reduction Reaction Intermediates at Defective TiO₂ Surfaces. Journal of Physical Chemistry C, 2019, 123, 19486-19492.	1.5	20

#	Article	IF	Citations
55	The charged interface between Pt and water: First principles molecular dynamics simulations. AIP Advances, 2012, 2, 032182.	0.6	19
56	Symmetry breaking and excitonic effects on optical properties of defective nanographenes. Journal of Chemical Physics, 2015, 142, 064313.	1.2	18
57	Effect of strain on band structure and electron transport in InAs. Solid-State Electronics, 1999, 43, 1813-1816.	0.8	17
58	A GW+Bethe-Salpeter calculation on photoabsorption spectra of (CdSe)3 and (CdSe)6 clusters. Journal of Chemical Physics, 2012, 137, 024306.	1.2	17
59	Performance of Tamm-Dancoff approximation on nonadiabatic couplings by time-dependent density functional theory. Journal of Chemical Physics, 2014, 140, 054106.	1.2	17
60	Validity of the broken-bond model for theDXcenter in GaAs. Physical Review B, 1992, 45, 13745-13748.	1.1	16
61	Molecular size insensitivity of optical gap of [n]cycloparaphenylenes (n = 3-16). Journal of Chemical Physics, 2017, 146, 144304.	1.2	16
62	Challenge of advanced low temperature fuel cells based on high degree of freedom of group 4 and 5 metal oxides. Current Opinion in Electrochemistry, 2020, 21, 234-241.	2.5	14
63	Real-time electron-ion dynamics for photoinduced reactivation of hydrogen-passivated donors in GaAs. Applied Physics Letters, 1999, 75, 2915-2917.	1.5	13
64	Self-Poisoning Dynamical Effects in the Oxygen Reduction Reaction on Pt(111) from a Top-Down Kinetic Analysis. Journal of Physical Chemistry C, 2014, 118, 13638-13643.	1.5	12
65	Quantitative characterization of exciton fromGW+Bethe-Salpeter calculation. Journal of Chemical Physics, 2017, 146, 044303.	1.2	12
66	Surface-state Coulomb repulsion accelerates a metal-insulator transition in topological semimetal nanofilms. Science Advances, 2020, 6, eaaz5015.	4.7	11
67	Exceptionally long-ranged lattice relaxation in oxygen-deficient Ta2O5. Solid State Communications, 2014, 195, 16-20.	0.9	10
68	Nuclear quantum effect for hydrogen adsorption on Pt(111). Physical Review B, 2020, 101, .	1.1	10
69	Favorable formation of the C49-TiSi2 phase on Si(001) determined by first-principles calculations. Applied Physics Letters, 1998, 72, 1176-1178.	1.5	9
70	Possible magnetic behavior in oxygen-deficient<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>-PtO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	1.1	9
71	Atomic and Electronic Structures of Deformed Graphite Sheets. Journal of the Physical Society of Japan, 1998, 67, 3976-3984.	0.7	8
72	Symmetric Tensor Decomposition Description of Fermionic Many-Body Wave Functions. Physical Review Letters, 2012, 109, 253001.	2.9	8

#	Article	IF	Citations
73	Configuration interaction with antisymmetrized geminal powers. Physical Review A, 2015, 91, .	1.0	8
74	High-Lying Triplet Excitons of Thermally Activated Delayed Fluorescence Molecules. Journal of Physical Chemistry C, 2017, 121, 20687-20695.	1.5	8
75	Novel Pathway to the Growth of Diamond on CubicÎ²-SiC(001). Physical Review Letters, 2002, 88, 125504.	2.9	7
76	Formation of dihydride chains on H-terminatedSi(100)â˜2Ã—1surfaces: Scanning tunneling microscopy and first-principles calculations. Physical Review B, 2006, 74, .	1.1	7
77	The effect of dynamical fluctuations of hydration structures on the absorption spectra of oxyluciferin anions in an aqueous solution. Physical Chemistry Chemical Physics, 2017, 19, 10028-10035.	1.3	7
78	Direct coupling of first-principles calculations with replica exchange Monte Carlo sampling of ion disorder in solids. Journal of Physics Condensed Matter, 2019, 31, 085901.	0.7	7
79	First Principles Study of Atomic-Scale Al2O3 Films as Insulators for Magnetic Tunnel Junctions. Japanese Journal of Applied Physics, 2000, 39, L479-L481.	0.8	6
80	Ab initiostudy of the oxidation on vicinal Si(001) surfaces: The step-selective oxidation. Physical Review B, 2007, 76, .	1.1	6
81	Nonadiabatic couplings from time-dependent density functional theory: Formulation by the Kohn-Sham derivative matrix within density functional perturbation theory. Physical Review B, 2013, 87, .	1.1	6
82	Four-body correlation embedded in antisymmetrized geminal power wave function. Journal of Chemical Physics, 2016, 145, 244110.	1.2	6
83	Reverse Stability of Oxyluciferin Isomers in Aqueous Solutions. Journal of Physical Chemistry B, 2016, 120, 8776-8783.	1.2	6
84	First-principles description of van der Waals bonded spin-polarized systems using the vdW-DF+ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> method: Application to solid oxygen at low pressure. Physical Review B, 2017, 95, .	1.1	6
85	Optical properties of six isomers of three dimensionally delocalized Ï€-conjugated carbon nanocage. European Physical Journal B, 2018, 91, 1.	0.6	6
86	Photoabsorption Spectra of Aqueous Oxyluciferin Anions Elucidated by Explicit Quantum Solvent. Journal of Chemical Theory and Computation, 2019, 15, 5474-5482.	2.3	6
87	Hydrogen at Electrochemical Interfaces. Journal of the Physical Society of Japan, 2020, 89, 051013.	0.7	6
88	Clarification of the alkali metal cluster's magic numbers using a â€œmetallic bond modelâ€• Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1989, 3, 443-455.	1.7	5
89	Vibrational fine structures in photoelectron spectra of carbon ring clusters. Physical Review B, 2000, 61, 12674-12677.	1.1	5
90	Molecular dynamics study of adatom diffusion on Si(100) surface â€" importance of the exchange mechanism. Surface Science, 1997, 391, L1199-L1204.	0.8	4

#	Article	IF	Citations
91	First-Principles Study of the Step Oxidation at Vicinal Si(001) Surfaces. Japanese Journal of Applied Physics, 2006, 45, 2144-2147.	0.8	4
92	Electronic hyperpolarizability calculation without the periodic images error for a large nonlinear molecule. Physical Review B, 2010, 81, .	1.1	4
93	Functional-renormalization-group approach to classical liquids with short-range repulsion: A scheme without repulsive reference system. Physical Review E, 2021, 104, 014124.	0.8	4
94	Fusion of ultra thin carbon nanotubes: tight-binding molecular dynamics simulations. Physica B: Condensed Matter, 2002, 323, 190-192.	1.3	3
95	Calculation of atomic excitation energies by time-dependent density functional theory within a modified linear response. Journal of Physics Condensed Matter, 2009, 21, 064229.	0.7	3
96	Title is missing!. Electrochemistry, 2009, 77, 241-247.	0.6	3
97	Analytical expression for the excited-state force from density-functional perturbation theory. Physical Review A, 2012, 86, .	1.0	3
98	First-Principles Calculation of Copper Oxide Superconductors That Supports the Kamimura-Suwa Model. Condensed Matter, 2020, 5, 69.	0.8	3
99	Quantum-mechanical hydration plays critical role in the stability of firefly oxyluciferin isomers: State-of-the-art calculations of the excited states. Journal of Chemical Physics, 2020, 153, 201103.	1.2	3
100	Pressure Dependence of Formation and Migration Enthalpies for Atomic Diffusion in Si: Conjugate Gradient Minimization of Total Energy. Materials Science Forum, 1992, 83-87, 469-474.	0.3	2
101	First principles band structure calculation and electron transport for strained InAs. , 0, , .		2
102	Anomalous temperature effect on the broad asymmetric Franck-Condon photoelectron spectrum of theC10â^'monocyclic ring cluster. Physical Review A, 2001, 63, .	1.0	2
103	First Principles Study of Dihydride Chains on H-Terminated Si(100)-2Ã—1 Surface. Japanese Journal of Applied Physics, 2006, 45, 2200-2203.	0.8	2
104	Effect of thermal motion on catalytic activity of nanoparticles in polar solvent. Journal of Chemical Physics, 2014, 140, 044703.	1.2	2
105	Jahn-Teller-Effect Induced Superconductivity in Copper Oxides: Theoretical Developments. Springer Series in Materials Science, 2017, , 129-150.	0.4	2
106	Development of the Bethe-Salpeter method considering second-order corrections for a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m electron-hole interaction kernel. Physical Review B, 2022, 106, .	1.1	2
107	A localized-orbital Hartree-Fock description of alkali metal clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 19, 67-70.	1.0	1
108	Quantum dissipative dynamics using the Doebnerâ€“Goldin equation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 3033-3037.	0.9	1

#	Article	IF	Citations
109	Towards First-Principles Understanding of Hydrogen Evolution Reaction at the Platinum Electrode. Hyomen Kagaku, 2013, 34, 638-643.	0.0	1
110	(Digital Presentation) Tuning Oxygen Reduction on Monoclinic and Tetragonal Zirconia Surfaces Using Oxygen Vacancy and Nitrogen Doping: A Density-Functional Study. ECS Meeting Abstracts, 2022, MA2022-01, 1517-1517.	0.0	1
111	Conjugate-Gradient Total-Energy Minimization: Defects in Silicon. Springer Series in Solid-state Sciences, 1993, , 57-66.	0.3	0
112	Erratum to â€œFirst principles study on energetics of cBN(001) reconstructed surfacesâ€•[Surface Science 341 (1995) L1037]. Surface Science, 1996, 348, L70.	0.8	0
113	First-principles dynamics of defect reactions triggered by electronic excitation. Physica B: Condensed Matter, 1999, 273-274, 991-994.	1.3	0
114	Dimer Reconstruction at Metal-Silicide/Silicon Interfaces: A First-Principles Study. Materials Research Society Symposia Proceedings, 1999, 564, 103.	0.1	0
115	Microscopic understanding of the electrochemical interfaces. , 2013, , .		0
116	Reply to â€œComment on â€˜Nonadiabatic couplings from the Kohn-Sham derivative matrix: Formulation by time-dependent density-functional theory and evaluation in the pseudopotential frameworkâ€™â€• Physical Review A, 2013, 88, .	1.0	0
117	Physical Model at the Electrode-Electrolyte Interface. Lecture Notes in Energy, 2016, , 93-101.	0.2	0
118	Oxygen reduction reaction (ORR) in acidic media with nanostructured metal oxide-based electrocatalysts. , 2021, , 37-59.		0
119	First Principles Description of Shell Structure in Metal Clusters. Few-Body Systems, 2000, , 15-24.	0.2	0
120	Time-dependent density-functional simulations of desorption dynamics of H and Br terminated Si surfaces induced by electronic excitations. Springer Proceedings in Physics, 2001, , 317-318.	0.1	0
121	A localized-orbital Hartree-Fock description of alkali metal clusters. , 1991, , 67-70.		0
122	Phase Transition of TiSi2 under Interfacial Stresses.. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 1998, 7, 181-186.	0.1	0
123	Ab-Initio Investigation of Polarization and Ion Conduction Mechanisms in the Bone Mineral and Electret Material Hydroxyapatite. ECS Meeting Abstracts, 2018, , .	0.0	0
124	Lattice Mismatch Pattern and the Dirac Point of a Monolayer Borophene. Vacuum and Surface Science, 2018, 61, 712-715.	0.0	0
125	Optical representation of thermal nuclear fluctuation effect on band-gap renormalization. Physical Review B, 2021, 104, .	1.1	0