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	Machine-learning-based exchange correlation functional with physical asymptotic constraints. Physical Review Research, 2022, 4, .	1.3	21
2	(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
3	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 electron-hole interaction kernel. Physical Review B, 2022, 106, .	1.1	2
4	Oxygen reduction reaction (ORR) in acidic media with nanostructured metal oxide-based electrocatalysts. , 2021, , 37-59.		0
5	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
6	Optical representation of thermal nuclear fluctuation effect on band-gap renormalization. Physical Review B, 2021, 104, .	1.1	0
7	First-Principles Calculation of Copper Oxide Superconductors That Supports the Kamimura-Suwa Model. Condensed Matter, 2020, 5, 69.	0.8	3
8	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
9	Hydrogen at Electrochemical Interfaces. Journal of the Physical Society of Japan, 2020, 89, 051013.	0.7	6
10	Completing density functional theory by machine learning hidden messages from molecules. Npj Computational Materials, 2020, 6, .	3.5	121
11	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
12	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
13	Surface-state Coulomb repulsion accelerates a metal-insulator transition in topological semimetal nanofilms. Science Advances, 2020, 6, eaaz5015.	4.7	11
14	Nuclear quantum effect for hydrogen adsorption on Pt(111). Physical Review B, 2020, 101, .	1.1	10
15	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
16	Scaling Relation of Oxygen Reduction Reaction Intermediates at Defective TiO₂ Surfaces. Journal of Physical Chemistry C, 2019, 123, 19486-19492.	1.5	20
17	Photoabsorption Spectra of Aqueous Oxyluciferin Anions Elucidated by Explicit Quantum Solvent. Journal of Chemical Theory and Computation, 2019, 15, 5474-5482.	2.3	6
18	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

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19	First-principles investigation of polarization and ion conduction mechanisms in hydroxyapatite. Physical Chemistry Chemical Physics, 2018, 20, 8744-8752.	1.3	20
20	Discovery of 2D Anisotropic Dirac Cones. Advanced Materials, 2018, 30, 1704025.	11.1	91
21	Hydrogen adsorption on Pt(111) revisited from random phase approximation. Journal of Chemical Physics, 2018, 149, 164702.	1.2	24
22	Optical properties of six isomers of three dimensionally delocalized Ï€-conjugated carbon nanocage. European Physical Journal B, 2018, 91, 1.	0.6	6
23	Ab-Initio Investigation of Polarization and Ion Conduction Mechanisms in the Bone Mineral and Electret Material Hydroxyapatite. ECS Meeting Abstracts, 2018, , .	0.0	0
24	Lattice Mismatch Pattern and the Dirac Point of a Monolayer Borophene. Vacuum and Surface Science, 2018, 61, 712-715.	0.0	0
25	Quantitative characterization of exciton fromGW+Bethe-Salpeter calculation. Journal of Chemical Physics, 2017, 146, 044303.	1.2	12
26	Dirac Fermions in Borophene. Physical Review Letters, 2017, 118, 096401.	2.9	353
27	Molecular size insensitivity of optical gap of [n]cycloparaphenylenes (n = 3-16). Journal of Chemical Physics, 2017, 146, 144304.	1.2	16
28	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
29	Jahn-Teller-Effect Induced Superconductivity in Copper Oxides: Theoretical Developments. Springer Series in Materials Science, 2017, , 129-150.	0.4	2
30	Experimental realization of two-dimensional Dirac nodal line fermions in monolayer Cu2Si. Nature Communications, 2017, 8, 1007.	5.8	219
31	High-Lying Triplet Excitons of Thermally Activated Delayed Fluorescence Molecules. Journal of Physical Chemistry C, 2017, 121, 20687-20695.	1.5	8
32	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
33	Four-body correlation embedded in antisymmetrized geminal power wave function. Journal of Chemical Physics, 2016, 145, 244110.	1.2	6
34	Reverse Stability of Oxyluciferin Isomers in Aqueous Solutions. Journal of Physical Chemistry B, 2016, 120, 8776-8783.	1.2	6
35	Pressure dependence of the magnetic ground states in MnP. Physical Review B, 2016, 93, .	1.1	36
36	Physical Model at the Electrode-Electrolyte Interface. Lecture Notes in Energy, 2016, , 93-101.	0.2	0

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37	Configuration interaction with antisymmetrized geminal powers. Physical Review A, 2015, 91, .	1.0	8
38	All-electronGW+Bethe-Salpeter calculations on small molecules. Physical Review B, 2015, 91, .	1.1	49
39	Symmetry breaking and excitonic effects on optical properties of defective nanographenes. Journal of Chemical Physics, 2015, 142, 064313.	1.2	18
40	Effect of thermal motion on catalytic activity of nanoparticles in polar solvent. Journal of Chemical Physics, 2014, 140, 044703.	1.2	2
41	Exceptionally long-ranged lattice relaxation in oxygen-deficient Ta2O5. Solid State Communications, 2014, 195, 16-20.	0.9	10
42	Performance of Tamm-Dancoff approximation on nonadiabatic couplings by time-dependent density functional theory. Journal of Chemical Physics, 2014, 140, 054106.	1.2	17
43	First-principles thermodynamic description of hydrogen electroadsorption on the Pt(111) surface. Surface Science, 2014, 625, 104-111.	0.8	41
44	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
45	Improved modeling of electrified interfaces using the effective screening medium method. Physical Review B, 2013, 88, .	1.1	49
46	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
47	Microscopic understanding of the electrochemical interfaces. , 2013, , .		0
48	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
49	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
50	Towards First-Principles Understanding of Hydrogen Evolution Reaction at the Platinum Electrode. Hyomen Kagaku, 2013, 34, 638-643.	0.0	1
51	Electronic structures of oxygen-deficient Ta2O5. AIP Advances, 2013, 3, .	0.6	26
52	Band gap of Î²-PtO2 from first-principles. AIP Advances, 2012, 2, 022172.	0.6	22
53	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
54	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

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55	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
56	Analytical expression for the excited-state force from density-functional perturbation theory. Physical Review A, 2012, 86, .	1.0	3
57	Symmetric Tensor Decomposition Description of Fermionic Many-Body Wave Functions. Physical Review Letters, 2012, 109, 253001.	2.9	8
58	First-Principles Molecular Dynamics at a Constant Electrode Potential. Physical Review Letters, 2012, 109, 266101.	2.9	165
59	The charged interface between Pt and water: First principles molecular dynamics simulations. AIP Advances, 2012, 2, 032182.	0.6	19
60	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
61	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
62	Electronic hyperpolarizability calculation without the periodic images error for a large nonlinear molecule. Physical Review B, 2010, 81, .	1.1	4
63	Hyper-Volcano Surface for Oxygen Reduction Reactions over Noble Metals. Journal of Physical Chemistry C, 2010, 114, 4473-4478.	1.5	37
64	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
65	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
66	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
67	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
68	Title is missing!. Electrochemistry, 2009, 77, 241-247.	0.6	3
69	Structure of the water/platinum interfaceâ€“â€“a first principles simulation under bias potential. Physical Chemistry Chemical Physics, 2008, 10, 3609.	1.3	124
70	Electrode Dynamics from First Principles. Journal of the Physical Society of Japan, 2008, 77, 024802.	0.7	133
71	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
72	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

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73	Ab initiostudy of the oxidation on vicinal Si(001) surfaces: The step-selective oxidation. Physical Review B, 2007, 76, .	1.1	6
74	Average excitation energies from time-dependent density functional response theory. Journal of Chemical Physics, 2007, 126, 074112.	1.2	21
75	First-principles molecular dynamics simulation of biased electrode/solution interface. Surface Science, 2007, 601, 5237-5240.	0.8	96
76	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
77	First-principles calculations of charged surfaces and interfaces: A plane-wave nonrepeated slab approach. Physical Review B, 2006, 73, .	1.1	616
78	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
79	First-Principles Study of the Step Oxidation at Vicinal Si(001) Surfaces. Japanese Journal of Applied Physics, 2006, 45, 2144-2147.	0.8	4
80	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
81	Modified linear response for time-dependent density-functional theory: Application to Rydberg and charge-transfer excitations. Physical Review A, 2006, 74, .	1.0	37
82	Ab initiostudy of incorporation ofO2molecules intoSi(001)surfaces: Oxidation bySiejection. Physical Review B, 2004, 70, .	1.1	23
83	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
84	General Sum Rule for Chiral Index of Coalescing Ultrathin Nanotubes. Physical Review Letters, 2002, 89, 085901.	2.9	26
85	Novel Pathway to the Growth of Diamond on CubicÎ²-SiC(001). Physical Review Letters, 2002, 88, 125504.	2.9	7
86	Nanotube and nanohorn nucleation from graphitic patches: Tight-binding molecular-dynamics simulations. Physical Review B, 2002, 66, .	1.1	40
87	Fusion of ultra thin carbon nanotubes: tight-binding molecular dynamics simulations. Physica B: Condensed Matter, 2002, 323, 190-192.	1.3	3
88	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
89	Anomalous temperature effect on the broad asymmetric Franck-Condon photoelectron spectrum of theC10â˜monocyclic ring cluster. Physical Review A, 2001, 63, .	1.0	2
90	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

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91	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
92	Graphitic ribbons without hydrogen-termination: Electronic structures and stabilities. Physical Review B, 2000, 62, R16349-R16352.	1.1	236
93	Efficient n-type doping of diamond using surfactant-mediated epitaxial growth. Applied Physics Letters, 2000, 76, 976-978.	1.5	30
94	First-principles electron-ion dynamics of excited systems: H-terminated Si(111) surfaces. Physical Review B, 2000, 62, 2039-2044.	1.1	20
95	Vibrational fine structures in photoelectron spectra of carbon ring clusters. Physical Review B, 2000, 61, 12674-12677.	1.1	5
96	First Principles Description of Shell Structure in Metal Clusters. Few-Body Systems, 2000, , 15-24.	0.2	0
97	Real-time electron-ion dynamics for photoinduced reactivation of hydrogen-passivated donors in GaAs. Applied Physics Letters, 1999, 75, 2915-2917.	1.5	13
98	Density-functional approach to electron dynamics: Stable simulation under a self-consistent field. Physical Review B, 1999, 59, 2579-2586.	1.1	221
99	Effect of strain on band structure and electron transport in InAs. Solid-State Electronics, 1999, 43, 1813-1816.	0.8	17
100	First-principles dynamics of defect reactions triggered by electronic excitation. Physica B: Condensed Matter, 1999, 273-274, 991-994.	1.3	0
101	Dimer Reconstruction at Metal-Silicide/Silicon Interfaces: A First-Principles Study. Materials Research Society Symposia Proceedings, 1999, 564, 103.	0.1	0
102	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
103	Unusual Ti adsorption on Si(001) and subsequent activation of Si ejection. Physical Review B, 1998, 58, 3549-3552.	1.1	25
104	Atomic and Electronic Structures of Deformed Graphite Sheets. Journal of the Physical Society of Japan, 1998, 67, 3976-3984.	0.7	8
105	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
106	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
107	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
108	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

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109	First-principles study on energetics ofc-BN(001) reconstructed surfaces. Physical Review B, 1996, 54, 5586-5603.	1.1	460
110	Covalency, elasticity and electron correlation in Si vacancies. Applied Surface Science, 1995, 85, 239-245.	3.1	31
111	Ab InitioMolecular Dynamics Study of First-Order Phase Transitions: Melting of Silicon. Physical Review Letters, 1995, 74, 1823-1826.	2.9	246
112	First-principles study on energetics of cBN(001) reconstructed surfaces. Surface Science, 1995, 341, L1037-L1041.	0.8	52
113	Energetics and local vibrations of theDXcenter in GaAs. Physical Review B, 1993, 47, 13205-13214.	1.1	22
114	Conjugate-Gradient Total-Energy Minimization: Defects in Silicon. Springer Series in Solid-state Sciences, 1993, , 57-66.	0.3	0
115	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
116	Vacancy in Si: Successful description within the local-density approximation. Physical Review Letters, 1992, 68, 1858-1861.	2.9	220
117	Validity of the broken-bond model for theDXcenter in GaAs. Physical Review B, 1992, 45, 13745-13748.	1.1	16
118	Microscopic mechanism of atomic diffusion in Si under pressure. Physical Review B, 1992, 46, 12335-12341.	1.1	56
119	Real-space-partitioned separable pseudopotential. Physical Review B, 1992, 46, 2606-2609.	1.1	31
120	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
121	A localized-orbital Hartree-Fock description of alkali metal clusters. , 1991, , 67-70.		0
122	Localized-orbital Hartree-Fock description of alkali-metal clusters. Physical Review Letters, 1990, 65, 2696-2699.	2.9	25
123	Electronic structure of the silicon divacancy. Physical Review B, 1990, 42, 11869-11874.	1.1	20
124	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
125	First principles band structure calculation and electron transport for strained InAs. , 0, , .		2