Hirofumi Sato

List of Publications by Year
in descending order

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		257101	288905
118	2,098	24	40
papers	citations	h-index	g-index

123	123	123	1484
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Analytical energy gradient for the reference interaction site model multiconfigurational selfâ€consistentâ€field method: Application to 1,2â€difluoroethylene in aqueous solution. Journal of Chemical Physics, 1996, 105, 1546-1551.	1.2	242
2	New generation of the reference interaction site model self-consistent field method: Introduction of spatial electron density distribution to the solvation theory. Journal of Chemical Physics, 2007, 126, 244504.	1.2	103
3	Self-consistent field, ab initio molecular orbital and three-dimensional reference interaction site model study for solvation effect on carbon monoxide in aqueous solution. Journal of Chemical Physics, 2000, 112, 9463-9468.	1.2	102
4	Geometries and Energies of Nitrobenzene Studied by CAS-SCF Calculations. Journal of Physical Chemistry A, 1997, 101, 5190-5195.	1.1	71
5	Ab initio study of water. II. Liquid structure, electronic and thermodynamic properties over a wide range of temperature and density. Journal of Chemical Physics, 1999, 111, 8545-8555.	1.2	63
6	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. Organometallics, 2009, 28, 2583-2594.	1.1	60
7	A modern solvation theory: quantum chemistry and statistical chemistry. Physical Chemistry Chemical Physics, 2013, 15, 7450.	1.3	57
8	Comparison of Electronic Structure Theories for Solvated Molecules:â€‰ RISM-SCF versus PCM. Journal of Physical Chemistry A, 2004, 108, 1629-1634.	1.1	53
9	A Theoretical Analysis of a Dielsâ^'Alder Reaction in Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 8227-8230.	1.2	47
10	Excitation Wavelength Dependence of Excited State Intramolecular Proton Transfer Reaction of 4â€²-N,N-Diethylamino-3-hydroxyflavone in Room Temperature Ionic Liquids Studied by Optical Kerr Gate Fluorescence Measurement. Journal of Physical Chemistry B, 2013, 117, 12567-12582.	1.2	41
11	Ab Initio Study on an Excited-State Intramolecular Proton-Transfer Reaction in Ionic Liquid. Journal of Physical Chemistry B, 2013, 117, 6759-6767.	1.2	41
12	Analytical energy gradient for reference interaction site model self-consistent field explicitly including spatial electron density distribution. Journal of Chemical Physics, 2009, 131, 214504.	1.2	40
13	Navigated Self-Assembly of a Pd₂L₄ Cage by Modulation of an Energy Landscape under Kinetic Control. Journal of the American Chemical Society, 2019, 141, 19669-19676.	6.6	39
14	Self-consistent parametrization of DFT +<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>framework using linear response approach: Application to evaluation of redox potentials of battery cathodes. Physical Review B, 2016, 93, .	1.1	36
15	The barrier origin on the reaction of CO2+OHâ^' in aqueous solution. Chemical Physics Letters, 2007, 443, 264-268.	1.2	35
16	Solvation effects in oxidative addition reaction of Methyliodide to Pt(II) complex: A theoretical study with RISMâ€“SCF method. Chemical Physics Letters, 2008, 458, 329-332.	1.2	35
17	Self-Assembly Processes of Octahedron-Shaped Pd₆L₄ Cages. Journal of the American Chemical Society, 2019, 141, 3178-3186.	6.6	34
18	Equilibrium and Nonequilibrium Solvation Structure of Hexaammineruthenium (II, III) in Aqueous Solution:Â Ab Initio RISM-SCF Studyâ€. Journal of Physical Chemistry A, 2002, 106, 2300-2304.	1.1	33

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19	A highly parallelizable integral equation theory for three dimensional solvent distribution function: Application to biomolecules. Journal of Chemical Physics, 2009, 130, 064111.	1.2	32
20	Proton Transfer Step in the Carbon Dioxide Capture by Monoethanol Amine: A Theoretical Study at the Molecular Level. Journal of Physical Chemistry B, 2012, 116, 2244-2248.	1.2	31
21	Superexchange Electron Tunneling Mediated by Solvent Molecules:Â Pulsed Electron Paramagnetic Resonance Study on Electronic Coupling in Solvent-Separated Radical Ion Pairsâ€. Journal of Physical Chemistry B, 2004, 108, 10226-10240.	1.2	27
22	Phase evolution of electrochemically potassium intercalated graphite. Journal of Materials Chemistry A, 2021, 9, 11187-11200.	5.2	27
23	Enhanced growth of human vascular endothelial cells on negative ion (Ag?)-implanted hydrophobic surfaces. , 1999, 44, 22-30.		26
24	A reaction model on the self-assembly process of octahedron-shaped coordination capsules. Physical Chemistry Chemical Physics, 2017, 19, 20338-20342.	1.3	25
25	Solvatochromic Shift of Brookerâ€™s Merocyanine: Hartreeâ€“Fock Exchange in Time Dependent Density Functional Calculation and Hydrogen Bonding Effect. Journal of Chemical Theory and Computation, 2014, 10, 4535-4547.	2.3	24
26	Unraveling the Role of Doping in Selective Stabilization of NaMnO₂ Polymorphs: Combined Theoretical and Experimental Study. Chemistry of Materials, 2018, 30, 1257-1264.	3.2	24
27	Theoretical Study of Tungsten Î·³-Silaallyl/Î·³-Vinylsilyl and Vinyl Silylene Complexes:â€‰ Interesting Bonding Nature and Relative Stability. Organometallics, 2007, 26, 4413-4423.	1.1	23
28	Ab initio study on SN2 reaction of methyl p-nitrobenzenesulfonate and chloride anion in [mmim][PF6]. Physical Chemistry Chemical Physics, 2010, 12, 1822.	1.3	23
29	Theoretical study of electronic and solvent reorganization associated with a charging process of organic compounds. I. Molecular and atomic level description of solvent reorganization. Journal of Chemical Physics, 2003, 119, 2753-2760.	1.2	21
30	Bifurcation of self-assembly pathways to sheet or cage controlled by kinetic template effect. Communications Chemistry, 2019, 2, .	2.0	21
31	A kinetics study of ligand substitution reaction on dinuclear platinum complexes: Stochastic versus deterministic approach. Journal of Computational Chemistry, 2019, 40, 279-285.	1.5	21
32	A New Analysis of Molecular Orbital Wave Functions Based on Resonance Theory. Journal of Physical Chemistry A, 2006, 110, 9028-9030.	1.1	20
33	Theoretical study on aquation reaction of cis-platin complex: RISMâ€“SCFâ€“SEDD, a hybrid approach of accurate quantum chemical method and statistical mechanics. Dalton Transactions, 2011, 40, 11125.	1.6	20
34	Solvation structure of coroneneâ€“transition metal complex: a RISM-SCF study. Physical Chemistry Chemical Physics, 2011, 13, 309-313.	1.3	20
35	A chemical potential equalization approach to constant potential polarizable electrodes for electrochemical-cell simulations. Journal of Chemical Physics, 2019, 151, 164123.	1.2	19
36	Analysis on Solvated Molecules with a New Energy Partitioning Scheme for Intra- and Intermolecular Interactions. Journal of Physical Chemistry B, 2006, 110, 12714-12720.	1.2	18

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37	NMR chemical shifts in solution: a RISM-SCF approach. Chemical Physics Letters, 2000, 325, 668-674.	1.2	17
38	Solvent effect on the nuclear magnetic shielding:ab initiostudy by the combined reference interaction site model and electronic structure theories. Journal of Chemical Physics, 2001, 115, 8949-8957.	1.2	17
39	Regularized regression analysis of digitized molecular structures in organic reactions for quantification of steric effects. Journal of Computational Chemistry, 2017, 38, 1825-1833.	1.5	17
40	Aqueous Solvation of p-Aminobenzonitrile in the Excited States: A Molecular Level Theory on Density Dependence. Journal of Physical Chemistry B, 2010, 114, 910-914.	1.2	15
41	Ab Initio Study of Stability of Na₂Fe₂(SO₄)₃, a High Potential Na-Ion Battery Cathode Material. Journal of Physical Chemistry C, 2017, 121, 20067-20074.	1.5	15
42	DFT+U in Dudarevâ€™s formulation with corrected interactions between the electrons with opposite spins: The form of Hamiltonian, calculation of forces, and bandgap adjustments. Journal of Chemical Physics, 2019, 151, 024102.	1.2	15
43	A stochastic model study on the self-assembly process of a Pd₂L₄ cage consisting of rigid ditopic ligands. Physical Chemistry Chemical Physics, 2019, 21, 6341-6347.	1.3	14
44	Theoretical Study on Electronic and Solvent Reorganization Associated with a Charging Process of Organic Compounds. 2. A New Decomposition Procedure into Electrostatic and Nonelectrostatic Responses. Journal of Physical Chemistry B, 2004, 108, 11709-11715.	1.2	13
45	Solvation effect on the interaction between sodium and chloride ions in aqueous solution: An analysis based on the new resonance theory. International Journal of Quantum Chemistry, 2007, 107, 3132-3136.	1.0	13
46	First Principle Theory for pK_a Prediction at Molecular Level: pH Effects Based on Explicit Solvent Model. Journal of Physical Chemistry B, 2009, 113, 10509-10514.	1.2	13
47	Theoretical Study of Magnesium Fluoride in Aqueous Solution. Journal of Physical Chemistry B, 2011, 115, 10553-10559.	1.2	13
48	Coordination Selfâ€Assembly Processes Revealed by Collaboration of Experiment and Theory: Toward Kinetic Control of Molecular Selfâ€Assembly. Chemical Record, 2021, 21, 443-459.	2.9	13
49	A systematic understanding of orbital energy shift in polar solvent. Journal of Chemical Physics, 2009, 130, 044107.	1.2	12
50	A resonance theory consistent with Mulliken-population concept. Chemical Physics Letters, 2011, 505, 148-153.	1.2	12
51	Constant-potential molecular dynamics simulations on an electrode-electrolyte system: Calculation of static quantities and comparison of two polarizable metal electrode models. Chemical Physics Letters, 2017, 681, 80-85.	1.2	12
52	A Catalytic Alkylation of Ketones via sp³ Câ€“H Bond Activation. Journal of Organic Chemistry, 2023, 88, 6333-6346.	1.7	12
53	A quantum soluteâ€“solvent interaction using spectral representation technique applied to the electronic structure theory in solution. Journal of Chemical Physics, 2003, 119, 6663-6670.	1.2	11
54	An integral equation theory for structural fluctuation in molecular liquid. Chemical Physics Letters, 2010, 487, 241-245.	1.2	11

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55	Development of three-dimensional site-site Smoluchowski-Vlasov equation and application to electrolyte solutions. Journal of Chemical Physics, 2014, 140, 244110.	1.2	11
56	Generalization of the New Resonance Theory: Second Quantization Operator, Localization Scheme, and Basis Set. Journal of Chemical Theory and Computation, 2009, 5, 1741-1748.	2.3	10
57	Solvent effect on (2,2,6,6-Tetramethylpiperidine-1-yl)oxyl (TEMPO): a RISM-SCF-SEDD study. Theoretical Chemistry Accounts, 2011, 130, 299-304.	0.5	10
58	An Ab Initio QM/MM-Based Approach to Efficiently Evaluate Vertical Excitation Energies in Condensed Phases Including the Nonequilibrium Solvation Effect. Journal of Physical Chemistry B, 2016, 120, 1670-1678.	1.2	10
59	A polarizable molecular dynamics method for electrodeâ€“electrolyte interfacial electron transfer under the constant chemical-potential-difference condition on the electrode electrons. Journal of Chemical Physics, 2020, 153, 054126.	1.2	10
60	Controlling potential difference between electrodes based on self-consistent-charge density functional tight binding. Journal of Chemical Physics, 2021, 154, 144107.	1.2	10
61	Theoretical study of the mechanism of the solvent dependency of ESIPT in HBT. Physical Chemistry Chemical Physics, 2021, 23, 20080-20085.	1.3	10
62	Theoretical Studies on the Electronic States and Liquid Structures of Ferrocenium-Based Ionic Liquids. Journal of Physical Chemistry A, 2015, 119, 5181-5188.	1.1	9
63	A theory of diffusion controlled reactions in polyatomic molecule system. Journal of Chemical Physics, 2016, 145, 194502.	1.2	9
64	Introducing the mean field approximation to CDFT/MMpol method: Statistically converged equilibrium and nonequilibrium free energy calculation for electron transfer reactions in condensed phases. Journal of Chemical Physics, 2017, 146, 154101.	1.2	9
65	Dynamics theory for molecular liquids based on an interaction site model. Physical Chemistry Chemical Physics, 2017, 19, 27917-27929.	1.3	9
66	A theoretical study on the electronic structure of PYP chromophore in low barrier hydrogen bonding model. Chemical Physics, 2013, 419, 163-166.	0.9	8
67	Towards kinetic control of coordination self-assembly: a case study of a Pd3L6 double-walled triangle to predict the outcomes by a reaction network model. Physical Chemistry Chemical Physics, 2020, 22, 26614-26626.	1.3	8
68	A hybrid framework of first principles molecular orbital calculations and a three-dimensional integral equation theory for molecular liquids: Multi-center molecular Ornsteinâ€“Zernike self-consistent field approach. Journal of Chemical Physics, 2015, 143, 014103.	1.2	7
69	Challenges in computational evaluation of redox and magnetic properties of Fe-based sulfate cathode materials of Li- and Na-ion batteries. Journal of Physics Condensed Matter, 2017, 29, 215701.	0.7	7
70	Theoretical Study of the Solvation Effect on the Reductive Reaction of Vinylene Carbonate in the Electrolyte Solution of Lithium Ion Batteries. Journal of Physical Chemistry B, 2017, 121, 5293-5299.	1.2	7
71	Experimental observation of the unique solvation process along multiple solvation coordinates of photodissociated products. Physical Chemistry Chemical Physics, 2021, 23, 4569-4579.	1.3	7
72	A catalyzed E/Z isomerization mechanism of stilbene using para-benzoquinone as a triplet sensitizer. Physical Chemistry Chemical Physics, 2022, 24, 1712-1721.	1.3	7

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73	Beyond the Continuum Approach. , 0, , 499-605.		6
74	Systematic assessment on aqueous pK_a and pK_b of an amino acid base on RISMâ€SCFâ€SEDD method: Toward first principles calculations. International Journal of Quantum Chemistry, 2012, 112, 103-112.	1.0	6
75	Photo absorption of â€coumaric acid in aqueous solution: RISMâ€SCFâ€SEDD theory approach. Journal of Computational Chemistry, 2017, 38, 1567-1573.	1.5	6
76	SCC-DFTB-PIMD Method To Evaluate a Multidimensional Quantum Free-Energy Surface for a Proton-Transfer Reaction. Journal of Chemical Theory and Computation, 2019, 15, 4965-4973.	2.3	6
77	Enhanced Surfaces for Endothelial Cell Seeding. Journal of Biomaterials Applications, 1999, 14, 169-183.	1.2	5
78	A theory for time-dependent solvation structure near solid-liquid interface. Journal of Chemical Physics, 2012, 136, 244502.	1.2	5
79	Theoretical study on the ionization of aniline in aqueous solutions. Chemical Physics Letters, 2013, 584, 103-107.	1.2	5
80	Chiral effects on the final step of an octahedron-shaped coordination capsule self-assembly. Physical Chemistry Chemical Physics, 2018, 20, 7383-7386.	1.3	5
81	Theoretical approaches for dynamical ordering of biomolecular systems. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 212-228.	1.1	5
82	Self-Assembly of Nanocubic Molecular Capsules via Solvent-Guided Formation of Rectangular Blocks. Journal of Physical Chemistry Letters, 2018, 9, 6082-6088.	2.1	5
83	Nuclear magnetic shielding of molecule in solution based on reference interaction site model self-consistent field with spatial electron density distribution. Journal of Chemical Physics, 2020, 152, 194102.	1.2	5
84	Theoretical study on isomerization of Î±-acids: A DFT calculation. Food Chemistry, 2021, 364, 130418.	4.2	5
85	An extended formula of site-site Smoluchowski-Vlasov equation for electrolyte solution and infinitely dilute solution. Journal of Chemical Physics, 2012, 137, 034506.	1.2	4
86	An integral equation theory for solvation effects on the molecular structural fluctuation. Journal of Chemical Physics, 2015, 143, 014104.	1.2	4
87	Potential energy landscapes of tetragonal pyramid molecules. Chemical Physics Letters, 2016, 664, 5-9.	1.2	4
88	Solvation Structure of LiClO₄/Ethylene Carbonate Solution near a Graphite Electrode in Lithium-ion Batteries: 3D-RISM Study. Chemistry Letters, 2018, 47, 311-314.	0.7	4
89	A model electronic Hamiltonian for the self-assembly of an octahedron-shaped coordination capsule. Physical Chemistry Chemical Physics, 2018, 20, 1164-1172.	1.3	4
90	Redox, Magnetic, and Structural Properties of Î±-NaMnO2 Cathode Material Analyzed by Fitting-Free DFT+U Calculations, Parameterized by the Linear Response Approach. Journal of Physical Chemistry C, 2021, 125, 1531-1543.	1.5	4

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91	A quantum chemical model for a series of self-assembled nanocages: the origin of stability behind the coordination-driven formation of transition metal complexes up to [M₁₂L₂₄]²⁴⁺. Physical Chemistry Chemical Physics, 2021, 23, 866-877.	1.3	4
92	Coarse-grained modeling of nanocube self-assembly system and transition network analyses. Chemical Physics Letters, 2020, 742, 137135.	1.2	4
93	Unexpected Self-Assembly Pathway to a Pd(II) Coordination Square-Based Pyramid and Its Preferential Formation beyond the Boltzmann Distribution. Inorganic Chemistry, 2021, 60, 16678-16685.	1.9	4
94	Unified polarizable electrode models for open and closed circuits: Revisiting the effects of electrode polarization and different circuit conditions on electrode-electrolyte interfaces. Journal of Chemical Physics, 0, , .	1.2	4
95	Self-consistent construction of bridge functional based on the weighted density approximation. Journal of Chemical Physics, 2021, 154, 124113.	1.2	3
96	An analysis of valence electronic structure from a viewpoint of resonance theory: Tautomerization of formamide and diazadiboretidine. Journal of Computational Chemistry, 2021, 42, 1662-1669.	1.5	3
97	Cyclization or bridging: which occurs faster is the key to the self-assembly mechanism of Pd₆L₃ coordination prisms. Physical Chemistry Chemical Physics, 2022, 24, 2997-3006.	1.3	3
98	Extraction of local spin-coupled states by second quantized operators. Journal of Chemical Physics, 2022, 157, 014112.	1.2	3
99	Timeâ€dependent pair distribution functions based on Smoluchowski equation and application to an electrolyte solution. Journal of Computational Chemistry, 2018, 39, 1491-1497.	1.5	2
100	Theoretical Analysis of Materials, used in Energy Storage Applications: the Quest for Robust and Accurate Computational Methodologies. Chemical Record, 2019, 19, 779-791.	2.9	2
101	Evaluation of redox potentials of cathode materials of alkali-ion batteries using extended DFT+U+Uâ†'â†" method: The role of interactions between the electrons with opposite spins. Journal of Chemical Physics, 2021, 154, 114709.	1.2	2
102	Experimental and theoretical study on p-aminophenylthyil radical geminate recombination in ionic liquids; analysis using the Smoluchowskiâ€"Collinsâ€"Kimball equation. Journal of Chemical Physics, 2021, 154, 154504.	1.2	2
103	Self-consistent construction of grand potential functional with hierarchical integral equations and its application to solvation thermodynamics. Journal of Chemical Physics, 2022, 156, 054116.	1.2	2
104	Solvation in nitration of benzene and the valence electronic structure of the Wheland intermediate. Physical Chemistry Chemical Physics, 2022, 24, 16453-16461.	1.3	2
105	Reply to â€œComment on â€˜Analysis on Solvated Molecules with a New Energy Partitioning Scheme for Intra- and Intermolecular Interactions'â€• Journal of Physical Chemistry B, 2007, 111, 672-674.	1.2	1
106	A molecular level study of selective cation capture by a hostâ€"guest mechanism for 25,26,27,28-tetramethoxycalix[4]arene in MClO₄solution (MÂ=ÂNa, K). Molecular Simulation, 2015, 41, 881-891.	0.9	1
107	A theoretical study on the optical absorption of green fluorescent protein chromophore in solutions. Molecular Simulation, 2017, 43, 997-1003.	0.9	1
108	A simple model of planar membrane: An integral equation investigation. Journal of Computational Chemistry, 2018, 39, 2576-2581.	1.5	1

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109	An Integral Equation Theory for Two Dimensional Molecular Fluids. Chemistry Letters, 2018, 47, 901-904.	0.7	1
110	Pseudo-Jahn-Teller effect on the lowest triplet state of para-benzoquinone involving inequivalent carbonyl bonds. Chemical Physics Letters, 2020, 741, 137072.	1.2	1
111	Density functional theory for molecular liquids based on interaction site model and self-consistent integral equations for siteâ€“site pair correlation functions. Journal of Chemical Physics, 2020, 153, 164102.	1.2	1
112	Energy landscape study of water splitting and H₂ evolution at a ruthenium(<scp>II</scp>) pincer complex. Journal of Computational Chemistry, 2020, 41, 2240-2250.	1.5	1
113	Uniform potential difference scheme to evaluate effective electronic couplings for superexchange electron transfer in donorâ€“bridgeâ€“acceptor systems. Journal of Chemical Physics, 2020, 152, 224103.	1.2	1
114	Chemical Shift of Solvated Hydride Ion: Comparative Study with Solvated Fluoride Ion. Journal of Physical Chemistry B, 2022, 126, 3090-3098.	1.2	1
115	Coronene-transition metal complex: View from quantum chemistry and statistical mechanics. , 2012, , .		0
116	Classical Molecular Dynamics Simulation of Metal Electrodes-Electrolyte Interface. Journal of Computer Chemistry Japan, 2019, 18, 9-17.	0.0	0
117	Distance as coordinate: A distance geometry study on isomerizations of small Lennard-Jones and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si10.svg"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>Au</mml:mtext></mml:mrow><mml:mrow><mml:mn>6</mml:mn> clusters. Chemical Physics Letters, 2021, 780, 138942.	1.2	0
118	(Invited) Titanium-Catalyzed Intermolecular Radical Addition to Ketones Via Sp ³ C-H Bond Activation. ECS Meeting Abstracts, 2022, MA2022-01, 914-914.	0.0	0