Hirofumi Sato

List of Publications by Citations

112 papers	1,694 citations	22 h-index	37 g-index
123 ext. papers	1,880 ext. citations	3.8 avg, IF	5.08 L-index

#	Paper	IF	Citations
112	Analytical energy gradient for the reference interaction site model multiconfigurational self-consistent-field method: Application to 1,2-difluoroethylene in aqueous solution. *Journal of Chemical Physics*, **1996**, 105, 1546-1551	3.9	227
111	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	3.9	91
110	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	3.9	90
109	Geometries and Energies of Nitrobenzene Studied by CAS-SCF Calculations. *Journal of Physical Chemistry A*, **1997**, 101, 5190-5195	2.8	62
108	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	3.9	59
107	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. *Organometallics*, **2009**, 28, 2583-2594	3.8	52
106	A modern solvation theory: quantum chemistry and statistical chemistry. *Physical Chemistry Chemical Physics*, **2013**, 15, 7450-65	3.6	49
105	Comparison of Electronic Structure Theories for Solvated Molecules: RISM-SCF versus PCM. *Journal of Physical Chemistry A*, **2004**, 108, 1629-1634	2.8	49
104	A theoretical analysis of a Diels-Alder reaction in ionic liquids. *Journal of Physical Chemistry B*, **2009**, 113, 8227-30	3.4	43
103	Excitation wavelength dependence of excited state intramolecular proton transfer reaction of 4′-N,N-diethylamino-3-hydroxyflavone in room temperature ionic liquids studied by optical Kerr gate fluorescence measurement. *Journal of Physical Chemistry B*, **2013**, 117, 12567-82	3.4	38
102	Ab initio study on an excited-state intramolecular proton-transfer reaction in ionic liquid. *Journal of Physical Chemistry B*, **2013**, 117, 6759-67	3.4	37
101	Analytical energy gradient for reference interaction site model self-consistent field explicitly including spatial electron density distribution. *Journal of Chemical Physics*, **2009**, 131, 214504	3.9	35
100	Solvation effects in oxidative addition reaction of Methyliodide to Pt(II) complex: A theoretical study with RISM□CF method. *Chemical Physics Letters*, **2008**, 458, 329-332	2.5	34
99	The barrier origin on the reaction of CO2+OH□n aqueous solution. *Chemical Physics Letters*, **2007**, 443, 264-268	2.5	33
98	Equilibrium and Nonequilibrium Solvation Structure of Hexaammineruthenium (II, III) in Aqueous Solution: Ab Initio RISM-SCF Study□*Journal of Physical Chemistry A*, **2002**, 106, 2300-2304	2.8	31
97	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, 2244-8	3.4	28
96	Self-consistent parametrization of DFT + U framework using linear response approach: Application to evaluation of redox potentials of battery cathodes. *Physical Review B*, **2016**, 93,	3.3	27

95	A highly parallelizable integral equation theory for three dimensional solvent distribution function: application to biomolecules. *Journal of Chemical Physics*, **2009**, 130, 064111	3.9	27
94	Superexchange Electron Tunneling Mediated by Solvent Molecules: Pulsed Electron Paramagnetic Resonance Study on Electronic Coupling in Solvent-Separated Radical Ion Pairs *Journal of Physical Chemistry B*, **2004**, 108, 10226-10240	3.4	24
93	Enhanced growth of human vascular endothelial cells on negative ion (Ag-)-implanted hydrophobic surfaces. *Journal of Biomedical Materials Research Part B*, **1999**, 44, 22-30		24
92	Ab initio study on SN2 reaction of methyl p-nitrobenzenesulfonate and chloride anion in [mmim][PF6]. *Physical Chemistry Chemical Physics*, **2010**, 12, 1822-6	3.6	23
91	Navigated Self-Assembly of a PdL Cage by Modulation of an Energy Landscape under Kinetic Control. *Journal of the American Chemical Society*, **2019**, 141, 19669-19676	16.4	23
90	Self-Assembly Processes of Octahedron-Shaped PdL Cages. *Journal of the American Chemical Society*, **2019**, 141, 3178-3186	16.4	22
89	A reaction model on the self-assembly process of octahedron-shaped coordination capsules. *Physical Chemistry Chemical Physics*, **2017**, 19, 20338-20342	3.6	20
88	Solvation structure of coronene-transition metal complex: a RISM-SCF study. *Physical Chemistry Chemical Physics*, **2011**, 13, 309-13	3.6	20
87	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	3.9	20
86	Unraveling the Role of Doping in Selective Stabilization of NaMnO2 Polymorphs: Combined Theoretical and Experimental Study. *Chemistry of Materials*, **2018**, 30, 1257-1264	9.6	19
85	Solvatochromic Shift of Brooker's Merocyanine: Hartree-Fock Exchange in Time Dependent Density Functional Calculation and Hydrogen Bonding Effect. *Journal of Chemical Theory and Computation*, **2014**, 10, 4535-47	6.4	19
84	Theoretical study on aquation reaction of cis-platin complex: RISM-SCF-SEDD, a hybrid approach of accurate quantum chemical method and statistical mechanics. *Dalton Transactions*, **2011**, 40, 11125-30	4.3	18
83	Theoretical Study of Tungsten β-Silaallyl/β-Vinylsilyl and Vinyl Silylene Complexes: Interesting Bonding Nature and Relative Stability. *Organometallics*, **2007**, 26, 4413-4423	3.8	17
82	Analysis on solvated molecules with a new energy partitioning scheme for intra- and intermolecular interactions. *Journal of Physical Chemistry B*, **2006**, 110, 12714-20	3.4	17
81	A new analysis of molecular orbital wave functions based on resonance theory. *Journal of Physical Chemistry A*, **2006**, 110, 9028-30	2.8	17
80	Solvent effect on the nuclear magnetic shielding: ab initio study by the combined reference interaction site model and electronic structure theories. *Journal of Chemical Physics*, **2001**, 115, 8949-8957	3.9	15
79	NMR chemical shifts in solution: a RISM-SCF approach. *Chemical Physics Letters*, **2000**, 325, 668-674	2.5	15
78	Aqueous solvation of p-aminobenzonitrile in the excited states: a molecular level theory on density dependence. *Journal of Physical Chemistry B*, **2010**, 114, 910-4	3.4	14

77	Regularized regression analysis of digitized molecular structures in organic reactions for quantification of steric effects. *Journal of Computational Chemistry*, **2017**, 38, 1825-1833	3.5	13
76	First principle theory for pKa prediction at molecular level: pH effects based on explicit solvent model. *Journal of Physical Chemistry B*, **2009**, 113, 10509-14	3.4	13
75	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	2.1	13
74	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	3.4	12
73	A systematic understanding of orbital energy shift in polar solvent. *Journal of Chemical Physics*, **2009**, 130, 044107	3.9	11
72	Bifurcation of self-assembly pathways to sheet or cage controlled by kinetic template effect. *Communications Chemistry*, **2019**, 2,	6.3	11
71	Development of three-dimensional site-site Smoluchowski-Vlasov equation and application to electrolyte solutions. *Journal of Chemical Physics*, **2014**, 140, 244110	3.9	10
70	Solvent effect on (2,2,6,6-Tetramethylpiperidine-1-yl)oxyl (TEMPO): a RISM-SCF-SEDD study. *Theoretical Chemistry Accounts*, **2011**, 130, 299-304	1.9	10
69	Theoretical study of magnesium fluoride in aqueous solution. *Journal of Physical Chemistry B*, **2011**, 115, 10553-9	3.4	10
68	A quantum solute–solvent interaction using spectral representation technique applied to the electronic structure theory in solution. *Journal of Chemical Physics*, **2003**, 119, 6663-6670	3.9	10
67	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, 1670-8	3.4	9
66	A chemical potential equalization approach to constant potential polarizable electrodes for electrochemical-cell simulations. *Journal of Chemical Physics*, **2019**, 151, 164123	3.9	9
65	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	3.8	9
64	A resonance theory consistent with Mulliken-population concept. *Chemical Physics Letters*, **2011**, 505, 148-153	2.5	9
63	An integral equation theory for structural fluctuation in molecular liquid. *Chemical Physics Letters*, **2010**, 487, 241-245	2.5	9
62	Phase evolution of electrochemically potassium intercalated graphite. *Journal of Materials Chemistry A*, **2021**, 9, 11187-11200	13	9
61	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	3.9	8
60	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	2.5	8

59	A stochastic model study on the self-assembly process of a PdL cage consisting of rigid ditopic ligands. *Physical Chemistry Chemical Physics*, **2019**, 21, 6341-6347	3.6	8
58	A theoretical study on the electronic structure of PYP chromophore in low barrier hydrogen bonding model. *Chemical Physics*, **2013**, 419, 163-166	2.3	8
57	Generalization of the New Resonance Theory: Second Quantization Operator, Localization Scheme, and Basis Set. *Journal of Chemical Theory and Computation*, **2009**, 5, 1741-8	6.4	8
56	DFT+U in Dudarev'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	3.9	7
55	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	1.8	6
54	Theoretical studies on the electronic states and liquid structures of ferrocenium-based ionic liquids. *Journal of Physical Chemistry A*, **2015**, 119, 5181-8	2.8	6
53	Systematic assessment on aqueous pKa and pKb of an amino acid base on RISM-SCF-SEDD method: Toward first principles calculations. *International Journal of Quantum Chemistry*, **2012**, 112, 103-112	2.1	6
52	Dynamics theory for molecular liquids based on an interaction site model. *Physical Chemistry Chemical Physics*, **2017**, 19, 27917-27929	3.6	5
51	Theoretical approaches for dynamical ordering of biomolecular systems. *Biochimica Et Biophysica Acta - General Subjects*, **2018**, 1862, 212-228	4	5
50	A theory for time-dependent solvation structure near solid-liquid interface. *Journal of Chemical Physics*, **2012**, 136, 244502	3.9	5
49	Enhanced surfaces for endothelial cell seeding. *Journal of Biomaterials Applications*, **1999**, 14, 169-83	2.9	5
48	A polarizable molecular dynamics method for electrode-electrolyte interfacial electron transfer under the constant chemical-potential-difference condition on the electrode electrons. *Journal of Chemical Physics*, **2020**, 153, 054126	3.9	5
47	Controlling potential difference between electrodes based on self-consistent-charge density functional tight binding. *Journal of Chemical Physics*, **2021**, 154, 144107	3.9	5
46	A theory of diffusion controlled reactions in polyatomic molecule system. *Journal of Chemical Physics*, **2016**, 145, 194502	3.9	5
45	A kinetics study of ligand substitution reaction on dinuclear platinum complexes: Stochastic versus deterministic approach. *Journal of Computational Chemistry*, **2019**, 40, 279-285	3.5	5
44	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	3.4	4
43	Photo absorption of p-coumaric acid in aqueous solution: RISM-SCF-SEDD theory approach. *Journal of Computational Chemistry*, **2017**, 38, 1567-1573	3.5	4
42	Chiral effects on the final step of an octahedron-shaped coordination capsule self-assembly. *Physical Chemistry Chemical Physics*, **2018**, 20, 7383-7386	3.6	4

41	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	6.4	4
40	A hybrid framework of first principles molecular orbital calculations and a three-dimensional integral equation theory for molecular liquids: multi-center molecular Ornstein-Zernike self-consistent field approach. *Journal of Chemical Physics*, **2015**, 143, 014103	3.9	4
39	An extended formula of site-site Smoluchowski-Vlasov equation for electrolyte solution and infinitely dilute solution. *Journal of Chemical Physics*, **2012**, 137, 034506	3.9	4
38	Coordination Self-Assembly Processes Revealed by Collaboration of Experiment and Theory: Toward Kinetic Control of Molecular Self-Assembly. *Chemical Record*, **2021**, 21, 443-459	6.6	4
37	Experimental observation of the unique solvation process along multiple solvation coordinates of photodissociated products. *Physical Chemistry Chemical Physics*, **2021**, 23, 4569-4579	3.6	4
36	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	3.9	3
35	Solvation Structure of LiClO4/Ethylene Carbonate Solution near a Graphite Electrode in Lithium-ion Batteries: 3D-RISM Study. *Chemistry Letters*, **2018**, 47, 311-314	1.7	3
34	Beyond the Continuum Approach499-605		3
33	Potential energy landscapes of tetragonal pyramid molecules. *Chemical Physics Letters*, **2016**, 664, 5-9	2.5	3
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31	Self-Assembly of Nanocubic Molecular Capsules via Solvent-Guided Formation of Rectangular Blocks. *Journal of Physical Chemistry Letters*, **2018**, 9, 6082-6088	6.4	3
30	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 [ML]. *Physical Chemistry Chemical Physics*, **2021**, 23, 866-877	3.6	3
29	Challenges in computational evaluation of redox and magnetic properties of Fe-based sulfate cathode materials of Li- and Na-ion batteries [J. Phys.: Condens. Matter 29 (2017) 215701]. *Journal of Physics Condensed Matter*, **2017**,	1.8	2
28	An integral equation theory for solvation effects on the molecular structural fluctuation. *Journal of Chemical Physics*, **2015**, 143, 014104	3.9	2
27	Theoretical study on the ionization of aniline in aqueous solutions. *Chemical Physics Letters*, **2013**, 584, 103-107	2.5	2
26	Towards kinetic control of coordination self-assembly: a case study of a PdL double-walled triangle to predict the outcomes by a reaction network model. *Physical Chemistry Chemical Physics*, **2020**, 22, 26614-26626	3.6	2
25	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	5.1	2
24	Redox, Magnetic, and Structural Properties of □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	3.8	2

23	Theoretical study of the mechanism of the solvent dependency of ESIPT in HBT. *Physical Chemistry Chemical Physics*, **2021**, 23, 20080-20085	3.6	2
22	A molecular level study of selective cation capture by a host□guest mechanism for 25,26,27,28-tetramethoxycalix[4]arene in MClO4 solution (M = Na, K). *Molecular Simulation*, **2015**, 41, 881-891	2	1
21	Uniform potential difference scheme to evaluate effective electronic couplings for superexchange electron transfer in donor-bridge-acceptor systems. *Journal of Chemical Physics*, **2020**, 152, 224103	3.9	1
20	Time-dependent pair distribution functions based on Smoluchowski equation and application to an electrolyte solution. *Journal of Computational Chemistry*, **2018**, 39, 1491-1497	3.5	1
19	A theoretical study on the optical absorption of green fluorescent protein chromophore in solutions. *Molecular Simulation*, **2017**, 43, 997-1003	2	1
18	Reply to □comment on □Analysis on Solvated Molecules with a New Energy Partitioning Scheme for Intra- and Intermolecular Interactions'□*Journal of Physical Chemistry B*, **2007**, 111, 672-674	3.4	1
17	Coarse-grained modeling of nanocube self-assembly system and transition network analyses. *Chemical Physics Letters*, **2020**, 742, 137135	2.5	1
16	Energy landscape study of water splitting and H evolution at a ruthenium(II) pincer complex. *Journal of Computational Chemistry*, **2020**, 41, 2240-2250	3.5	1
15	Self-consistent construction of bridge functional based on the weighted density approximation. *Journal of Chemical Physics*, **2021**, 154, 124113	3.9	1
14	Theoretical Analysis of Materials, used in Energy Storage Applications: the Quest for Robust and Accurate Computational Methodologies. *Chemical Record*, **2018**, 19, 779	6.6	1
13	A simple model of planar membrane: An integral equation investigation. *Journal of Computational Chemistry*, **2018**, 39, 2576-2581	3.5	1
12	An Integral Equation Theory for Two Dimensional Molecular Fluids. *Chemistry Letters*, **2018**, 47, 901-904	1.7	1
11	Pseudo-Jahn-Teller effect on the lowest triplet state of para-benzoquinone involving inequivalent carbonyl bonds. *Chemical Physics Letters*, **2020**, 741, 137072	2.5	0
10	Experimental and theoretical study on p-aminophenylthyil radical geminate recombination in ionic liquids; analysis using the Smoluchowski-Collins-Kimball equation. *Journal of Chemical Physics*, **2021**, 154, 154504	3.9	0
9	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	3.5	0
8	Evaluation of redox potentials of cathode materials of alkali-ion batteries using extended DFT+U+U method: The role of interactions between the electrons with opposite spins. *Journal of Chemical Physics*, **2021**, 154, 114709	3.9	0
7	Theoretical study on isomerization of □acids: A DFT calculation. *Food Chemistry*, **2021**, 364, 130418	8.5	0
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5	Self-consistent construction of grand potential functional with hierarchical integral equations and its application to solvation thermodynamics.. *Journal of Chemical Physics*, **2022**, 156, 054116	3.9
4	Theoretical Approach to Chemical Reactions and Photochemical Processes in Ionic Liquid. *Physical Chemistry in Action*, **2021**, 255-287	
3	Multiscale Solvation Theory for Nano- and Biomolecules. *Physical Chemistry in Action*, **2021**, 17-37	
2	Density functional theory for molecular liquids based on interaction site model and self-consistent integral equations for site-site pair correlation functions. *Journal of Chemical Physics*, **2020**, 153, 164102	3.9
1	Distance as coordinate: A distance geometry study on isomerizations of small Lennard-Jones and Au6+ clusters. *Chemical Physics Letters*, **2021**, 780, 138942	2.5