

# Hirofumi Sato

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Self-consistent construction of grand potential functional with hierarchical integral equations and its application to solvation thermodynamics.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 054116	3.9	
111	Theoretical Approach to Chemical Reactions and Photochemical Processes in Ionic Liquid. <i>Physical Chemistry in Action</i> , <b>2021</b> , 255-287		
110	Multiscale Solvation Theory for Nano- and Biomolecules. <i>Physical Chemistry in Action</i> , <b>2021</b> , 17-37		
109	Unexpected Self-Assembly Pathway to a Pd(II) Coordination Square-Based Pyramid and Its Preferential Formation beyond the Boltzmann Distribution. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 16678-16685	5.1	2
108	Self-consistent construction of bridge functional based on the weighted density approximation. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 124113	3.9	1
107	Controlling potential difference between electrodes based on self-consistent-charge density functional tight binding. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 144107	3.9	5
106	Experimental and theoretical study on p-aminophenylthiyl radical geminate recombination in ionic liquids; analysis using the Smoluchowski-Collins-Kimball equation. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 154504	3.9	0
105	An analysis of valence electronic structure from a viewpoint of resonance theory: Tautomerization of formamide and diazadiboretidine. <i>Journal of Computational Chemistry</i> , <b>2021</b> , 42, 1662-1669	3.5	0
104	Coordination Self-Assembly Processes Revealed by Collaboration of Experiment and Theory: Toward Kinetic Control of Molecular Self-Assembly. <i>Chemical Record</i> , <b>2021</b> , 21, 443-459	6.6	4
103	Experimental observation of the unique solvation process along multiple solvation coordinates of photodissociated products. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 4569-4579	3.6	4
102	Redox, Magnetic, and Structural Properties of $\text{NaMnO}_2$ Cathode Material Analyzed by Fitting-Free DFT+U Calculations, Parameterized by the Linear Response Approach. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 1531-1543	3.8	2
101	Phase evolution of electrochemically potassium intercalated graphite. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 11187-11200	13	9
100	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. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 114709	3.9	0
99	Distance as coordinate: A distance geometry study on isomerizations of small Lennard-Jones and $\text{Au}_6^+$ clusters. <i>Chemical Physics Letters</i> , <b>2021</b> , 780, 138942	2.5	
98	Theoretical study on isomerization of $\text{H}_2\text{O}$ acids: A DFT calculation. <i>Food Chemistry</i> , <b>2021</b> , 364, 130418	8.5	0
97	Theoretical study of the mechanism of the solvent dependency of ESIPT in HBT. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 20080-20085	3.6	2
96	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]. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 866-877	3.6	3

95	Uniform potential difference scheme to evaluate effective electronic couplings for superexchange electron transfer in donor-bridge-acceptor systems. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 224103	3.9	1
94	Nuclear magnetic shielding of molecule in solution based on reference interaction site model self-consistent field with spatial electron density distribution. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 194102	3.9	3
93	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. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 26614-26626	3.6	2
92	Coarse-grained modeling of nanocube self-assembly system and transition network analyses. <i>Chemical Physics Letters</i> , <b>2020</b> , 742, 137135	2.5	1
91	Pseudo-Jahn-Teller effect on the lowest triplet state of para-benzoquinone involving inequivalent carbonyl bonds. <i>Chemical Physics Letters</i> , <b>2020</b> , 741, 137072	2.5	0
90	A polarizable molecular dynamics method for electrode-electrolyte interfacial electron transfer under the constant chemical-potential-difference condition on the electrode electrons. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 054126	3.9	5
89	Density functional theory for molecular liquids based on interaction site model and self-consistent integral equations for site-site pair correlation functions. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 164102 <sup>3.9</sup>	3.9	
88	Energy landscape study of water splitting and H evolution at a ruthenium(II) pincer complex. <i>Journal of Computational Chemistry</i> , <b>2020</b> , 41, 2240-2250	3.5	1
87	A stochastic model study on the self-assembly process of a PdL cage consisting of rigid ditopic ligands. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 6341-6347	3.6	8
86	Self-Assembly Processes of Octahedron-Shaped PdL Cages. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 3178-3186	16.4	22
85	SCC-DFTB-PIMD Method To Evaluate a Multidimensional Quantum Free-Energy Surface for a Proton-Transfer Reaction. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 4965-4973	6.4	4
84	Classical Molecular Dynamics Simulation of Metal Electrodes-Electrolyte Interface. <i>Journal of Computer Chemistry Japan</i> , <b>2019</b> , 18, 9-17	0.2	
83	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. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 024102	3.9	7
82	A chemical potential equalization approach to constant potential polarizable electrodes for electrochemical-cell simulations. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 164123	3.9	9
81	Bifurcation of self-assembly pathways to sheet or cage controlled by kinetic template effect. <i>Communications Chemistry</i> , <b>2019</b> , 2,	6.3	11
80	Navigated Self-Assembly of a PdL Cage by Modulation of an Energy Landscape under Kinetic Control. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 19669-19676	16.4	23
79	A kinetics study of ligand substitution reaction on dinuclear platinum complexes: Stochastic versus deterministic approach. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 279-285	3.5	5
78	Time-dependent pair distribution functions based on Smoluchowski equation and application to an electrolyte solution. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 1491-1497	3.5	1

77	Unraveling the Role of Doping in Selective Stabilization of NaMnO <sub>2</sub> Polymorphs: Combined Theoretical and Experimental Study. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 1257-1264	9.6	19
76	Chiral effects on the final step of an octahedron-shaped coordination capsule self-assembly. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 7383-7386	3.6	4
75	Solvation Structure of LiClO <sub>4</sub> /Ethylene Carbonate Solution near a Graphite Electrode in Lithium-ion Batteries: 3D-RISM Study. <i>Chemistry Letters</i> , <b>2018</b> , 47, 311-314	1.7	3
74	Theoretical approaches for dynamical ordering of biomolecular systems. <i>Biochimica Et Biophysica Acta - General Subjects</i> , <b>2018</b> , 1862, 212-228	4	5
73	Theoretical Analysis of Materials, used in Energy Storage Applications: the Quest for Robust and Accurate Computational Methodologies. <i>Chemical Record</i> , <b>2018</b> , 19, 779	6.6	1
72	A model electronic Hamiltonian for the self-assembly of an octahedron-shaped coordination capsule. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 1164-1172	3.6	3
71	A simple model of planar membrane: An integral equation investigation. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 2576-2581	3.5	1
70	Self-Assembly of Nanocubic Molecular Capsules via Solvent-Guided Formation of Rectangular Blocks. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 6082-6088	6.4	3
69	An Integral Equation Theory for Two Dimensional Molecular Fluids. <i>Chemistry Letters</i> , <b>2018</b> , 47, 901-904	1.7	1
68	Challenges in computational evaluation of redox and magnetic properties of Fe-based sulfate cathode materials of Li- and Na-ion batteries. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 215701	1.8	6
67	Introducing the mean field approximation to CDFT/MMpol method: Statistically converged equilibrium and nonequilibrium free energy calculation for electron transfer reactions in condensed phases. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 154101	3.9	8
66	Theoretical Study of the Solvation Effect on the Reductive Reaction of Vinylene Carbonate in the Electrolyte Solution of Lithium Ion Batteries. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 5293-5299	3.4	4
65	Constant-potential molecular dynamics simulations on an electrode-electrolyte system: Calculation of static quantities and comparison of two polarizable metal electrode models. <i>Chemical Physics Letters</i> , <b>2017</b> , 681, 80-85	2.5	8
64	Photo absorption of p-coumaric acid in aqueous solution: RISM-SCF-SEDD theory approach. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 1567-1573	3.5	4
63	Regularized regression analysis of digitized molecular structures in organic reactions for quantification of steric effects. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 1825-1833	3.5	13
62	Dynamics theory for molecular liquids based on an interaction site model. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 27917-27929	3.6	5
61	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]. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> ,	1.8	2
60	Ab Initio Study of Stability of Na <sub>2</sub> Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> , a High Potential Na-Ion Battery Cathode Material. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 20067-20074	3.8	9

59	A reaction model on the self-assembly process of octahedron-shaped coordination capsules. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 20338-20342	3.6	20
58	A theoretical study on the optical absorption of green fluorescent protein chromophore in solutions. <i>Molecular Simulation</i> , <b>2017</b> , 43, 997-1003	2	1
57	Self-consistent parametrization of DFT + U framework using linear response approach: Application to evaluation of redox potentials of battery cathodes. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	27
56	An Ab Initio QM/MM-Based Approach to Efficiently Evaluate Vertical Excitation Energies in Condensed Phases Including the Nonequilibrium Solvation Effect. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 1670-8	3.4	9
55	A theory of diffusion controlled reactions in polyatomic molecule system. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 194502	3.9	5
54	Potential energy landscapes of tetragonal pyramid molecules. <i>Chemical Physics Letters</i> , <b>2016</b> , 664, 5-9	2.5	3
53	An integral equation theory for solvation effects on the molecular structural fluctuation. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 014104	3.9	2
52	Theoretical studies on the electronic states and liquid structures of ferrocenium-based ionic liquids. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 5181-8	2.8	6
51	A molecular level study of selective cation capture by a host-guest mechanism for 25,26,27,28-tetramethoxycalix[4]arene in MClO <sub>4</sub> solution (M = Na, K). <i>Molecular Simulation</i> , <b>2015</b> , 41, 881-891	2	1
50	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. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 014103	3.9	4
49	Solvatochromic Shift of Brooker's Merocyanine: Hartree-Fock Exchange in Time Dependent Density Functional Calculation and Hydrogen Bonding Effect. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 4535-47	6.4	19
48	Development of three-dimensional site-site Smoluchowski-Vlasov equation and application to electrolyte solutions. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 244110	3.9	10
47	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. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 12567-82	3.4	38
46	A theoretical study on the electronic structure of PYP chromophore in low barrier hydrogen bonding model. <i>Chemical Physics</i> , <b>2013</b> , 419, 163-166	2.3	8
45	Theoretical study on the ionization of aniline in aqueous solutions. <i>Chemical Physics Letters</i> , <b>2013</b> , 584, 103-107	2.5	2
44	A modern solvation theory: quantum chemistry and statistical chemistry. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 7450-65	3.6	49
43	Ab initio study on an excited-state intramolecular proton-transfer reaction in ionic liquid. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 6759-67	3.4	37
42	Proton transfer step in the carbon dioxide capture by monoethanol amine: a theoretical study at the molecular level. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 2244-8	3.4	28

4 <sup>1</sup>	A theory for time-dependent solvation structure near solid-liquid interface. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 244502	3.9	5
4 <sup>0</sup>	Systematic assessment on aqueous pKa and pKb of an amino acid base on RISM-SCF-SEDD method: Toward first principles calculations. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 103-112	2.1	6
39	An extended formula of site-site Smoluchowski-Vlasov equation for electrolyte solution and infinitely dilute solution. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 034506	3.9	4
38	Solvation structure of coronene-transition metal complex: a RISM-SCF study. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 309-13	3.6	20
37	Solvent effect on (2,2,6,6-Tetramethylpiperidine-1-yl)oxyl (TEMPO): a RISM-SCF-SEDD study. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 130, 299-304	1.9	10
36	Theoretical study on aquation reaction of cis-platin complex: RISM-SCF-SEDD, a hybrid approach of accurate quantum chemical method and statistical mechanics. <i>Dalton Transactions</i> , <b>2011</b> , 40, 11125-30	4.3	18
35	Theoretical study of magnesium fluoride in aqueous solution. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 10553-9	3.4	10
34	A resonance theory consistent with Mulliken-population concept. <i>Chemical Physics Letters</i> , <b>2011</b> , 505, 148-153	2.5	9
33	Aqueous solvation of p-aminobenzonitrile in the excited states: a molecular level theory on density dependence. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 910-4	3.4	14
32	Ab initio study on SN2 reaction of methyl p-nitrobenzenesulfonate and chloride anion in [mim][PF6]. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 1822-6	3.6	23
3 <sup>1</sup>	An integral equation theory for structural fluctuation in molecular liquid. <i>Chemical Physics Letters</i> , <b>2010</b> , 487, 241-245	2.5	9
3 <sup>0</sup>	Analytical energy gradient for reference interaction site model self-consistent field explicitly including spatial electron density distribution. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 214504	3.9	35
29	Generalization of the New Resonance Theory: Second Quantization Operator, Localization Scheme, and Basis Set. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 1741-8	6.4	8
28	A systematic understanding of orbital energy shift in polar solvent. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 044107	3.9	11
27	First principle theory for pKa prediction at molecular level: pH effects based on explicit solvent model. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 10509-14	3.4	13
26	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. <i>Organometallics</i> , <b>2009</b> , 28, 2583-2594	3.8	52
25	A highly parallelizable integral equation theory for three dimensional solvent distribution function: application to biomolecules. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 064111	3.9	27
24	A theoretical analysis of a Diels-Alder reaction in ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 8227-30	3.4	43



23	Solvation effects in oxidative addition reaction of Methyl iodide to Pt(II) complex: A theoretical study with RISM-SCF method. <i>Chemical Physics Letters</i> , <b>2008</b> , 458, 329-332	2.5	34
22	Reply to 'Comment on 'Analysis on Solvated Molecules with a New Energy Partitioning Scheme for Intra- and Intermolecular Interactions'' <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 672-674	3.4	1
21	New generation of the reference interaction site model self-consistent field method: introduction of spatial electron density distribution to the solvation theory. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 244504	3.9	90
20	Theoretical Study of Tungsten $\beta$ -Silallyl/ $\beta$ -Vinylsilyl and Vinyl Silylene Complexes: Interesting Bonding Nature and Relative Stability. <i>Organometallics</i> , <b>2007</b> , 26, 4413-4423	3.8	17
19	The barrier origin on the reaction of CO <sub>2</sub> +OH <sup>-</sup> in aqueous solution. <i>Chemical Physics Letters</i> , <b>2007</b> , 443, 264-268	2.5	33
18	Solvation effect on the interaction between sodium and chloride ions in aqueous solution: An analysis based on the new resonance theory. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 107, 3132-3136	2.1	13
17	Analysis on solvated molecules with a new energy partitioning scheme for intra- and intermolecular interactions. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 12714-20	3.4	17
16	A new analysis of molecular orbital wave functions based on resonance theory. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 9028-30	2.8	17
15	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. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 11709-11715	3.4	12
14	Superexchange Electron Tunneling Mediated by Solvent Molecules: Pulsed Electron Paramagnetic Resonance Study on Electronic Coupling in Solvent-Separated Radical Ion Pairs <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 10226-10240	3.4	24
13	Comparison of Electronic Structure Theories for Solvated Molecules: RISM-SCF versus PCM. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 1629-1634	2.8	49
12	Theoretical study of electronic and solvent reorganization associated with a charging process of organic compounds. I. Molecular and atomic level description of solvent reorganization. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 2753-2760	3.9	20
11	A quantum solute-solvent interaction using spectral representation technique applied to the electronic structure theory in solution. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 6663-6670	3.9	10
10	Equilibrium and Nonequilibrium Solvation Structure of Hexaammineruthenium (II, III) in Aqueous Solution: Ab Initio RISM-SCF Study <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 2300-2304	2.8	31
9	Solvent effect on the nuclear magnetic shielding: ab initio study by the combined reference interaction site model and electronic structure theories. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 8949-8957	3.9	15
8	NMR chemical shifts in solution: a RISM-SCF approach. <i>Chemical Physics Letters</i> , <b>2000</b> , 325, 668-674	2.5	15
7	Self-consistent field, ab initio molecular orbital and three-dimensional reference interaction site model study for solvation effect on carbon monoxide in aqueous solution. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 9463-9468	3.9	91
6	Enhanced surfaces for endothelial cell seeding. <i>Journal of Biomaterials Applications</i> , <b>1999</b> , 14, 169-83	2.9	5

5	Ab initio study of water. II. Liquid structure, electronic and thermodynamic properties over a wide range of temperature and density. <i>Journal of Chemical Physics</i> , <b>1999</b> , 111, 8545-8555	3.9	59
4	Enhanced growth of human vascular endothelial cells on negative ion (Ag <sup>-</sup> )-implanted hydrophobic surfaces. <i>Journal of Biomedical Materials Research Part B</i> , <b>1999</b> , 44, 22-30		24
3	Geometries and Energies of Nitrobenzene Studied by CAS-SCF Calculations. <i>Journal of Physical Chemistry A</i> , <b>1997</b> , 101, 5190-5195	2.8	62
2	Analytical energy gradient for the reference interaction site model multiconfigurational self-consistent-field method: Application to 1,2-difluoroethylene in aqueous solution. <i>Journal of Chemical Physics</i> , <b>1996</b> , 105, 1546-1551	3.9	227
1	Beyond the Continuum Approach		3