

# Shinji Saito

## List of Publications by Citations

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95  
papers

3,468  
citations

30  
h-index

57  
g-index

104  
ext. papers

3,763  
ext. citations

5.8  
avg, IF

5.52  
L-index

#	Paper	IF	Citations
95	Molecular dynamics simulation of the ice nucleation and growth process leading to water freezing. <i>Nature</i> , <b>2002</b> , 416, 409-13	50.4	649
94	Instantaneous normal mode analysis of liquid water. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 6672-6683	3.9	315
93	Water Dynamics: Fluctuation, Relaxation, and Chemical Reactions in Hydrogen Bond Network Rearrangement. <i>Accounts of Chemical Research</i> , <b>1999</b> , 32, 741-749	24.3	229
92	Off-resonant fifth-order nonlinear response of water and CS <sub>2</sub> : Analysis based on normal modes. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 240-251	3.9	145
91	Off-resonant fifth-order response function for two-dimensional Raman spectroscopy of liquids CS <sub>2</sub> and H <sub>2</sub> O. <i>Physical Review Letters</i> , <b>2002</b> , 88, 207401	7.4	104
90	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. <i>Chemical Reviews</i> , <b>2020</b> , 120, 7152-7218	68.1	87
89	Circadian rhythms. Atomic-scale origins of slowness in the cyanobacterial circadian clock. <i>Science</i> , <b>2015</b> , 349, 312-6	33.3	76
88	Anisotropic cooperative structural rearrangements in sheared supercooled liquids. <i>Physical Review Letters</i> , <b>2009</b> , 102, 016001	7.4	70
87	Multiple length and time scales of dynamic heterogeneities in model glass-forming liquids: a systematic analysis of multi-point and multi-time correlations. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 12A506	3.9	63
86	Slow dynamics in random media: Crossover from glass to localization transition. <i>Europhysics Letters</i> , <b>2009</b> , 88, 36002	1.6	61
85	Mechanism of fast proton transfer in ice: Potential energy surface and reaction coordinate analyses. <i>Journal of Chemical Physics</i> , <b>2000</b> , 113, 9090-9100	3.9	60
84	Third order nonlinear response of liquid water. <i>Journal of Chemical Physics</i> , <b>1997</b> , 106, 4889-4893	3.9	58
83	Off-resonant two-dimensional fifth-order Raman spectroscopy of liquid CS <sub>2</sub> : Detection of anharmonic dynamics. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 9073-9087	3.9	58
82	Translational and orientational dynamics of a water cluster (H <sub>2</sub> O) <sub>108</sub> and liquid water: Analysis of neutron scattering and depolarized light scattering. <i>Journal of Chemical Physics</i> , <b>1995</b> , 102, 3566-3579	3.9	56
81	Insights in quantum dynamical effects in the infrared spectroscopy of liquid water from a semiclassical study with an ab initio-based flexible and polarizable force field. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 244503	3.9	54
80	Ultrafast intermolecular dynamics of liquid water: a theoretical study on two-dimensional infrared spectroscopy. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 154521	3.9	53
79	Direct Simulation of Excited-State Intramolecular Proton Transfer and Vibrational Coherence of 10-Hydroxybenzo[h]quinoline in Solution. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 2366-2371	6.4	49

78	Molecular dynamics simulation of nonlinear spectroscopies of intermolecular motions in liquid water. <i>Accounts of Chemical Research</i> , <b>2009</b> , 42, 1250-8	24.3	48
77	A theoretical study on anomalous temperature dependence of pK <sub>w</sub> of water. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 144504	3.9	44
76	Multi-time density correlation functions in glass-forming liquids: Probing dynamical heterogeneity and its lifetime. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 044511	3.9	41
75	Probing the Spectral Diffusion of Vibrational Transitions of OCN- and SCN- in Methanol by Three-Pulse Infrared Photon Echo Spectroscopy. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 5643-5649	2.8	40
74	Crucial role of fragmented and isolated defects in persistent relaxation of deeply supercooled water. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 124504	3.9	40
73	Molecular origin of the difference in the HOH bend of the IR spectra between liquid water and ice. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 054506	3.9	37
72	Fluctuations and relaxation dynamics of liquid water revealed by linear and nonlinear spectroscopy. <i>Annual Review of Physical Chemistry</i> , <b>2013</b> , 64, 55-75	15.7	37
71	Dynamics of proton attachment to water cluster: Proton transfer, evaporation, and relaxation. <i>Journal of Chemical Physics</i> , <b>1996</b> , 105, 6358-6366	3.9	37
70	Slow dynamics, dynamic heterogeneities, and fragility of supercooled liquids confined in random media. <i>Journal of Physics Condensed Matter</i> , <b>2011</b> , 23, 234123	1.8	35
69	Ultrafast energy relaxation and anisotropy decay of the librational motion in liquid water: A molecular dynamics study. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 164511	3.9	35
68	Mechanism of proton transfer in ice. II. Hydration, modes, and transport. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 4742-4749	3.9	34
67	Dynamics and relaxation of an intermediate size water cluster (H <sub>2</sub> O) <sub>108</sub> . <i>Journal of Chemical Physics</i> , <b>1994</b> , 101, 6063-6075	3.9	33
66	Molecular Mechanism Behind the Fast Folding/Unfolding Transitions of Villin Headpiece Subdomain: Hierarchy and Heterogeneity. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 11683-11691	3.4	33
65	Vibrational frequency fluctuation of ions in aqueous solutions studied by three-pulse infrared photon echo method. <i>Accounts of Chemical Research</i> , <b>2012</b> , 45, 1982-91	24.3	30
64	Fifth-order two-dimensional Raman spectroscopy of liquid water, crystalline ice Ih and amorphous ices: sensitivity to anharmonic dynamics and local hydrogen bond network structure. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 084506	3.9	30
63	Quantitative Evaluation of Site Energies and Their Fluctuations of Pigments in the Fenna-Matthews-Olson Complex with an Efficient Method for Generating a Potential Energy Surface. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4128-37	6.4	30
62	Theoretical study on excited states of bacteriochlorophyll a in solutions with density functional assessment. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 10906-18	3.4	29
61	Ultrafast dynamics of liquid water: frequency fluctuations of the OH stretch and the HOH bend. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 044503	3.9	29

60	A theoretical study on decomposition of formic acid in sub- and supercritical water. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 7631-7639	3.9	29
59	Multiple time scales hidden in heterogeneous dynamics of glass-forming liquids. <i>Physical Review E</i> , <b>2009</b> , 79, 060501	2.4	28
58	Ultrafast Dynamics of Liquid Water: Energy Relaxation and Transfer Processes of the OH Stretch and the HOH Bend. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 11068-78	3.4	27
57	A novel method for analyzing energy relaxation in condensed phases using nonequilibrium molecular dynamics simulations: application to the energy relaxation of intermolecular motions in liquid water. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 184503	3.9	26
56	Mechanism of ion permeation in a model channel: Free energy surface and dynamics of K <sup>+</sup> ion transport in an anion-doped carbon nanotube. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 20671-7	3.4	26
55	Excited and ionized states of RuO <sub>4</sub> and OsO <sub>4</sub> studied by SAC and SAC-CI theories. <i>International Journal of Quantum Chemistry</i> , <b>1991</b> , 39, 93-113	2.1	26
54	Relation between the conformational heterogeneity and reaction cycle of Ras: molecular simulation of Ras. <i>Biophysical Journal</i> , <b>2010</b> , 99, 3726-34	2.9	25
53	Effects of nonadditive interactions on ion solvation at the water/vapor interface: a molecular dynamics study. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 12573-84	2.8	25
52	Temperature dependence of vibrational frequency fluctuation of N(3) (-) in D(2)O. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 014505	3.9	23
51	Theoretical study for the excited states of MoO <sub>4</sub> <sup>2-</sup> (n=0~4) and MoSe <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>1990</b> , 93, 1865-1875	3.9	23
50	Thermodynamic picture of vitrification of water through complex specific heat and entropy: A journey through "no man's land". <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 054502	3.9	22
49	Frequency dependence of specific heat in supercooled liquid water and emergence of correlated dynamics. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 094503	3.9	22
48	Electronic origin of molybdenum-95 NMR chemical shifts in molybdenum complexes. Relationship between excitation energy and chemical shift. <i>Inorganic Chemistry</i> , <b>1990</b> , 29, 3095-3097	5.1	21
47	Theory of coherent two-dimensional vibrational spectroscopy. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 100901	3.9	20
46	Site-Dependent Fluctuations Optimize Electronic Energy Transfer in the Fenna-Matthews-Olson Protein. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 9762-9772	3.4	19
45	Molecular dynamics studies of slow dynamics in random media: Type A-B and reentrant transitions. <i>European Physical Journal: Special Topics</i> , <b>2010</b> , 189, 135-139	2.3	19
44	Fluctuation, relaxation and rearrangement dynamics of a model (H <sub>2</sub> O) <sub>20</sub> cluster: Non-statistical dynamical behavior. <i>Journal of Chemical Physics</i> , <b>1997</b> , 106, 3329-3337	3.9	18
43	Proton transfer and associated molecular rearrangements in the photocycle of photoactive yellow protein: role of water molecular migration on the proton transfer reaction. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 2948-56	3.4	18

42	Reconsideration of the relaxational and vibrational line shapes of liquid water based on ultrabroadband dielectric spectroscopy. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 26200-26209	3.6	18
41	Dynamic heterogeneity in the folding/unfolding transitions of FIP35. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 135101	3.9	17
40	Role of the Lifetime of Dynamical Heterogeneity in the Frequency-Dependent Stokes-Einstein Relation of Supercooled Liquids. <i>Journal of the Physical Society of Japan</i> , <b>2010</b> , 79, 093601	1.5	16
39	Temperature and hydration dependence of low-frequency spectra of poly-L-glutamic acid with different secondary structures studied by terahertz time-domain spectroscopy. <i>Soft Matter</i> , <b>2012</b> , 8, 1997-2006	3.6	15
38	Couplings between hierarchical conformational dynamics from multi-time correlation functions and two-dimensional lifetime spectra: Application to adenylate kinase. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 212404	3.9	13
37	Energy relaxation of intermolecular motions in supercooled water and ice: a molecular dynamics study. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 244511	3.9	13
36	Intermolecular vibrational mode of the benzoic acid dimer in solution observed by terahertz time-domain spectroscopy. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 14742-9	3.6	11
35	Isotope dilution effects on the hydroxyl-stretch bands of alcohols. <i>Molecular Physics</i> , <b>2005</b> , 103, 37-44	1.7	11
34	Global potential energy surfaces of water clusters; reaction coordinate and annealing analyses. <i>Journal of Molecular Liquids</i> , <b>1998</b> , 77, 95-103	6	9
33	Origin of slow relaxation in liquid-water dynamics: A possible scenario for the presence of bottleneck in phase space. <i>Europhysics Letters</i> , <b>2006</b> , 73, 826-832	1.6	9
32	Mechanism of ion permeation through a model channel: roles of energetic and entropic contributions. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 165106	3.9	7
31	Theoretical investigation on vibrational frequency fluctuations of SCN-derivatized vibrational probe molecule in water. <i>Chemical Physics</i> , <b>2018</b> , 512, 82-87	2.3	6
30	Dynamic length scales in glass-forming liquids: an inhomogeneous molecular dynamics simulation approach. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 13259-67	3.4	6
29	Computational strategy for studying structural change of tritium-substituted macromolecules by a beta decay to helium-3. <i>Journal of Advanced Simulation in Science and Engineering</i> , <b>2019</b> , 6, 94-99	0.4	6
28	Structure and dynamics of solvent molecules inside the polytheonamide B channel in different environments: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 3334-3348	3.6	6
27	Hidden slow time scale of correlated motions in supercooled liquids: Multi-time correlation function approach. <i>Journal of Non-Crystalline Solids</i> , <b>2011</b> , 357, 371-375	3.9	5
26	Tautomeric Effect of Histidine on $\beta$ -Sheet Formation of Amyloid Beta 1-40: 2D-IR Simulations. <i>Biophysical Journal</i> , <b>2020</b> , 119, 831-842	2.9	5
25	Conformational Excitation and Nonequilibrium Transition Facilitate Enzymatic Reactions: Application to Pin1 Peptidyl-Prolyl Isomerase. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 474-480	6.4	5

24	Vibrational frequency fluctuations of ionic vibrational probe in water: Theoretical study with molecular dynamics simulation. <i>Chemical Physics Letters</i> , <b>2017</b> , 683, 547-552	2.5	4
23	Theoretical and experimental studies on vibrational energy relaxation of the CO stretching mode of acetone in alcohol solutions. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 4723-31	3.4	4
22	Molecular dynamics study on DNA damage by tritium disintegration. <i>Japanese Journal of Applied Physics</i> , <b>2020</b> , 59, SAAE01	1.4	4
21	An alternative interpretation of the slow KaiB-KaiC binding of the cyanobacterial clock proteins. <i>Scientific Reports</i> , <b>2020</b> , 10, 10439	4.9	3
20	Dissecting the Dynamics during Enzyme Catalysis: A Case Study of Pin1 Peptidyl-Prolyl Isomerase. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 3396-3407	6.4	3
19	Structural Changes in Tritium-Substituted Polymeric Materials by Beta Decays: A Molecular Dynamics Study. <i>Plasma and Fusion Research</i> , <b>2019</b> , 14, 3401106-3401106	0.5	3
18	Structural change of damaged polyethylene by beta-decay of substituted tritium using reactive force field. <i>Japanese Journal of Applied Physics</i> , <b>2021</b> , 60, SAAB06	1.4	2
17	Heterodyne detected fifth-order nonresonant Raman spectroscopy of CS <sub>2</sub> : Evidence for anharmonic coupling. <i>Springer Series in Chemical Physics</i> , <b>2003</b> , 554-556	0.3	2
16	Effects of interfaces on structure and dynamics of water droplets on a graphene surface: A molecular dynamics study. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 164704	3.9	2
15	Vibrational Frequency Fluctuations of Ionic and Non-ionic Vibrational Probe Molecules in Aqueous Solutions. <i>Springer Series in Optical Sciences</i> , <b>2019</b> , 259-285	0.5	1
14	Sufficiency of unidirectional allostery in KaiC in generating the cyanobacterial circadian rhythm		1
13	Molecular Mechanism of Acceleration and Retardation of Collective Orientation Relaxation of Water Molecules in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 11730-11737	3.4	1
12	Microscopic insights into dynamic disorder in the isomerization dynamics of the protein BPTI. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 224113	3.9	1
11	Vectorial insertion of a helical peptide into membrane: a theoretical study on polytheonamide B. <i>Biophysical Journal</i> , <b>2021</b> , 120, 4786-4797	2.9	1
10	Tetrahedral structure of supercooled water at ambient pressure and its influence on dynamic relaxation: Comparative study of water models. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 341, 117269	6	1
9	Inverse Kohn-Sham Equations Derived from the Density Equation Theory. <i>Journal of the Physical Society of Japan</i> , <b>2020</b> , 89, 024301	1.5	0
8	What We can Learn about Protein Folding from Ultra-long Molecular Dynamics Simulations. <i>Seibutsu Butsuri</i> , <b>2017</b> , 57, 030-032	0	
7	Terahertz Radiation Spectroscopy on Chloroform Confined in Porous Silica Glasses. <i>Materials Research Society Symposia Proceedings</i> , <b>2003</b> , 790, 1		

- 6 Slow Relaxation in Hamiltonian Systems with Internal Degrees of Freedom. *Advances in Chemical Physics*, **2005**, 373-421
- 5 Dynamical Behavior of Water; Fluctuation, Reactions and Phase Transitions. *Bulletin of the Chemical Society of Japan*, **2021**, 94, 2575-2601 5.1
- 4 Hybrid Monte Carlo method with potential scaling for sampling from the canonical multimodal distribution and imitating the relaxation process.. *Journal of Chemical Physics*, **2022**, 156, 104111 3.9
- 3 Excited states of chlorophyll a and b in solution by time-dependent density functional theory.. *Journal of Chemical Physics*, **2022**, 156, 124111 3.9
- 2 Multimeric structure enables the acceleration of KaiB-KaiC complex formation induced by ADP/ATP exchange inhibition.. *PLoS Computational Biology*, **2022**, 18, e1009243 5
- 1 Regulation mechanisms of the dual ATPase in KaiC.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2119627119 11.5