Shinji Saito

List of Publications by Year in Descending Order

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	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	
94	Excited states of chlorophyll a and b in solution by time-dependent density functional theory.. *Journal of Chemical Physics*, **2022**, 156, 124111	3.9	
93	Multimeric structure enables the acceleration of KaiB-KaiC complex formation induced by ADP/ATP exchange inhibition.. *PLoS Computational Biology*, **2022**, 18, e1009243	5	
92	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	
91	Structural change of damaged polyethylene by beta-decay of substituted tritium using reactive force field. *Japanese Journal of Applied Physics*, **2021**, 60, SAAB06	1.4	2
90	Dynamical Behavior of Water; Fluctuation, Reactions and Phase Transitions. *Bulletin of the Chemical Society of Japan*, **2021**, 94, 2575-2601	5.1	
89	Effects of interfaces on structure and dynamics of water droplets on a graphene surface: A molecular dynamics study. *Journal of Chemical Physics*, **2021**, 154, 164704	3.9	2
88	Microscopic insights into dynamic disorder in the isomerization dynamics of the protein BPTI. *Journal of Chemical Physics*, **2021**, 154, 224113	3.9	1
87	Vectorial insertion of a helical peptide into membrane: a theoretical study on polytheonamide B. *Biophysical Journal*, **2021**, 120, 4786-4797	2.9	1
86	Tetrahedral structure of supercooled water at ambient pressure and its influence on dynamic relaxation: Comparative study of water models. *Journal of Molecular Liquids*, **2021**, 341, 117269	6	1
85	Inverse KohnSham Equations Derived from the Density Equation Theory. *Journal of the Physical Society of Japan*, **2020**, 89, 024301	1.5	0
84	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. *Chemical Reviews*, **2020**, 120, 7152-7218	68.1	87
83	An alternative interpretation of the slow KaiB-KaiC binding of the cyanobacterial clock proteins. *Scientific Reports*, **2020**, 10, 10439	4.9	3
82	Dissecting the Dynamics during Enzyme Catalysis: A Case Study of Pin1 Peptidyl-Prolyl Isomerase. *Journal of Chemical Theory and Computation*, **2020**, 16, 3396-3407	6.4	3
81	Tautomeric Effect of Histidine on Sheet Formation of Amyloid Beta 1-40: 2D-IR Simulations. *Biophysical Journal*, **2020**, 119, 831-842	2.9	5
80	Molecular Mechanism of Acceleration and Retardation of Collective Orientation Relaxation of Water Molecules in Aqueous Solutions. *Journal of Physical Chemistry B*, **2020**, 124, 11730-11737	3.4	1
79	Molecular dynamics study on DNA damage by tritium disintegration. *Japanese Journal of Applied Physics*, **2020**, 59, SAAE01	1.4	4

78	Theory of coherent two-dimensional vibrational spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 100901	3.9	20
77	Thermodynamic picture of vitrification of water through complex specific heat and entropy: A journey through "no man's land". *Journal of Chemical Physics*, **2019**, 150, 054502	3.9	22
76	Site-Dependent Fluctuations Optimize Electronic Energy Transfer in the Fenna-Matthews-Olson Protein. *Journal of Physical Chemistry B*, **2019**, 123, 9762-9772	3.4	19
75	Computational strategy for studying structural change of tritium-substituted macromolecules by a beta decay to helium-3. *Journal of Advanced Simulation in Science and Engineering*, **2019**, 6, 94-99	0.4	6
74	Structural Changes in Tritium-Substituted Polymeric Materials by Beta Decays: A Molecular Dynamics Study. *Plasma and Fusion Research*, **2019**, 14, 3401106-3401106	0.5	3
73	Vibrational Frequency Fluctuations of Ionic and Non-ionic Vibrational Probe Molecules in Aqueous Solutions. *Springer Series in Optical Sciences*, **2019**, 259-285	0.5	1
72	Conformational Excitation and Nonequilibrium Transition Facilitate Enzymatic Reactions: Application to Pin1 Peptidyl-Prolyl Isomerase. *Journal of Physical Chemistry Letters*, **2019**, 10, 474-480	6.4	5
71	Theoretical investigation on vibrational frequency fluctuations of SCN-derivatized vibrational probe molecule in water. *Chemical Physics*, **2018**, 512, 82-87	2.3	6
70	Structure and dynamics of solvent molecules inside the polytheonamide B channel in different environments: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2018**, 20, 3334-3348	3.6	6
69	Reconsideration of the relaxational and vibrational line shapes of liquid water based on ultrabroadband dielectric spectroscopy. *Physical Chemistry Chemical Physics*, **2018**, 20, 26200-26209	3.6	18
68	Crucial role of fragmented and isolated defects in persistent relaxation of deeply supercooled water. *Journal of Chemical Physics*, **2018**, 149, 124504	3.9	40
67	Vibrational frequency fluctuations of ionic vibrational probe in water: Theoretical study with molecular dynamics simulation. *Chemical Physics Letters*, **2017**, 683, 547-552	2.5	4
66	What We can Learn about Protein Folding from Ultra-long Molecular Dynamics Simulations. *Seibutsu Butsuri*, **2017**, 57, 030-032	0	
65	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. *Journal of Chemical Theory and Computation*, **2016**, 12, 4128-37	6.4	30
64	Molecular Mechanism Behind the Fast Folding/Unfolding Transitions of Villin Headpiece Subdomain: Hierarchy and Heterogeneity. *Journal of Physical Chemistry B*, **2016**, 120, 11683-11691	3.4	33
63	Ultrafast Dynamics of Liquid Water: Energy Relaxation and Transfer Processes of the OH Stretch and the HOH Bend. *Journal of Physical Chemistry B*, **2015**, 119, 11068-78	3.4	27
62	Circadian rhythms. Atomic-scale origins of slowness in the cyanobacterial circadian clock. *Science*, **2015**, 349, 312-6	33.3	76
61	Couplings between hierarchical conformational dynamics from multi-time correlation functions and two-dimensional lifetime spectra: Application to adenylate kinase. *Journal of Chemical Physics*, **2015** , 142, 212404	3.9	13

60	Dynamic heterogeneity in the folding/unfolding transitions of FiP35. *Journal of Chemical Physics*, **2015**, 142, 135101	3.9	17
59	Theoretical study on excited states of bacteriochlorophyll a in solutions with density functional assessment. *Journal of Physical Chemistry B*, **2014**, 118, 10906-18	3.4	29
58	Ultrafast dynamics of liquid water: frequency fluctuations of the OH stretch and the HOH bend. *Journal of Chemical Physics*, **2013**, 139, 044503	3.9	29
57	Molecular origin of the difference in the HOH bend of the IR spectra between liquid water and ice. *Journal of Chemical Physics*, **2013**, 138, 054506	3.9	37
56	Dynamic length scales in glass-forming liquids: an inhomogeneous molecular dynamics simulation approach. *Journal of Physical Chemistry B*, **2013**, 117, 13259-67	3.4	6
55	Frequency dependence of specific heat in supercooled liquid water and emergence of correlated dynamics. *Journal of Chemical Physics*, **2013**, 138, 094503	3.9	22
54	Fluctuations and relaxation dynamics of liquid water revealed by linear and nonlinear spectroscopy. *Annual Review of Physical Chemistry*, **2013**, 64, 55-75	15.7	37
53	Theoretical and experimental studies on vibrational energy relaxation of the CO stretching mode of acetone in alcohol solutions. *Journal of Physical Chemistry B*, **2013**, 117, 4723-31	3.4	4
52	Multiple length and time scales of dynamic heterogeneities in model glass-forming liquids: a systematic analysis of multi-point and multi-time correlations. *Journal of Chemical Physics*, **2013**, 138, 12A506	3.9	63
51	Mechanism of ion permeation through a model channel: roles of energetic and entropic contributions. *Journal of Chemical Physics*, **2013**, 139, 165106	3.9	7
50	Vibrational frequency fluctuation of ions in aqueous solutions studied by three-pulse infrared photon echo method. *Accounts of Chemical Research*, **2012**, 45, 1982-91	24.3	30
49	Temperature and hydration dependence of low-frequency spectra of poly-L-glutamic acid with different secondary structures studied by terahertz time-domain spectroscopy. *Soft Matter*, **2012**, 8, 1997-2006	3.6	15
48	Slow dynamics, dynamic heterogeneities, and fragility of supercooled liquids confined in random media. *Journal of Physics Condensed Matter*, **2011**, 23, 234123	1.8	35
47	Intermolecular vibrational mode of the benzoic acid dimer in solution observed by terahertz time-domain spectroscopy. *Physical Chemistry Chemical Physics*, **2011**, 13, 14742-9	3.6	11
46	Hidden slow time scale of correlated motions in supercooled liquids: Multi-time correlation function approach. *Journal of Non-Crystalline Solids*, **2011**, 357, 371-375	3.9	5
45	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. *Journal of Chemical Physics*, **2011**, 134, 184503	3.9	26
44	Direct Simulation of Excited-State Intramolecular Proton Transfer and Vibrational Coherence of 10-Hydroxybenzo[h]quinoline in Solution. *Journal of Physical Chemistry Letters*, **2011**, 2, 2366-2371	6.4	49
43	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. *Journal of Chemical Physics*, **2011**, 135, 244503	3.9	54

42	Energy relaxation of intermolecular motions in supercooled water and ice: a molecular dynamics study. *Journal of Chemical Physics*, **2011**, 135, 244511	3.9	13
41	Temperature dependence of vibrational frequency fluctuation of N(3) (-) in D(2)O. *Journal of Chemical Physics*, **2010**, 133, 014505	3.9	23
40	Relation between the conformational heterogeneity and reaction cycle of Ras: molecular simulation of Ras. *Biophysical Journal*, **2010**, 99, 3726-34	2.9	25
39	Effects of nonadditive interactions on ion solvation at the water/vapor interface: a molecular dynamics study. *Journal of Physical Chemistry A*, **2010**, 114, 12573-84	2.8	25
38	Multi-time density correlation functions in glass-forming liquids: Probing dynamical heterogeneity and its lifetime. *Journal of Chemical Physics*, **2010**, 133, 044511	3.9	41
37	Role of the Lifetime of Dynamical Heterogeneity in the Frequency-Dependent Stokes□Einstein Relation of Supercooled Liquids. *Journal of the Physical Society of Japan*, **2010**, 79, 093601	1.5	16
36	Molecular dynamics studies of slow dynamics in random media: Type A-B and reentrant transitions. *European Physical Journal: Special Topics*, **2010**, 189, 135-139	2.3	19
35	Multiple time scales hidden in heterogeneous dynamics of glass-forming liquids. *Physical Review E*, **2009**, 79, 060501	2.4	28
34	Anisotropic cooperative structural rearrangements in sheared supercooled liquids. *Physical Review Letters*, **2009**, 102, 016001	7.4	70
33	Slow dynamics in random media: Crossover from glass to localization transition. *Europhysics Letters*, **2009**, 88, 36002	1.6	61
32	Ultrafast energy relaxation and anisotropy decay of the librational motion in liquid water: A molecular dynamics study. *Journal of Chemical Physics*, **2009**, 131, 164511	3.9	35
31	Molecular dynamics simulation of nonlinear spectroscopies of intermolecular motions in liquid water. *Accounts of Chemical Research*, **2009**, 42, 1250-8	24.3	48
30	Ultrafast intermolecular dynamics of liquid water: a theoretical study on two-dimensional infrared spectroscopy. *Journal of Chemical Physics*, **2008**, 128, 154521	3.9	53
29	Proton transfer and associated molecular rearrangements in the photocycle of photoactive yellow protein: role of water molecular migration on the proton transfer reaction. *Journal of Physical Chemistry B*, **2007**, 111, 2948-56	3.4	18
28	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. *Journal of Chemical Physics*, **2006**, 125, 084506	3.9	30
27	Mechanism of ion permeation in a model channel: Free energy surface and dynamics of K+ ion transport in an anion-doped carbon nanotube. *Journal of Physical Chemistry B*, **2006**, 110, 20671-7	3.4	26
26	Origin of slow relaxation in liquid-water dynamics: A possible scenario for the presence of bottleneck in phase space. *Europhysics Letters*, **2006**, 73, 826-832	1.6	9
25	Isotope dilution effects on the hydroxyl-stretch bands of alcohols. *Molecular Physics*, **2005**, 103, 37-44	1.7	11

24	A theoretical study on anomalous temperature dependence of pKw of water. *Journal of Chemical Physics*, **2005**, 122, 144504	3.9	44
23	Slow Relaxation in Hamiltonian Systems with Internal Degrees of Freedom. *Advances in Chemical Physics*, **2005**, 373-421		
22	Probing the Spectral Diffusion of Vibrational Transitions of OCN- and SCN- in Methanol by Three-Pulse Infrared Photon Echo Spectroscopy. *Journal of Physical Chemistry A*, **2003**, 107, 5643-5649	2.8	40
21	Off-resonant two-dimensional fifth-order Raman spectroscopy of liquid CS2: Detection of anharmonic dynamics. *Journal of Chemical Physics*, **2003**, 119, 9073-9087	3.9	58
20	Terahertz Radiation Spectroscopy on Chloroform Confined in Porous Silica Glasses. *Materials Research Society Symposia Proceedings*, **2003**, 790, 1		
19	Heterodyne detected fifth-order nonresonant Raman spectroscopy of CS2: Evidence for anharmonic coupling. *Springer Series in Chemical Physics*, **2003**, 554-556	0.3	2
18	Molecular dynamics simulation of the ice nucleation and growth process leading to water freezing. *Nature*, **2002**, 416, 409-13	50.4	649
17	A theoretical study on decomposition of formic acid in sub- and supercritical water. *Journal of Chemical Physics*, **2002**, 117, 7631-7639	3.9	29
16	Off-resonant fifth-order response function for two-dimensional Raman spectroscopy of liquids CS2 and H2O. *Physical Review Letters*, **2002**, 88, 207401	7.4	104
15	Mechanism of proton transfer in ice. II. Hydration, modes, and transport. *Journal of Chemical Physics* , **2001**, 115, 4742-4749	3.9	34
14	Mechanism of fast proton transfer in ice: Potential energy surface and reaction coordinate analyses. *Journal of Chemical Physics*, **2000**, 113, 9090-9100	3.9	60
13	Water Dynamics: Fluctuation, Relaxation, and Chemical Reactions in Hydrogen Bond Network Rearrangement. *Accounts of Chemical Research*, **1999**, 32, 741-749	24.3	229
12	Global potential energy surfaces of water clusters; reaction coordinate and annealing analyses. *Journal of Molecular Liquids*, **1998**, 77, 95-103	6	9
11	Off-resonant fifth-order nonlinear response of water and CS2: Analysis based on normal modes. *Journal of Chemical Physics*, **1998**, 108, 240-251	3.9	145
10	Fluctuation, relaxation and rearrangement dynamics of a model (H2O)20 cluster: Non-statistical dynamical behavior. *Journal of Chemical Physics*, **1997**, 106, 3329-3337	3.9	18
9	Third order nonlinear response of liquid water. *Journal of Chemical Physics*, **1997**, 106, 4889-4893	3.9	58
8	Dynamics of proton attachment to water cluster: Proton transfer, evaporation, and relaxation. *Journal of Chemical Physics*, **1996**, 105, 6358-6366	3.9	37
7	Translational and orientational dynamics of a water cluster (H2O)108 and liquid water: Analysis of neutron scattering and depolarized light scattering. *Journal of Chemical Physics*, **1995**, 102, 3566-3579	3.9	56

6	Dynamics and relaxation of an intermediate size water cluster (H2O)108. *Journal of Chemical Physics*, **1994**, 101, 6063-6075	3.9	33
5	Instantaneous normal mode analysis of liquid water. *Journal of Chemical Physics*, **1994**, 100, 6672-6683	3.9	315
4	Excited and ionized states of RuO4 and OsO4 studied by SAC and SAC-CI theories. *International Journal of Quantum Chemistry*, **1991**, 39, 93-113	2.1	26
3	Theoretical study for the excited states of MoO_4^{2-} and MoS_4^{2-} (n=0~4) and $MoSe_4^{2-}$. *Journal of Chemical Physics*, **1990**, 93, 1865-1875	3.9	23
2	Electronic origin of molybdenum-95 NMR chemical shifts in molybdenum complexes. Relationship between excitation energy and chemical shift. *Inorganic Chemistry*, **1990**, 29, 3095-3097	5.1	21
1	Sufficiency of unidirectional allostery in KaiC in generating the cyanobacterial circadian rhythm		1