Shinji Saito

List of Publications by Year
in descending order

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95	4,092	117625	118850
papers	citations	34 h-index	62 g-index

104	104	104	3563
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular dynamics simulation of the ice nucleation and growth process leading to water freezing. Nature, 2002, 416, 409-413.	27.8	772
2	Instantaneous normal mode analysis of liquid water. Journal of Chemical Physics, 1994, 100, 6672-6683.	3.0	350
3	Water Dynamics:â€‰ Fluctuation, Relaxation, and Chemical Reactions in Hydrogen Bond Network Rearrangement. Accounts of Chemical Research, 1999, 32, 741-749.	15.6	259
4	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
5	Off-resonant fifth-order nonlinear response of water and CS2: Analysis based on normal modes. Journal of Chemical Physics, 1998, 108, 240-251.	3.0	155
6	Off-Resonant Fifth-Order Response Function for Two-Dimensional Raman Spectroscopy of LiquidsCS2andH2O. Physical Review Letters, 2002, 88, 207401.	7.8	107
7	Atomic-scale origins of slowness in the cyanobacterial circadian clock. Science, 2015, 349, 312-316.	12.6	103
8	Anisotropic Cooperative Structural Rearrangements in Sheared Supercooled Liquids. Physical Review Letters, 2009, 102, 016001.	7.8	76
9	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.	3.0	76
10	Mechanism of fast proton transfer in ice: Potential energy surface and reaction coordinate analyses. Journal of Chemical Physics, 2000, 113, 9090-9100.	3.0	65
11	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.	3.0	63
12	Slow dynamics in random media: Crossover from glass to localization transition. Europhysics Letters, 2009, 88, 36002.	2.0	62
13	Translational and orientational dynamics of a water cluster (H2O)108and liquid water: Analysis of neutron scattering and depolarized light scattering. Journal of Chemical Physics, 1995, 102, 3566-3579.	3.0	60
14	Off-resonant two-dimensional fifth-order Raman spectroscopy of liquid CS2: Detection of anharmonic dynamics. Journal of Chemical Physics, 2003, 119, 9073-9087.	3.0	60
15	Third order nonlinear response of liquid water. Journal of Chemical Physics, 1997, 106, 4889-4893.	3.0	59
16	Ultrafast intermolecular dynamics of liquid water: A theoretical study on two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2008, 128, 154521.	3.0	58
17	Molecular Dynamics Simulation of Nonlinear Spectroscopies of Intermolecular Motions in Liquid Water. Accounts of Chemical Research, 2009, 42, 1250-1258.	15.6	56
18	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.	4.6	56

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19	A theoretical study on anomalous temperature dependence of pKw of water. Journal of Chemical Physics, 2005, 122, 144504.	3.0	54
20	Multi-time density correlation functions in glass-forming liquids: Probing dynamical heterogeneity and its lifetime. Journal of Chemical Physics, 2010, 133, 044511.	3.0	46
21	Crucial role of fragmented and isolated defects in persistent relaxation of deeply supercooled water. Journal of Chemical Physics, 2018, 149, 124504.	3.0	46
22	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.	3.0	43
23	Theoretical Study on Excited States of Bacteriochlorophyll a in Solutions with Density Functional Assessment. Journal of Physical Chemistry B, 2014, 118, 10906-10918.	2.6	42
24	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.	2.5	40
25	Theory of coherent two-dimensional vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 100901.	3.0	40
26	Slow dynamics, dynamic heterogeneities, and fragility of supercooled liquids confined in random media. Journal of Physics Condensed Matter, 2011, 23, 234123.	1.8	39
27	Fluctuations and Relaxation Dynamics of Liquid Water Revealed by Linear and Nonlinear Spectroscopy. Annual Review of Physical Chemistry, 2013, 64, 55-75.	10.8	39
28	Dynamics of proton attachment to water cluster: Proton transfer, evaporation, and relaxation. Journal of Chemical Physics, 1996, 105, 6358-6366.	3.0	38
29	Dynamics and relaxation of an intermediate size water cluster (H2O)108. Journal of Chemical Physics, 1994, 101, 6063-6075.	3.0	37
30	Ultrafast energy relaxation and anisotropy decay of the librational motion in liquid water: A molecular dynamics study. Journal of Chemical Physics, 2009, 131, 164511.	3.0	37
31	A theoretical study on decomposition of formic acid in sub- and supercritical water. Journal of Chemical Physics, 2002, 117, 7631-7639.	3.0	36
32	Quantitative Evaluation of Site Energies and Their Fluctuations of Pigments in the Fennaâ€“Matthewsâ€“Olson Complex with an Efficient Method for Generating a Potential Energy Surface. Journal of Chemical Theory and Computation, 2016, 12, 4128-4137.	5.3	36
33	Molecular Mechanism Behind the Fast Folding/Unfolding Transitions of Villin Headpiece Subdomain: Hierarchy and Heterogeneity. Journal of Physical Chemistry B, 2016, 120, 11683-11691.	2.6	36
34	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, 11068-11078.	2.6	35
35	Mechanism of proton transfer in ice. II. Hydration, modes, and transport. Journal of Chemical Physics, 2001, 115, 4742-4749.	3.0	34
36	Relation between the Conformational Heterogeneity and Reaction Cycle of Ras: Molecular Simulation of Ras. Biophysical Journal, 2010, 99, 3726-3734.	0.5	33

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37	Vibrational Frequency Fluctuation of Ions in Aqueous Solutions Studied by Three-Pulse Infrared Photon Echo Method. Accounts of Chemical Research, 2012, 45, 1982-1991.	15.6	33
38	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.	3.0	31
39	Ultrafast dynamics of liquid water: Frequency fluctuations of the OH stretch and the HOH bend. Journal of Chemical Physics, 2013, 139, 044503.	3.0	30
40	Multiple time scales hidden in heterogeneous dynamics of glass-forming liquids. Physical Review E, 2009, 79, 060501.	2.1	29
41	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.	3.0	29
42	Effects of Nonadditive Interactions on Ion Solvation at the Water/Vapor Interface: A Molecular Dynamics Study. Journal of Physical Chemistry A, 2010, 114, 12573-12584.	2.5	28
43	Reconsideration of the relaxational and vibrational line shapes of liquid water based on ultrabroadband dielectric spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 26200-26209.	2.8	28
44	Mechanism of Ion Permeation in a Model Channel:Â Free Energy Surface and Dynamics of K+Ion Transport in an Anion-Doped Carbon Nanotube. Journal of Physical Chemistry B, 2006, 110, 20671-20677.	2.6	27
45	Electronic origin of molybdenum-95 NMR chemical shifts in molybdenum complexes. Relationship between excitation energy and chemical shift. Inorganic Chemistry, 1990, 29, 3095-3097.	4.0	26
46	Excited and ionized states of RuO4 and OsO4 studied bySAC andSAC-CI theories. International Journal of Quantum Chemistry, 1991, 39, 93-113.	2.0	26
47	Site-Dependent Fluctuations Optimize Electronic Energy Transfer in the Fennaâ€“Matthewsâ€“Olson Protein. Journal of Physical Chemistry B, 2019, 123, 9762-9772.	2.6	25
48	Temperature dependence of vibrational frequency fluctuation of N3â^' in D2O. Journal of Chemical Physics, 2010, 133, 014505.	3.0	24
49	Thermodynamic picture of vitrification of water through complex specific heat and entropy: A journey through â€œno manâ€™s landâ€. Journal of Chemical Physics, 2019, 150, 054502.	3.0	24
50	Theoretical study for the excited states of MoO4â^'nS2â^'n(n=0â^¼4) and MoSe2â^'4. Journal of Chemical Physics, 1990, 93, 1865-1875.	3.0	23
51	Frequency dependence of specific heat in supercooled liquid water and emergence of correlated dynamics. Journal of Chemical Physics, 2013, 138, 094503.	3.0	22
52	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.	2.7	20
53	Dynamic heterogeneity in the folding/unfolding transitions of FiP35. Journal of Chemical Physics, 2015, 142, 135101.	3.0	20
54	Fluctuation, relaxation and rearrangement dynamics of a model (H2O)20 cluster: Non-statistical dynamical behavior. Journal of Chemical Physics, 1997, 106, 3329-3337.	3.0	19

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55	Proton Transfer and Associated Molecular Rearrangements in the Photocycle of Photoactive Yellow Protein:Â Role of Water Molecular Migration on the Proton Transfer Reaction. Journal of Physical Chemistry B, 2007, 111, 2948-2956.	2.6	19
56	Molecular dynamics studies of slow dynamics in random media: Type A-B and reentrant transitions. European Physical Journal: Special Topics, 2010, 189, 135-139.	2.6	19
57	Role of the Lifetime of Dynamical Heterogeneity in the Frequency-Dependent Stokesâ€“Einstein Relation of Supercooled Liquids. Journal of the Physical Society of Japan, 2010, 79, 093601.	1.6	17
58	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.	3.0	17
59	Energy relaxation of intermolecular motions in supercooled water and ice: A molecular dynamics study. Journal of Chemical Physics, 2011, 135, 244511.	3.0	14
60	Isotope dilution effects on the hydroxyl-stretch bands of alcohols. Molecular Physics, 2005, 103, 37-44.	1.7	13
61	Intermolecular vibrational mode of the benzoic acid dimer in solution observed by terahertz time-domain spectroscopy. Physical Chemistry Chemical Physics, 2011, 13, 14742.	2.8	12
62	Global potential energy surfaces of water clusters; reaction coordinate and annealing analyses. Journal of Molecular Liquids, 1998, 77, 95-103.	4.9	9
63	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.	2.0	9
64	Mechanism of ion permeation through a model channel: Roles of energetic and entropic contributions. Journal of Chemical Physics, 2013, 139, 165106.	3.0	9
65	Tautomeric Effect of Histidine on Î²-Sheet Formation of Amyloid Beta 1â€“40: 2D-IR Simulations. Biophysical Journal, 2020, 119, 831-842.	0.5	9
66	Conformational Excitation and Nonequilibrium Transition Facilitate Enzymatic Reactions: Application to Pin1 Peptidylâ€“Prolyl Isomerase. Journal of Physical Chemistry Letters, 2019, 10, 474-480.	4.6	8
67	Dissecting the Dynamics during Enzyme Catalysis: A Case Study of Pin1 Peptidyl-Prolyl Isomerase. Journal of Chemical Theory and Computation, 2020, 16, 3396-3407.	5.3	8
68	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.	3.0	8
69	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.	0.2	8
70	Dynamic Length Scales in Glass-Forming Liquids: An Inhomogeneous Molecular Dynamics Simulation Approach. Journal of Physical Chemistry B, 2013, 117, 13259-13267.	2.6	7
71	Molecular dynamics study on DNA damage by tritium disintegration. Japanese Journal of Applied Physics, 2020, 59, SAAE01.	1.5	7
72	Theoretical investigation on vibrational frequency fluctuations of SCN-derivatized vibrational probe molecule in water. Chemical Physics, 2018, 512, 82-87.	1.9	6

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73	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.	2.8	6
74	Hidden slow time scale of correlated motions in supercooled liquids: Multi-time correlation function approach. Journal of Non-Crystalline Solids, 2011, 357, 371-375.	3.1	5
75	An alternative interpretation of the slow KaiB-KaiC binding of the cyanobacterial clock proteins. Scientific Reports, 2020, 10, 10439.	3.3	5
76	Structural Changes in Tritium-Substituted Polymeric Materials by Beta Decays: A Molecular Dynamics Study. Plasma and Fusion Research, 2019, 14, 3401106-3401106.	0.7	5
77	Regulation mechanisms of the dual ATPase in KaiC. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2119627119.	7.1	5
78	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, 4723-4731.	2.6	4
79	Vibrational frequency fluctuations of ionic vibrational probe in water: Theoretical study with molecular dynamics simulation. Chemical Physics Letters, 2017, 683, 547-552.	2.6	4
80	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.	4.9	4
81	Structural change of damaged polyethylene by beta-decay of substituted tritium using reactive force field. Japanese Journal of Applied Physics, 2021, 60, SAAB06.	1.5	4
82	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.	2.6	3
83	Molecular Insights into the Intrinsic Dynamics and Their Roles During Catalysis in Pin1 Peptidyl-prolyl Isomerase. Journal of Physical Chemistry B, 2022, 126, 5185-5193.	2.6	3
84	Microscopic insights into dynamic disorder in the isomerization dynamics of the protein BPTI. Journal of Chemical Physics, 2021, 154, 224113.	3.0	2
85	Heterodyne detected fifth-order nonresonant Raman spectroscopy of CS2: Evidence for anharmonic coupling. Springer Series in Chemical Physics, 2003, , 554-556.	0.2	2
86	Dynamical Behavior of Water; Fluctuation, Reactions and Phase Transitions. Bulletin of the Chemical Society of Japan, 2021, 94, 2575-2601.	3.2	2
87	Excited states of chlorophyll a and b in solution by time-dependent density functional theory. Journal of Chemical Physics, 2022, 156, 124111.	3.0	2
88	Inverse Kohnâ€“Sham Equations Derived from the Density Equation Theory. Journal of the Physical Society of Japan, 2020, 89, 024301.	1.6	1
89	Vectorial insertion of a Î²-helical peptide into membrane: a theoretical study on polytheonamide B. Biophysical Journal, 2021, 120, 4786-4797.	0.5	1
90	Vibrational Frequency Fluctuations of Ionic and Non-ionic Vibrational Probe Molecules in Aqueous Solutions. Springer Series in Optical Sciences, 2019, , 259-285.	0.7	1

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91	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.	3.0	1
92	Terahertz Radiation Spectroscopy on Chloroform Confined in Porous Silica Glasses. Materials Research Society Symposia Proceedings, 2003, 790, 1.	0.1	0
93	Slow Relaxation in Hamiltonian Systems with Internal Degrees of Freedom. Advances in Chemical Physics, 2005, , 373-421.	0.3	0
94	What We can Learn about Protein Folding from Ultra-long Molecular Dynamics Simulations. Seibutsu Butsuri, 2017, 57, 030-032.	0.1	0
95	Multimeric structure enables the acceleration of KaiB-KaiC complex formation induced by ADP/ATP exchange inhibition. PLoS Computational Biology, 2022, 18, e1009243.	3.2	0