# 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | Microscopic insights into dynamic disorder in the isomerization dynamics of the protein BPTI. Journal of Chemical Physics, 2021, 154, 224113. | 3.0 | 2 |
| 8 | Vectorial insertion of a Î²-helical peptide into membrane: a theoretical study on polytheonamide B. Biophysical Journal, 2021, 120, 4786-4797. | 0.5 | 1 |
| 9 | 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 |
| 10 | 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 |
| 11 | Dynamical Behavior of Water; Fluctuation, Reactions and Phase Transitions. Bulletin of the Chemical Society of Japan, 2021, 94, 2575-2601. | 3.2 | 2 |
| 12 | Molecular dynamics study on DNA damage by tritium disintegration. Japanese Journal of Applied Physics, 2020, 59, SAAE01. | 1.5 | 7 |
| 13 | 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 |
| 14 | 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 |
| 15 | Inverse Kohnâ€“Sham Equations Derived from the Density Equation Theory. Journal of the Physical Society of Japan, 2020, 89, 024301. | 1.6 | 1 |
| 16 | Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218. | 47.7 | 205 |
| 17 | An alternative interpretation of the slow KaiB-KaiC binding of the cyanobacterial clock proteins. Scientific Reports, 2020, 10, 10439. | 3.3 | 5 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | Theory of coherent two-dimensional vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 100901. | 3.0 | 40 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | Theoretical investigation on vibrational frequency fluctuations of SCN-derivatized vibrational probe molecule in water. Chemical Physics, 2018, 512, 82-87. | 1.9 | 6 |
| 27 | 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 |
| 28 | 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 |
| 29 | Crucial role of fragmented and isolated defects in persistent relaxation of deeply supercooled water. Journal of Chemical Physics, 2018, 149, 124504. | 3.0 | 46 |
| 30 | 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 |
| 31 | What We can Learn about Protein Folding from Ultra-long Molecular Dynamics Simulations. Seibutsu Butsuri, 2017, 57, 030-032. | 0.1 | 0 |
| 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 | Atomic-scale origins of slowness in the cyanobacterial circadian clock. Science, 2015, 349, 312-316. | 12.6 | 103 |
| 36 | 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 |

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| 37 | Dynamic heterogeneity in the folding/unfolding transitions of FiP35. Journal of Chemical Physics, 2015, 142, 135101. | 3.0 | 20 |
| 38 | 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 |
| 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 | 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 |
| 41 | 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 |
| 42 | Frequency dependence of specific heat in supercooled liquid water and emergence of correlated dynamics. Journal of Chemical Physics, 2013, 138, 094503. | 3.0 | 22 |
| 43 | 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 |
| 44 | 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 |
| 45 | 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 |
| 46 | Mechanism of ion permeation through a model channel: Roles of energetic and entropic contributions. Journal of Chemical Physics, 2013, 139, 165106. | 3.0 | 9 |
| 47 | 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 |
| 48 | 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 |
| 49 | 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 |
| 50 | Slow dynamics, dynamic heterogeneities, and fragility of supercooled liquids confined in random media. Journal of Physics Condensed Matter, 2011, 23, 234123. | 1.8 | 39 |
| 51 | 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 |
| 52 | 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 |
| 53 | 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 |
| 54 | 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 |

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| 55 | Energy relaxation of intermolecular motions in supercooled water and ice: A molecular dynamics study. Journal of Chemical Physics, 2011, 135, 244511. | 3.0 | 14 |
| 56 | 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 |
| 57 | 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 |
| 58 | Temperature dependence of vibrational frequency fluctuation of N3â^' in D2O. Journal of Chemical Physics, 2010, 133, 014505. | 3.0 | 24 |
| 59 | Relation between the Conformational Heterogeneity and Reaction Cycle of Ras: Molecular Simulation of Ras. Biophysical Journal, 2010, 99, 3726-3734. | 0.5 | 33 |
| 60 | 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 |
| 61 | 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 |
| 62 | Multiple time scales hidden in heterogeneous dynamics of glass-forming liquids. Physical Review E, 2009, 79, 060501. | 2.1 | 29 |
| 63 | Anisotropic Cooperative Structural Rearrangements in Sheared Supercooled Liquids. Physical Review Letters, 2009, 102, 016001. | 7.8 | 76 |
| 64 | Slow dynamics in random media: Crossover from glass to localization transition. Europhysics Letters, 2009, 88, 36002. | 2.0 | 62 |
| 65 | 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 |
| 66 | Molecular Dynamics Simulation of Nonlinear Spectroscopies of Intermolecular Motions in Liquid Water. Accounts of Chemical Research, 2009, 42, 1250-1258. | 15.6 | 56 |
| 67 | Ultrafast intermolecular dynamics of liquid water: A theoretical study on two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2008, 128, 154521. | 3.0 | 58 |
| 68 | 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 |
| 69 | 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 |
| 70 | 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 |
| 71 | 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 |
| 72 | Slow Relaxation in Hamiltonian Systems with Internal Degrees of Freedom. Advances in Chemical Physics, 2005, , 373-421. | 0.3 | 0 |

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| 73 | Isotope dilution effects on the hydroxyl-stretch bands of alcohols. Molecular Physics, 2005, 103, 37-44. | 1.7 | 13 |
| 74 | A theoretical study on anomalous temperature dependence of pKw of water. Journal of Chemical Physics, 2005, 122, 144504. | 3.0 | 54 |
| 75 | 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 |
| 76 | 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 |
| 77 | Terahertz Radiation Spectroscopy on Chloroform Confined in Porous Silica Glasses. Materials Research Society Symposia Proceedings, 2003, 790, 1. | 0.1 | 0 |
| 78 | Heterodyne detected fifth-order nonresonant Raman spectroscopy of CS2: Evidence for anharmonic coupling. Springer Series in Chemical Physics, 2003, , 554-556. | 0.2 | 2 |
| 79 | A theoretical study on decomposition of formic acid in sub- and supercritical water. Journal of Chemical Physics, 2002, 117, 7631-7639. | 3.0 | 36 |
| 80 | Off-Resonant Fifth-Order Response Function for Two-Dimensional Raman Spectroscopy of LiquidsCS2andH2O. Physical Review Letters, 2002, 88, 207401. | 7.8 | 107 |
| 81 | Molecular dynamics simulation of the ice nucleation and growth process leading to water freezing. Nature, 2002, 416, 409-413. | 27.8 | 772 |
| 82 | Mechanism of proton transfer in ice. II. Hydration, modes, and transport. Journal of Chemical Physics, 2001, 115, 4742-4749. | 3.0 | 34 |
| 83 | 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 |
| 84 | Water Dynamics:â€‰ Fluctuation, Relaxation, and Chemical Reactions in Hydrogen Bond Network Rearrangement. Accounts of Chemical Research, 1999, 32, 741-749. | 15.6 | 259 |
| 85 | Global potential energy surfaces of water clusters; reaction coordinate and annealing analyses. Journal of Molecular Liquids, 1998, 77, 95-103. | 4.9 | 9 |
| 86 | 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 |
| 87 | 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 |
| 88 | Third order nonlinear response of liquid water. Journal of Chemical Physics, 1997, 106, 4889-4893. | 3.0 | 59 |
| 89 | Dynamics of proton attachment to water cluster: Proton transfer, evaporation, and relaxation. Journal of Chemical Physics, 1996, 105, 6358-6366. | 3.0 | 38 |
| 90 | 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 |

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| 91 | Dynamics and relaxation of an intermediate size water cluster (H2O)108. Journal of Chemical Physics, 1994, 101, 6063-6075. | 3.0 | 37 |
| 92 | Instantaneous normal mode analysis of liquid water. Journal of Chemical Physics, 1994, 100, 6672-6683. | 3.0 | 350 |
| 93 | 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 |
| 94 | 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 |
| 95 | 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 |