

Akihiro Morita

List of Publications by Year in descending order

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110
papers

4,613
citations

81900

39
h-index

106344

65
g-index

114
all docs

114
docs citations

114
times ranked

2773
citing authors

#	ARTICLE	IF	CITATIONS
1	A theoretical analysis of the sum frequency generation spectrum of the water surface. <i>Chemical Physics</i> , 2000, 258, 371-390.	1.9	340
2	A Theoretical Analysis of the Sum Frequency Generation Spectrum of the Water Surface. II. Time-Dependent Approach. <i>Journal of Physical Chemistry B</i> , 2002, 106, 673-685.	2.6	251
3	Unified Molecular View of the Air/Water Interface Based on Experimental and Theoretical $\ddot{\Gamma}^{\langle 2 \rangle}$ Spectra of an Isotopically Diluted Water Surface. <i>Journal of the American Chemical Society</i> , 2011, 133, 16875-16880.	13.7	245
4	Ab Initio Molecular Orbital Theory on Intramolecular Charge Polarization: Effect of Hydrogen Abstraction on the Charge Sensitivity of Aromatic and Nonaromatic Species. <i>Journal of the American Chemical Society</i> , 1997, 119, 4021-4032.	13.7	152
5	Molecular Dynamics Study of Gas-Liquid Aqueous Sodium Halide Interfaces. I. Flexible and Polarizable Molecular Modeling and Interfacial Properties. <i>Journal of Physical Chemistry C</i> , 2007, 111, 721-737.	3.1	150
6	Theoretical Studies of Structures and Vibrational Sum Frequency Generation Spectra at Aqueous Interfaces. <i>Chemical Reviews</i> , 2014, 114, 8447-8470.	47.7	132
7	Experimental and theoretical evidence for bilayer-by-bilayer surface melting of crystalline ice. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 227-232.	7.1	131
8	Recent progress in theoretical analysis of vibrational sum frequency generation spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5801.	2.8	121
9	Analysis of anisotropic local field in sum frequency generation spectroscopy with the charge response kernel water model. <i>Journal of Chemical Physics</i> , 2009, 131, 244714.	3.0	121
10	Vibrational relaxation of azide ion in water: The role of intramolecular charge fluctuation and solvent-induced vibrational coupling. <i>Journal of Chemical Physics</i> , 1998, 109, 5511-5523.	3.0	113
11	Solute-solvent interaction in nonpolar supercritical fluid: a clustering model and size distribution. <i>The Journal of Physical Chemistry</i> , 1990, 94, 6420-6425.	2.9	84
12	Molecular Dynamics Study of Gas-Liquid Aqueous Sodium Halide Interfaces. II. Analysis of Vibrational Sum Frequency Generation Spectra. <i>Journal of Physical Chemistry C</i> , 2007, 111, 738-748.	3.1	83
13	Vibrational Spectroscopic Response of Intermolecular Orientational Correlation at the Water Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16299-16302.	3.1	82
14	Molecular dynamics simulation with the charge response kernel: Diffusion dynamics of pyrazine and pyrazinyl radical in methanol. <i>Journal of Chemical Physics</i> , 1998, 108, 6809-6818.	3.0	81
15	Theory of Sum Frequency Generation Spectroscopy. <i>Lecture Notes in Quantum Chemistry II</i> , 2018, , .	0.3	81
16	Mass Accommodation Coefficient of Water: Molecular Dynamics Simulation and Revised Analysis of Droplet Train/Flow Reactor Experiment. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9111-9120.	2.6	79
17	An ab initio analysis of medium perturbation on molecular polarizabilities. <i>Journal of Chemical Physics</i> , 1999, 110, 11987-11998.	3.0	76
18	Improved Computation of Sum Frequency Generation Spectrum of the Surface of Water. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3158-3163.	2.6	74

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19	Effects of third-order susceptibility in sum frequency generation spectra: a molecular dynamics study in liquid water. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3040-3053.	2.8	74
20	Water polarizability in condensed phase: Ab initio evaluation by cluster approach. <i>Journal of Computational Chemistry</i> , 2002, 23, 1466-1471.	3.3	73
21	Bulk Contributions Modulate the Sum-Frequency Generation Spectra of Water on Model Sea-Spray Aerosols. <i>CheM</i> , 2018, 4, 1629-1644.	11.7	69
22	Hydrogen-Bonding Structure at Zwitterionic Lipid/Water Interface. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 216-220.	4.6	65
23	Origin of the Overpotential for the Oxygen Evolution Reaction on a Well-Defined Graphene Electrode Probed by in Situ Sum Frequency Generation Vibrational Spectroscopy. <i>Journal of the American Chemical Society</i> , 2018, 140, 15568-15571.	13.7	64
24	Molecular Dynamics Analysis of Interfacial Structures and Sum Frequency Generation Spectra of Aqueous Hydrogen Halide Solutions. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9277-9285.	2.5	62
25	Microscopic Barrier Mechanism of Ion Transport through Liquid-Liquid Interface. <i>Journal of the American Chemical Society</i> , 2015, 137, 8022-8025.	13.7	56
26	The Charge Response Kernel with Modified Electrostatic Potential Charge Model. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3909-3916.	2.5	54
27	Effect of solvent fluctuation on the electronic transitions of formaldehyde in aqueous solution. <i>Journal of Chemical Physics</i> , 1999, 110, 3484-3492.	3.0	53
28	Bend Vibration of Surface Water Investigated by Heterodyne-Detected Sum Frequency Generation and Theoretical Study: Dominant Role of Quadrupole. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2597-2601.	4.6	53
29	Origin of Vibrational Spectroscopic Response at Ice Surface. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3001-3006.	4.6	52
30	Molecular dynamics simulation of liquid methanol. I. Molecular modeling including C-H vibration and fermi resonance. <i>Journal of Chemical Physics</i> , 2011, 134, 024509.	3.0	51
31	Molecular Dynamics Simulation of Sum Frequency Generation Spectra of Aqueous Sulfuric Acid Solution. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13704-13716.	3.1	47
32	Uptake of the HO ₂ radical by water: Molecular dynamics calculations and their implications for atmospheric modeling. <i>Journal of Geophysical Research</i> , 2004, 109, .	3.3	46
33	Efficient Spectral Diffusion at the Air/Water Interface Revealed by Femtosecond Time-Resolved Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1811-1815.	4.6	45
34	Mechanisms of Sum Frequency Generation from Liquid Benzene: Symmetry Breaking at Interface and Bulk Contribution. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13169-13182.	3.1	43
35	Real-Time Observation of the Destruction of Hydration Shells under Electrochemical Force. <i>Journal of the American Chemical Society</i> , 2013, 135, 15033-15039.	13.7	43
36	Molecular dynamics simulation of liquid methanol. II. Unified assignment of infrared, raman, and sum frequency generation vibrational spectra in methyl C-H stretching region. <i>Journal of Chemical Physics</i> , 2011, 134, 024510.	3.0	42

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37	Toward computation of bulk quadrupolar signals in vibrational sum frequency generation spectroscopy. <i>Chemical Physics Letters</i> , 2004, 398, 361-366.	2.6	40
38	Extended treatment of charge response kernel comprising the density functional theory and charge regulation procedures. <i>Journal of Chemical Physics</i> , 2006, 125, 074112.	3.0	40
39	Unveiling subsurface hydrogen-bond structure of hexagonal water ice. <i>Physical Review B</i> , 2017, 96, .	3.2	40
40	Energetic Origin of Proton Affinity to the Air/Water Interface. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4745-4751.	2.6	39
41	Theory of Quadrupole Contributions from Interface and Bulk in Second-Order Optical Processes. <i>Bulletin of the Chemical Society of Japan</i> , 2012, 85, 1061-1076.	3.2	39
42	RISM-SCF study of the free-energy profile of the Menshutkin-type reaction $\text{NH}_3 + \text{CH}_3\text{Cl} \rightarrow \text{NH}_3\text{CH}_3 + \text{Cl}^-$ in aqueous solution. <i>Theoretical Chemistry Accounts</i> , 1999, 102, 165-169.	1.4	38
43	Surface Structure of Methanol/Water Solutions via Sum Frequency Orientational Analysis and Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9879-9889.	3.1	38
44	Metamaterials-Enhanced Infrared Spectroscopic Study of Nanoconfined Molecules by Plasmonics in Nanofluidics Hybrid Device. <i>ACS Photonics</i> , 2018, 5, 3179-3188.	6.6	35
45	Structure at the air/water interface in the presence of phenol: a study using heterodyne-detected vibrational sum frequency generation and molecular dynamics simulation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3002-3009.	2.8	34
46	Electrolyte and Temperature Effects on Third-Order Susceptibility in Sum-Frequency Generation Spectroscopy of Aqueous Salt Solutions. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11407-11413.	3.1	33
47	Computational Analysis of Vibrational Sum Frequency Generation Spectroscopy. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 355-377.	10.8	32
48	Intermolecular correlation effect in sum frequency generation spectroscopy of electrolyte aqueous solution. <i>Chemical Physics Letters</i> , 2006, 431, 78-82.	2.6	31
49	Molecular theory on dielectric constant at interfaces: A molecular dynamics study of the water/vapor interface. <i>Journal of Chemical Physics</i> , 2011, 134, 234705.	3.0	30
50	Molecular dynamics simulations of surface-specific bonding of the hydrogen network of water: A solution to the low sum-frequency spectra. <i>Physical Review B</i> , 2012, 86, .	3.2	28
51	Surface Structures of NaF and Na_2SO_4 Aqueous Solutions: Specific Effects of Hard Ions on Surface Vibrational Spectra. <i>Journal of Physical Chemistry C</i> , 2012, 116, 11082-11090.	3.1	27
52	Nonlinear vibrational spectroscopic studies on water/ionic liquid ($[\text{C}_n\text{mim}]\text{TFSA}$; $n = 4, 8$) interfaces. <i>Faraday Discussions</i> , 2012, 154, 289-301.	3.2	27
53	Theoretical Investigation of C-H Vibrational Spectroscopy. 1. Modeling of Methyl and Methylene Groups of Ethanol with Different Conformers. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6687-6700.	2.5	27
54	Why is Benzene Soluble in Water? Role of OH/π Interaction in Solvation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1181-1194.	5.3	25

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55	Theoretical and experimental examination of SFG polarization analysis at acetonitrile/water solution surfaces. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8941-8961.	2.8	25
56	Theoretical Investigation of C-H Vibrational Spectroscopy. 2. Unified Assignment Method of IR, Raman, and Sum Frequency Generation Spectra of Ethanol. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6701-6712.	2.5	25
57	Effect of Frequency-Dependent Fresnel Factor on the Vibrational Sum Frequency Generation Spectra for Liquid/Solid Interfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15665-15673.	3.1	25
58	Refractive index of nanoconfined water reveals its anomalous physical properties. <i>Nanoscale Horizons</i> , 2020, 5, 1016-1024.	8.0	25
59	Vibrational spectrum at a water surface: a hybrid quantum mechanics/molecular mechanics molecular dynamics approach. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 124107.	1.8	24
60	Half-hydration at the air/water interface revealed by heterodyne-detected electronic sum frequency generation spectroscopy, polarization second harmonic generation, and molecular dynamics simulation. <i>Journal of Chemical Physics</i> , 2010, 132, 144701.	3.0	23
61	Molecular dynamics study of phase transfer catalyst for ion transfer through water/chloroform interface. <i>Chemical Physics Letters</i> , 2012, 534, 19-22.	2.6	23
62	Computational study of effect of water finger on ion transport through water-oil interface. <i>Journal of Chemical Physics</i> , 2016, 145, 014702.	3.0	22
63	Molecular Dynamics Analysis of NaOH Aqueous Solution Surface and the Sum Frequency Generation Spectra: Is Surface OH Detected by SFG Spectroscopy?. <i>Journal of Physical Chemistry C</i> , 2014, 118, 29017-29027.	3.1	21
64	Surface Structure of Organic Carbonate Liquids Investigated by Molecular Dynamics Simulation and Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2016, 120, 15185-15197.	3.1	21
65	Molecular dynamics study of two-dimensional sum frequency generation spectra at vapor/water interface. <i>Journal of Chemical Physics</i> , 2015, 142, 212407.	3.0	19
66	In Situ Monitoring of the Unsaturated Phospholipid Monolayer Oxidation in Ambient Air by HD-SFG Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5246-5250.	2.6	19
67	Simple and exact approach to the electronic polarization effect on the solvation free energy: Formulation for quantum-mechanical/ molecular-mechanical system and its applications to aqueous solutions. <i>Journal of Chemical Physics</i> , 2012, 136, 214503.	3.0	17
68	Liquid/liquid interface layering of 1-butanol and [bmim]PF ₆ ionic liquid: a nonlinear vibrational spectroscopy and molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24587-24597.	2.8	17
69	Solvent electronic polarization effect on the electronic transitions in solution: Charge polarizable reference interaction site model self-consistent field approach. <i>Journal of Chemical Physics</i> , 1999, 111, 481-491.	3.0	16
70	Drastic Compensation of Electronic and Solvation Effects on ATP Hydrolysis Revealed through Large-Scale QM/MM Simulations Combined with a Theory of Solutions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 2279-2287.	2.6	16
71	Molecular structure and vibrational spectra at water/poly(2-methoxyethylacrylate) and water/poly(methyl methacrylate) interfaces: A molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2019, 150, 044707.	3.0	16
72	Why the Photochemical Reaction of Phenol Becomes Ultrafast at the Air/Water Interface: The Effect of Surface Hydration. <i>Journal of the American Chemical Society</i> , 2022, 144, 6321-6325.	13.7	16

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73	Improved Theory of Difference Vibrational Spectroscopy and Application to Water. Journal of Chemical Theory and Computation, 2016, 12, 5026-5036.	5.3	15
74	Molecular dynamics study of structure and vibrational spectra at zwitterionic lipid/aqueous KCl, NaCl, and CaCl ₂ solution interfaces. Journal of Chemical Physics, 2018, 148, 222801.	3.0	15
75	Nuclear Quantum Effect on the $\ddot{\text{T}}^{\text{2}}$ Band Shape of Vibrational Sum Frequency Generation Spectra of Normal and Deuterated Water Surfaces. Journal of Physical Chemistry Letters, 2019, 10, 5070-5075.	4.6	14
76	Theory and efficient computation of differential vibrational spectra. Journal of Chemical Physics, 2014, 140, 144109.	3.0	13
77	Topologically disordered mesophase at the topmost surface layer of crystalline ice between 120 and 200 K. Physical Review B, 2019, 99, .	3.2	13
78	Interfacial Structures and Vibrational Spectra at Liquid/Liquid Boundaries: Molecular Dynamics Study of Water/Carbon Tetrachloride and Water/1,2-Dichloroethane Interfaces. Journal of Physical Chemistry C, 2012, 116, 21439-21446.	3.1	11
79	Dispersion of Complex Refractive Indices for Intense Vibrational Bands. I. Quantitative Spectra. Journal of Physical Chemistry B, 2021, 125, 9794-9803.	2.6	11
80	A direct evidence of vibrationally delocalized response at ice surface. Journal of Chemical Physics, 2014, 141, 18C503.	3.0	10
81	A simple and effective solution to the constrained QM/MM simulations. Journal of Chemical Physics, 2018, 148, 134119.	3.0	10
82	Unraveling the Unstable Nature of Tetraglyme-Based Electrolytes toward Superoxide and the Inhibitory Effect of Lithium Ions by Using In Situ Vibrational Spectroscopies. Journal of Physical Chemistry C, 2022, 126, 2980-2989.	3.1	10
83	Hydrated Ion Clusters in Hydrophobic Liquid: Equilibrium Distribution, Kinetics, and Implications. Journal of Physical Chemistry B, 2018, 122, 3562-3571.	2.6	9
84	Quadrupole Contribution of $\text{C}=\text{O}$ Vibrational Band in Sum Frequency Generation Spectra of Organic Carbonates. Journal of Physical Chemistry Letters, 2020, 11, 8527-8531.	4.6	9
85	Bi-layering at ionic liquid surfaces: a sum-frequency generation vibrational spectroscopy- and molecular dynamics simulation-based study. Physical Chemistry Chemical Physics, 2020, 22, 12565-12576.	2.8	9
86	Computation of the free energy due to electron density fluctuation of a solute in solution: A QM/MM method with perturbation approach combined with a theory of solutions. Journal of Chemical Physics, 2014, 140, 134111.	3.0	8
87	Development of quadrupole susceptibility automatic calculator in sum frequency generation spectroscopy and application to methyl $\text{C}=\text{H}$ vibrations. Journal of Chemical Physics, 2020, 153, 174705.	3.0	8
88	Recent progress in simulating microscopic ion transport mechanisms at liquid-liquid interfaces. Journal of Chemical Physics, 2021, 154, 080901.	3.0	8
89	Dispersion of Complex Refractive Indices for Intense Vibrational Bands. II. Implication to Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry B, 2021, 125, 9804-9810.	2.6	8
90	Electron Transfer Mechanism at the Oil/Water Interface Revealed by Multidimensional Free Energy Calculations. Journal of Physical Chemistry B, 2020, 124, 3811-3827.	2.6	7

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91	Construction of exchange repulsion in terms of the wave functions at QM/MM boundary region. <i>Journal of Chemical Physics</i> , 2015, 143, 084104.	3.0	5
92	Efficient Computation of Difference Vibrational Spectra in Isothermal-Isobaric Ensemble. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11229-11238.	2.6	5
93	Role of the Photosystem II as an Environment in the Oxidation Free Energy of the Mn Cluster from $S_{1/2}$ to $S_{2/2}$. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7081-7091.	2.6	5
94	Nonlinear spectroscopy and interfacial structure and dynamics. <i>Journal of Chemical Physics</i> , 2019, 151, 150401.	3.0	5
95	Revealing Transient Shuttling Mechanism of Catalytic Ion Transport through Liquid-Liquid Interface. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1584-1588.	4.6	5
96	Exploration of Gas-Liquid Interfaces for Liquid Water and Methanol Using Extreme Ultraviolet Laser Photoemission Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10514-10526.	2.6	5
97	Calculation of solvation free energy utilizing a constrained QM/MM approach combined with a theory of solutions. <i>Journal of Chemical Physics</i> , 2019, 150, 114109.	3.0	4
98	Large-Scale Parallel Implementation of Hartree-Fock Exchange Energy on Real-Space Grids Using 3D-Parallel Fast Fourier Transform. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1376-1389.	5.4	4
99	Quadrupole Contributions from Interface and Bulk. <i>Lecture Notes in Quantum Chemistry II</i> , 2018, , 151-200.	0.3	4
100	Microscopic Investigation of Ethylene Carbonate Interface: A Molecular Dynamics and Vibrational Spectroscopic Study. <i>Wuli Huaxue Xuebao/ Acta Physico-Chimica Sinica</i> , 2018, 34, 1124-1135.	4.9	4
101	Condensed phase QM/MM simulations utilizing the exchange core functions to describe exchange repulsions at the QM boundary region. <i>Journal of Chemical Physics</i> , 2016, 145, 084107.	3.0	3
102	Comment on "Toward Unraveling the Puzzle of Sum Frequency Generation Spectra at Interface of Aqueous Methanol Solution: Effects of Concentration-Dependent Hyperpolarizability". <i>Journal of Physical Chemistry C</i> , 2020, 124, 25160-25162.	3.1	2
103	Boundary Effects and Quadrupole Contribution in Sum Frequency Generation Spectroscopy. <i>Journal of Chemical Physics</i> , 2022, 156, 154109.	3.0	2
104	A QM/MM study on the correlation between the polarisations of and electrons in a hydrated benzene. <i>Molecular Simulation</i> , 2017, 43, 1209-1217.	2.0	1
105	Singularity-free constraint on molecular dynamics beyond Lagrange multiplier. <i>Molecular Simulation</i> , 2018, 44, 965-972.	2.0	1
106	Reply to the "Comment on Bi-layering at ionic liquid surfaces: a sum-frequency generation vibrational spectroscopy- and molecular dynamics simulation-based study" by M. Deutsch, O. M. Magnussen, J. Haddad, D. Pontoni, B. M. Murphy and B. M. Ocko, <i>Phys. Chem. Chem. Phys.</i> , 2021, DOI: 10.1039/DOCP04882H. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5028-5030.	2.8	1
107	Other Topics. <i>Lecture Notes in Quantum Chemistry II</i> , 2018, , 201-218.	0.3	1
108	Applications: Aqueous Interfaces. <i>Lecture Notes in Quantum Chemistry II</i> , 2018, , 219-246.	0.3	0

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109	Applications: Organic Interfaces. Lecture Notes in Quantum Chemistry II, 2018, , 247-260.	0.3	0
110	Two Computational Schemes of $\ddot{\text{I}}\ddot{\text{t}}$ (2). Lecture Notes in Quantum Chemistry II, 2018, , 81-103.	0.3	0