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	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
2	Boundary Effects and Quadrupole Contribution in Sum Frequency Generation Spectroscopy. Journal of Chemical Physics, 2022, 156, 154109.	3.0	2
3	Why the Photochemical Reaction of Phenol Becomes Ultrafast at the Airâ€“Water Interface: The Effect of Surface Hydration. Journal of the American Chemical Society, 2022, 144, 6321-6325.	13.7	16
4	Recent progress in simulating microscopic ion transport mechanisms at liquidâ€“liquid interfaces. Journal of Chemical Physics, 2021, 154, 080901.	3.0	8
5	Dispersion of Complex Refractive Indices for Intense Vibrational Bands. I. Quantitative Spectra. Journal of Physical Chemistry B, 2021, 125, 9794-9803.	2.6	11
6	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
7	Exploration of Gasâ€“Liquid Interfaces for Liquid Water and Methanol Using Extreme Ultraviolet Laser Photoemission Spectroscopy. Journal of Physical Chemistry B, 2021, 125, 10514-10526.	2.6	5
8	Reply to the â€˜Comment on â€œBi-layering at ionic liquid surfaces: a sum-frequency generation vibrational spectroscopy- and molecular dynamics simulation-based studyâ€â€™ by M. Deutsch, O. M. Magnussen, J. Haddad, D. Pontoni, B. M. Murphy and B. M. Ocko, Phys. Chem. Chem. Phys., 2021, DOI: 10.1039/D0CP04882H. Physical Chemistry Chemical Physics, 2021, 23, 5028-5030.	2.8	1
9	Development of quadrupole susceptibility automatic calculator in sum frequency generation spectroscopy and application to methyl Câ€”H vibrations. Journal of Chemical Physics, 2020, 153, 174705.	3.0	8
10	Quadrupole Contribution of C•O Vibrational Band in Sum Frequency Generation Spectra of Organic Carbonates. Journal of Physical Chemistry Letters, 2020, 11, 8527-8531.	4.6	9
11	Refractive index of nanoconfined water reveals its anomalous physical properties. Nanoscale Horizons, 2020, 5, 1016-1024.	8.0	25
12	In Situ Monitoring of the Unsaturated Phospholipid Monolayer Oxidation in Ambient Air by HD-SFG Spectroscopy. Journal of Physical Chemistry B, 2020, 124, 5246-5250.	2.6	19
13	Revealing Transient Shuttling Mechanism of Catalytic Ion Transport through Liquidâ€“Liquid Interface. Journal of Physical Chemistry Letters, 2020, 11, 1584-1588.	4.6	5
14	Large-Scale Parallel Implementation of Hartreeâ€“Fock Exchange Energy on Real-Space Grids Using 3D-Parallel Fast Fourier Transform. Journal of Chemical Information and Modeling, 2020, 60, 1376-1389.	5.4	4
15	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
16	Comment on â€œToward Unraveling the Puzzle of Sum Frequency Generation Spectra at Interface of Aqueous Methanol Solution: Effects of Concentration-Dependent Hyperpolarizabilityâ€• Journal of Physical Chemistry C, 2020, 124, 25160-25162.	3.1	2
17	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
18	Nuclear Quantum Effect on the Ï‡⁽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

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19	Role of the Photosystem II as an Environment in the Oxidation Free Energy of the Mn Cluster from S₁ to S₂. Journal of Physical Chemistry B, 2019, 123, 7081-7091.	2.6	5
20	Molecular structure and vibrational spectra at water/poly(2-methoxyethylacrylate) and water/poly(methyl methacrylate) interfaces: A molecular dynamics simulation study. Journal of Chemical Physics, 2019, 150, 044707.	3.0	16
21	Effect of Frequency-Dependent Fresnel Factor on the Vibrational Sum Frequency Generation Spectra for Liquid/Solid Interfaces. Journal of Physical Chemistry C, 2019, 123, 15665-15673.	3.1	25
22	Calculation of solvation free energy utilizing a constrained QM/MM approach combined with a theory of solutions. Journal of Chemical Physics, 2019, 150, 114109.	3.0	4
23	Topologically disordered mesophase at the topmost surface layer of crystalline ice between 120 and 200 K. Physical Review B, 2019, 99, .	3.2	13
24	Nonlinear spectroscopy and interfacial structure and dynamics. Journal of Chemical Physics, 2019, 151, 150401.	3.0	5
25	Molecular dynamics study of structure and vibrational spectra at zwitterionoic lipid/aqueous KCl, NaCl, and CaCl2 solution interfaces. Journal of Chemical Physics, 2018, 148, 222801.	3.0	15
26	A simple and effective solution to the constrained QM/MM simulations. Journal of Chemical Physics, 2018, 148, 134119.	3.0	10
27	Hydrated Ion Clusters in Hydrophobic Liquid: Equilibrium Distribution, Kinetics, and Implications. Journal of Physical Chemistry B, 2018, 122, 3562-3571.	2.6	9
28	Electrolyte and Temperature Effects on Third-Order Susceptibility in Sum-Frequency Generation Spectroscopy of Aqueous Salt Solutions. Journal of Physical Chemistry C, 2018, 122, 11407-11413.	3.1	33
29	Effects of third-order susceptibility in sum frequency generation spectra: a molecular dynamics study in liquid water. Physical Chemistry Chemical Physics, 2018, 20, 3040-3053.	2.8	74
30	Structure at the air/water interface in the presence of phenol: a study using heterodyne-detected vibrational sum frequency generation and molecular dynamics simulation. Physical Chemistry Chemical Physics, 2018, 20, 3002-3009.	2.8	34
31	Origin of the Overpotential for the Oxygen Evolution Reaction on a Well-Defined Graphene Electrode Probed by in Situ Sum Frequency Generation Vibrational Spectroscopy. Journal of the American Chemical Society, 2018, 140, 15568-15571.	13.7	64
32	Theory of Sum Frequency Generation Spectroscopy. Lecture Notes in Quantum Chemistry II, 2018, , .	0.3	81
33	Applications: Aqueous Interfaces. Lecture Notes in Quantum Chemistry II, 2018, , 219-246.	0.3	0
34	Singularity-free constraint on molecular dynamics beyond Lagrange multiplier. Molecular Simulation, 2018, 44, 965-972.	2.0	1
35	Applications: Organic Interfaces. Lecture Notes in Quantum Chemistry II, 2018, , 247-260.	0.3	0
36	Two Computational Schemes of Ï‡ (2). Lecture Notes in Quantum Chemistry II, 2018, , 81-103.	0.3	0

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37	Metamaterials-Enhanced Infrared Spectroscopic Study of Nanoconfined Molecules by Plasmonicsâ€“Nanofluidics Hydrid Device. ACS Photonics, 2018, 5, 3179-3188.	6.6	35
38	Bulk Contributions Modulate the Sum-Frequency Generation Spectra of Water on Model Sea-Spray Aerosols. CheM, 2018, 4, 1629-1644.	11.7	69
39	Quadrupole Contributions from Interface and Bulk. Lecture Notes in Quantum Chemistry II, 2018, , 151-200.	0.3	4
40	Microscopic Investigation of Ethylene Carbonate Interface: A Molecular Dynamics and Vibrational Spectroscopic Study. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 1124-1135.	4.9	4
41	Other Topics. Lecture Notes in Quantum Chemistry II, 2018, , 201-218.	0.3	1
42	Theoretical and experimental examination of SFG polarization analysis at acetonitrileâ€“water solution surfaces. Physical Chemistry Chemical Physics, 2017, 19, 8941-8961.	2.8	25
43	Drastic Compensation of Electronic and Solvation Effects on ATP Hydrolysis Revealed through Large-Scale QM/MM Simulations Combined with a Theory of Solutions. Journal of Physical Chemistry B, 2017, 121, 2279-2287.	2.6	16
44	Computational Analysis of Vibrational Sum Frequency Generation Spectroscopy. Annual Review of Physical Chemistry, 2017, 68, 355-377.	10.8	32
45	Experimental and theoretical evidence for bilayer-by-bilayer surface melting of crystalline ice. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 227-232.	7.1	131
46	Unveiling subsurface hydrogen-bond structure of hexagonal water ice. Physical Review B, 2017, 96, .	3.2	40
47	Theoretical Investigation of Câ€“H Vibrational Spectroscopy. 1. Modeling of Methyl and Methylene Groups of Ethanol with Different Conformers. Journal of Physical Chemistry A, 2017, 121, 6687-6700.	2.5	27
48	A QM/MM study on the correlation between the polarisations of and electrons in a hydrated benzene. Molecular Simulation, 2017, 43, 1209-1217.	2.0	1
49	Theoretical Investigation of Câ€“H Vibrational Spectroscopy. 2. Unified Assignment Method of IR, Raman, and Sum Frequency Generation Spectra of Ethanol. Journal of Physical Chemistry A, 2017, 121, 6701-6712.	2.5	25
50	Computational study of effect of water finger on ion transport through water-oil interface. Journal of Chemical Physics, 2016, 145, 014702.	3.0	22
51	Efficient Spectral Diffusion at the Air/Water Interface Revealed by Femtosecond Time-Resolved Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 1811-1815.	4.6	45
52	Improved Theory of Difference Vibrational Spectroscopy and Application to Water. Journal of Chemical Theory and Computation, 2016, 12, 5026-5036.	5.3	15
53	Efficient Computation of Difference Vibrational Spectra in Isothermalâ€“Isobaric Ensemble. Journal of Physical Chemistry B, 2016, 120, 11229-11238.	2.6	5
54	Bend Vibration of Surface Water Investigated by Heterodyne-Detected Sum Frequency Generation and Theoretical Study: Dominant Role of Quadrupole. Journal of Physical Chemistry Letters, 2016, 7, 2597-2601.	4.6	53

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55	Surface Structure of Organic Carbonate Liquids Investigated by Molecular Dynamics Simulation and Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 15185-15197.	3.1	21
56	Hydrogen-Bonding Structure at Zwitterionic Lipid/Water Interface. Journal of Physical Chemistry Letters, 2016, 7, 216-220.	4.6	65
57	Condensed phase QM/MM simulations utilizing the exchange core functions to describe exchange repulsions at the QM boundary region. Journal of Chemical Physics, 2016, 145, 084107.	3.0	3
58	Construction of exchange repulsion in terms of the wave functions at QM/MM boundary region. Journal of Chemical Physics, 2015, 143, 084104.	3.0	5
59	Why is Benzene Soluble in Water? Role of OH/Ï€ Interaction in Solvation. Journal of Chemical Theory and Computation, 2015, 11, 1181-1194.	5.3	25
60	Surface Structure of Methanol/Water Solutions via Sum Frequency Orientational Analysis and Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2015, 119, 9879-9889.	3.1	38
61	Microscopic Barrier Mechanism of Ion Transport through Liquidâ€“Liquid Interface. Journal of the American Chemical Society, 2015, 137, 8022-8025.	13.7	56
62	Molecular dynamics study of two-dimensional sum frequency generation spectra at vapor/water interface. Journal of Chemical Physics, 2015, 142, 212407.	3.0	19
63	Liquid/liquid interface layering of 1-butanol and [bmim]PF6 ionic liquid: a nonlinear vibrational spectroscopy and molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2015, 17, 24587-24597.	2.8	17
64	Theory and efficient computation of differential vibrational spectra. Journal of Chemical Physics, 2014, 140, 144109.	3.0	13
65	A direct evidence of vibrationally delocalized response at ice surface. Journal of Chemical Physics, 2014, 141, 18C503.	3.0	10
66	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
67	Theoretical Studies of Structures and Vibrational Sum Frequency Generation Spectra at Aqueous Interfaces. Chemical Reviews, 2014, 114, 8447-8470.	47.7	132
68	Molecular Dynamics Analysis of NaOH Aqueous Solution Surface and the Sum Frequency Generation Spectra: Is Surface OH^{â€“} Detected by SFG Spectroscopy?. Journal of Physical Chemistry C, 2014, 118, 29017-29027.	3.1	21
69	Real-Time Observation of the Destruction of Hydration Shells under Electrochemical Force. Journal of the American Chemical Society, 2013, 135, 15033-15039.	13.7	43
70	Vibrational spectrum at a water surface: a hybrid quantum mechanics/molecular mechanics molecular dynamics approach. Journal of Physics Condensed Matter, 2012, 24, 124107.	1.8	24
71	Molecular dynamics simulations of surface-specific bonding of the hydrogen network of water: A solution to the low sum-frequency spectra. Physical Review B, 2012, 86, .	3.2	28
72	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. Journal of Chemical Physics, 2012, 136, 214503.	3.0	17

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73	Theory of Quadrupole Contributions from Interface and Bulk in Second-Order Optical Processes. Bulletin of the Chemical Society of Japan, 2012, 85, 1061-1076.	3.2	39
74	Surface Structures of NaF and Na₂SO₄ Aqueous Solutions: Specific Effects of Hard Ions on Surface Vibrational Spectra. Journal of Physical Chemistry C, 2012, 116, 11082-11090.	3.1	27
75	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
76	Mechanisms of Sum Frequency Generation from Liquid Benzene: Symmetry Breaking at Interface and Bulk Contribution. Journal of Physical Chemistry C, 2012, 116, 13169-13182.	3.1	43
77	Nonlinear vibrational spectroscopic studies on water/ionic liquid([C_nmim]TFSA: n = 4, 8) interfaces. Faraday Discussions, 2012, 154, 289-301.	3.2	27
78	Origin of Vibrational Spectroscopic Response at Ice Surface. Journal of Physical Chemistry Letters, 2012, 3, 3001-3006.	4.6	52
79	Molecular dynamics study of phase transfer catalyst for ion transfer through waterâ€“chloroform interface. Chemical Physics Letters, 2012, 534, 19-22.	2.6	23
80	Energetic Origin of Proton Affinity to the Air/Water Interface. Journal of Physical Chemistry B, 2011, 115, 4745-4751.	2.6	39
81	Molecular dynamics simulation of liquid methanol. I. Molecular modeling including Câ€“H vibration and fermi resonance. Journal of Chemical Physics, 2011, 134, 024509.	3.0	51
82	Molecular Dynamics Simulation of Sum Frequency Generation Spectra of Aqueous Sulfuric Acid Solution. Journal of Physical Chemistry C, 2011, 115, 13704-13716.	3.1	47
83	Unified Molecular View of the Air/Water Interface Based on Experimental and Theoretical Ï‡⁽²⁾ Spectra of an Isotopically Diluted Water Surface. Journal of the American Chemical Society, 2011, 133, 16875-16880.	13.7	245
84	Molecular dynamics simulation of liquid methanol. II. Unified assignment of infrared, raman, and sum frequency generation vibrational spectra in methyl Câ€“H stretching region. Journal of Chemical Physics, 2011, 134, 024510.	3.0	42
85	Molecular theory on dielectric constant at interfaces: A molecular dynamics study of the water/vapor interface. Journal of Chemical Physics, 2011, 134, 234705.	3.0	30
86	â€œHalf-hydrationâ€•at the air/water interface revealed by heterodyne-detected electronic sum frequency generation spectroscopy, polarization second harmonic generation, and molecular dynamics simulation. Journal of Chemical Physics, 2010, 132, 144701.	3.0	23
87	Analysis of anisotropic local field in sum frequency generation spectroscopy with the charge response kernel water model. Journal of Chemical Physics, 2009, 131, 244714.	3.0	121
88	Vibrational Spectroscopic Response of Intermolecular Orientational Correlation at the Water Surface. Journal of Physical Chemistry C, 2009, 113, 16299-16302.	3.1	82
89	Recent progress in theoretical analysis of vibrational sum frequency generation spectroscopy. Physical Chemistry Chemical Physics, 2008, 10, 5801.	2.8	121
90	Molecular Dynamics Study of Gasâˆ’Liquid Aqueous Sodium Halide Interfaces. II. Analysis of Vibrational Sum Frequency Generation Spectra. Journal of Physical Chemistry C, 2007, 111, 738-748.	3.1	83

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91	Molecular Dynamics Analysis of Interfacial Structures and Sum Frequency Generation Spectra of Aqueous Hydrogen Halide Solutions. Journal of Physical Chemistry A, 2007, 111, 9277-9285.	2.5	62
92	Molecular Dynamics Study of Gasâ^'Liquid Aqueous Sodium Halide Interfaces. I. Flexible and Polarizable Molecular Modeling and Interfacial Properties. Journal of Physical Chemistry C, 2007, 111, 721-737.	3.1	150
93	Improved Computation of Sum Frequency Generation Spectrum of the Surface of Water. Journal of Physical Chemistry B, 2006, 110, 3158-3163.	2.6	74
94	Intermolecular correlation effect in sum frequency generation spectroscopy of electrolyte aqueous solution. Chemical Physics Letters, 2006, 431, 78-82.	2.6	31
95	Extended treatment of charge response kernel comprising the density functional theory and charge regulation procedures. Journal of Chemical Physics, 2006, 125, 074112.	3.0	40
96	Toward computation of bulk quadrupolar signals in vibrational sum frequency generation spectroscopy. Chemical Physics Letters, 2004, 398, 361-366.	2.6	40
97	Mass Accommodation Coefficient of Water:Â Molecular Dynamics Simulation and Revised Analysis of Droplet Train/Flow Reactor Experiment. Journal of Physical Chemistry B, 2004, 108, 9111-9120.	2.6	79
98	Uptake of the HO2radical by water: Molecular dynamics calculations and their implications for atmospheric modeling. Journal of Geophysical Research, 2004, 109, .	3.3	46
99	The Charge Response Kernel with Modified Electrostatic Potential Charge Model. Journal of Physical Chemistry A, 2002, 106, 3909-3916.	2.5	54
100	A Theoretical Analysis of the Sum Frequency Generation Spectrum of the Water Surface. II. Time-Dependent Approach. Journal of Physical Chemistry B, 2002, 106, 673-685.	2.6	251
101	Water polarizability in condensed phase:Ab initio evaluation by cluster approach. Journal of Computational Chemistry, 2002, 23, 1466-1471.	3.3	73
102	A theoretical analysis of the sum frequency generation spectrum of the water surface. Chemical Physics, 2000, 258, 371-390.	1.9	340
103	An ab initio analysis of medium perturbation on molecular polarizabilities. Journal of Chemical Physics, 1999, 110, 11987-11998.	3.0	76
104	Effect of solvent fluctuation on the electronic transitions of formaldehyde in aqueous solution. Journal of Chemical Physics, 1999, 110, 3484-3492.	3.0	53
105	Solvent electronic polarization effect on the electronic transitions in solution: Charge polarizable reference interaction site model self-consistent field approach. Journal of Chemical Physics, 1999, 111, 481-491.	3.0	16
106	RISM-SCF study of the free-energy profile of the Menshutkin-type reaction NH 3 +CH 3 Clâ†'NH 3 CH 3 + +Cl â^' in aqueous solution. Theoretical Chemistry Accounts, 1999, 102, 165-169.	1.4	38
107	Vibrational relaxation of azide ion in water: The role of intramolecular charge fluctuation and solvent-induced vibrational coupling. Journal of Chemical Physics, 1998, 109, 5511-5523.	3.0	113
108	Molecular dynamics simulation with the charge response kernel: Diffusion dynamics of pyrazine and pyrazinyl radical in methanol. Journal of Chemical Physics, 1998, 108, 6809-6818.	3.0	81

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109	Ab Initio Molecular Orbital Theory on Intramolecular Charge Polarization:Â Effect of Hydrogen Abstraction on the Charge Sensitivity of Aromatic and Nonaromatic Species. Journal of the American Chemical Society, 1997, 119, 4021-4032.	13.7	152
110	Solute-solvent interaction in nonpolar supercritical fluid: a clustering model and size distribution. The Journal of Physical Chemistry, 1990, 94, 6420-6425.	2.9	84