Hajime Torii

List of Publications by Year
in descending order

82 papers	3,410 citations	186254 28 h-index	144002 57 g-index
84 all docs	84 docs citations	84 times ranked	2499 citing authors

#	Article	IF	Citations
1	Singular value decomposition analysis of the electron density changes occurring upon electrostatic polarization of water. RSC Advances, 2022, 12, 2564-2573.	3.6	3
2	Theoretical analysis toward better description of the wavenumber shifts of the OH stretch of hydrogenâ€bonded water. Journal of Raman Spectroscopy, 2022, 53, 1785-1792.	2.5	4
3	Infrared Spectra and Hydrogen-Bond Configurations of Water Molecules at the Interface of Water-Insoluble Polymers under Humidified Conditions. Journal of Physical Chemistry B, 2022, 126, 4143-4151.	2.6	24
4	Role of the electrostatic interactions in the changes in the CN stretching frequency of benzonitrile interacting with hydrogen-bond donating molecules. Journal of Molecular Liquids, 2022, 362, 119714.	4.9	3
5	Role of Intermolecular Charge Fluxes in the Hydrogen-Bond-Induced Frequency Shifts of the OH Stretching Mode of Water. Journal of Physical Chemistry B, 2021, 125, 1468-1475.	2.6	13
6	Hidden Halogen-Bonding Ability of Fluorine Manifesting in the Hydrogen-Bond Configurations of Hydrogen Fluoride. Journal of Physical Chemistry B, 2021, 125, 11742-11750.	2.6	6
7	Dissecting the electric quadrupolar and polarization effects operating in halogen bonding through electron density analysis with a focus on bromine. Journal of Chemical Physics, 2020, 153, 174302.	3.0	6
8	Hydrogen order at the surface of ice Ih revealed by vibrational spectroscopy. Chemical Communications, 2020, 56, 4563-4566.	4.1	12
9	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
10	Correlation of the partial charge-transfer and covalent nature of halogen bonding with the THz and IR spectral changes. Physical Chemistry Chemical Physics, 2019, 21, 17118-17125.	2.8	10
11	Theoretical analysis and modeling of the electrostatic responses of the vibrational and NMR spectroscopic properties of the cyanide anion. Journal of Molecular Liquids, 2019, 284, 773-779.	4.9	6
12	Strategy for Modeling the Electrostatic Responses of the Spectroscopic Properties of Proteins. Journal of Physical Chemistry B, 2018, 122, 154-164.	2.6	10
13	Intermolecular charge fluxes and far-infrared spectral intensities of liquid formamide. Physical Chemistry Chemical Physics, 2018, 20, 3029-3039.	2.8	8
14	Intermediate length-scale chirality related to the vibrational circular dichroism intensity enhancement upon fibril formation in a gelation process. Physical Chemistry Chemical Physics, 2018, 20, 14992-14996.	2.8	12
15	New twist in the theories on the secondary structure dependence and hydration effect of the vibrational properties of peptides. AIP Conference Proceedings, 2016, , .	0.4	0
16	Unified Electrostatic Understanding on the Solvation-Induced Changes in the CN Stretching Frequency and the NMR Chemical Shifts of a Nitrile. Journal of Physical Chemistry A, 2016, 120, 7137-7144.	2.5	17
17	Roles of the scalar and vector components of the solvation effects on the vibrational properties of hydrogen- or halogen-bond accepting stretching modes. Physical Chemistry Chemical Physics, 2016, 18, 10081-10096.	2.8	10
18	Secondary Structure Dependence and Hydration Effect of the Infrared Intensity of the Amide II Mode of Peptide Chains. Journal of Physical Chemistry B, 2016, 120, 1624-1634.	2.6	19

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19	Simulations of the THz spectrum of liquid water incorporating the effects of intermolecular charge fluxes through hydrogen bonds. AIP Conference Proceedings, 2015, , .	0.4	0
20	Electronic Structural Basis for the Atomic Partial Charges of Planar Molecular Systems Derived from Out-of-Plane Dipole Derivatives. Journal of Physical Chemistry A, 2015, 119, 3277-3284.	2.5	1
21	Amide I Vibrational Properties Affected by Hydrogen Bonding Out-of-Plane of the Peptide Group. Journal of Physical Chemistry Letters, 2015, 6, 727-733.	4.6	45
22	Delocalized electrons in infrared intensities. Journal of Molecular Structure, 2014, 1056-1057, 84-96.	3.6	12
23	Cooperative Contributions of the Intermolecular Charge Fluxes and Intramolecular Polarizations in the Far-Infrared Spectral Intensities of Liquid Water. Journal of Chemical Theory and Computation, 2014, 10, 1219-1227.	5.3	34
24	Extended Nature of the Molecular Dipole of Hydrogen-Bonded Water. Journal of Physical Chemistry A, 2013, 117, 2044-2051.	2.5	31
25	Vibrational polarizabilities of hydrogen-bonded water. Chemical Physics, 2013, 419, 90-96.	1.9	11
26	Time-domain calculations of the 1D and 2D spectra of resonantly-coupled vibrations in liquids and proteins. , 2012, , .		0
27	Properties of halogen atoms related to the electrostatic origin of halogen bonding: Basic aspects and some applications. AIP Conference Proceedings, 2012, , .	0.4	8
28	Merged- and Separate-Band Behavior of the Câ•Ọ Stretching Band in N,N-Dimethylformamide Isotopic Liquid Mixtures: DMF/DMF-d₁, DMF/DMF-d₆, and DMF/DMF-¹³Câ•Ọ. Journal of Physical Chemistry B, 2012, 116, 353-366.	2.6	7
29	Mechanism of the Secondary Structure Dependence of the Infrared Intensity of the Amide II Mode of Peptide Chains. Journal of Physical Chemistry Letters, 2012, 3, 112-116.	4.6	28
30	Intermolecular Electron Density Modulations in Water and Their Effects on the Far-Infrared Spectral Profiles at 6 THz. Journal of Physical Chemistry B, 2011, 115, 6636-6643.	2.6	58
31	Intra- and Intermolecular Charge Fluxes Induced by the OH Stretching Mode of Water and Their Effects on the Infrared Intensities and Intermolecular Vibrational Coupling. Journal of Physical Chemistry B, 2010, 114, 13403-13409.	2.6	33
32	Properties of halogen atoms for representing intermolecular electrostatic interactions related to halogen bonding and their substituent effects. Journal of Computational Chemistry, 2010, 31, 107-116.	3.3	62
33	Intermolecular charge flux as the origin of infrared intensity enhancement upon halogen-bond formation of the peptide group. Journal of Chemical Physics, 2010, 133, 034504.	3.0	28
34	Nature of vibrational frequency modulations and the related one- and two-dimensional vibrational spectral features analysed for the amide I mode of tetraalanine in aqueous solution. Molecular Physics, 2009, 107, 1855-1866.	1.7	7
35	Merged and separate band profiles arising from resonantly coupled vibrational modes of liquid mixtures: theoretical study. Journal of Raman Spectroscopy, 2008, 39, 1592-1599.	2.5	9
36	Amide I Infrared Spectral Features Characteristic of Some Untypical Conformations Appearing in the Structures Suggested for Amyloids. Journal of Physical Chemistry B, 2008, 112, 8737-8743.	2.6	23

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37	Scheme of detecting microscopic inhomogeneity in binary liquid mixtures utilizing resonantly coupled vibrational modes. Journal of Chemical Physics, 2007, 127, 054508.	3.0	2
38	1P008 Theoretical analysis of the inter-beta-sheet vibrational coupling involving glutamine side chains(Proteins-structure and structure-function relationship,Oral Presentations). Seibutsu Butsuri, 2007, 47, S25.	0.1	0
39	Time-Domain Calculations of the Infrared and Polarized Raman Spectra of Tetraalanine in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 5434-5444.	2.6	27
40	Time-Domain Calculations of the Polarized Raman Spectra, the Transient Infrared Absorption Anisotropy, and the Extent of Delocalization of the OH Stretching Mode of Liquid Water. Journal of Physical Chemistry A, 2006, 110, 9469-9477.	2.5	138
41	Effects of Intermolecular Vibrational Coupling and Liquid Dynamics on the Polarized Raman and Two-Dimensional Infrared Spectral Profiles of LiquidN,N-Dimethylformamide Analyzed with a Time-Domain Computational Method. Journal of Physical Chemistry A, 2006, 110, 4822-4832.	2.5	92
42	RESPONSES OF MOLECULAR VIBRATIONS TO INTERMOLECULAR ELECTROSTATIC INTERACTIONS AND THEIR EFFECTS ON VIBRATIONAL SPECTROSCOPIC FEATURES. , 2006, , 179-214.		14
43	Electrostatic origin of the cooperative effect on the CO bond lengths and the amide I vibrational frequencies of the N-methylacetamide oligomers. Journal of Molecular Structure, 2005, 735-736, 21-26.	3.6	17
44	Time-domain calculations of the polarized Raman and two-dimensional infrared spectra of liquid N,N-dimethylformamide. Chemical Physics Letters, 2005, 414, 417-422.	2.6	20
45	Molecular Conductors Based onperi-Ditellurium-Bridged Donors,2,3-DMTTeA and TMTTeN. European Journal of Inorganic Chemistry, 2005, 2005, 3435-3449.	2.0	5
46	Time-Domain Theoretical Analysis of the Noncoincidence Effect, Diagonal Frequency Shift, and the Extent of Delocalization of the CO Stretching Mode of Acetone/Dimethyl Sulfoxide Binary Liquid Mixtures. Journal of Physical Chemistry A, 2005, 109, 7797-7804.	2.5	38
47	Vibrational Interactions in the Amide I Subspace of the Oligomers and Hydration Clusters ofN-Methylacetamide. Journal of Physical Chemistry A, 2004, 108, 7272-7280.	2.5	56
48	Extent of Delocalization of Vibrational Modes in Liquids as a Result of Competition between Diagonal Disorder and Off-Diagonal Coupling. Journal of Physical Chemistry A, 2004, 108, 2103-2107.	2.5	23
49	The role of atomic quadrupoles in intermolecular electrostatic interactions of polar and nonpolar molecules. Journal of Chemical Physics, 2003, 119, 2192-2198.	3.0	63
50	Vibrational Polarization and Opsin Shift of Retinal Schiff Bases:Â Theoretical Study. Journal of the American Chemical Society, 2002, 124, 9272-9277.	13.7	9
51	Intensity-carrying modes important for vibrational polarizabilities and hyperpolarizabilities of molecules: Derivation from the algebraic properties of formulas and applications. Journal of Computational Chemistry, 2002, 23, 997-1006.	3.3	17
52	The role of electrical property derivatives in intermolecular vibrational interactions and their effects on vibrational spectra. Vibrational Spectroscopy, 2002, 29, 205-209.	2.2	11
53	Extended dipole-induced dipole mechanism for generating Raman and optical Kerr effect intensities of low-frequency dynamics in liquids. Chemical Physics Letters, 2002, 353, 431-438.	2.6	20
54	Low-Wavenumber Vibrational Dynamics of Liquid Formamide and N-Methylformamide:â€‰ Molecular Dynamics and Instantaneous Normal Mode Analysis. Journal of Physical Chemistry A, 2000, 104, 4174-4181.	2.5	52

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55	Model Hamiltonian Approach to the Infrared Intensities of Charged Conjugated Ï€-Electron Systems. Journal of Physical Chemistry A, 2000, 104, 413-421.	2.5	16
56	Ab initio molecular orbital study of the amide I vibrational interactions between the peptide groups in di- and tripeptides and considerations on the conformation of the extended helix. Journal of Raman Spectroscopy, 1998, 29, 81-86.	2.5	270
57	Effects of hydration on the structure, vibrational wavenumbers, vibrational force field and resonance raman intensities ofN-methylacetamide. Journal of Raman Spectroscopy, 1998, 29, 537-546.	2.5	137
58	Intermolecular hydrogen bonding and low-wave-number vibrational spectra of formamide,N-methylformamide, andN-methylacetamide in the liquid state. International Journal of Quantum Chemistry, 1998, 70, 241-252.	2.0	44
59	Raman Intensities Induced by Electrostatic Intermolecular Interaction and Related Nonlinear Optical Properties of a Conjugated Ï€-Electron System:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 1998, 102, 8422-8425.	2.5	18
60	Liquid Structure, Infrared and Isotropic/Anisotropic Raman Noncoincidence of the Amide I Band, and Low-Wavenumber Vibrational Spectra of Liquid Formamide:Â Molecular Dynamics and ab Initio Molecular Orbital Studies. Journal of Physical Chemistry B, 1998, 102, 315-321.	2.6	57
61	Effects of Intermolecular Hydrogen-Bonding Interactions on the Amide I Mode ofN-Methylacetamide:Â Matrix-Isolation Infrared Studies and ab Initio Molecular Orbital Calculations. Journal of Physical Chemistry B, 1998, 102, 309-314.	2.6	155
62	Coupling between amide I vibrations of neighboring peptide groups and conformation of an extended helix. , 1998, , .		0
63	Ab initio molecular orbital study of the amide I vibrational interactions between the peptide groups in di- and tripeptides and considerations on the conformation of the extended helix. , 1998, 29, 81.		1
64	Ab initio molecular orbital study of the amide I vibrational interactions between the peptide groups in di- and tripeptides and considerations on the conformation of the extended helix. , 1998, 29, 81.		2
65	Ab initio molecular orbital study of the amide I vibrational interactions between the peptide groups in di- and tripeptides and considerations on the conformation of the extended helix. Journal of Raman Spectroscopy, 1998, 29, 81-86.	2.5	8
66	Effects of hydration on the structure, vibrational wavenumbers, vibrational force field and resonance raman intensities of N-methylacetamide. Journal of Raman Spectroscopy, 1998, 29, 537-546.	2.5	1
67	Charge Fluxes and Changes in Electronic Structures as the Origin of Infrared Intensities in the Ground and Excited Electronic States. Journal of Physical Chemistry B, 1997, 101, 466-471.	2.6	25
68	Infrared Intensities of the CC and CN Stretching Modes of Conjugated Schiff Bases. A Study Based onab InitioMolecular Orbital Calculations. The Journal of Physical Chemistry, 1996, 100, 15335-15339.	2.9	22
69	Correlation between the Vibrational Frequencies of the Carboxylate Group and the Types of Its Coordination to a Metal Ion:Â Anab InitioMolecular Orbital Study. The Journal of Physical Chemistry, 1996, 100, 19812-19817.	2.9	401
70	Vibrational Analysis of a Schiff Base Based onab InitioMolecular Orbital Calculations:Â Effect of Electron Correlation on the CN Stretching Force Constant and the Origin of the Shift of the CN Stretching Frequency upon Protonation and Hydrogen-Bond Formation. The Journal of Physical Chemistry, 1996, 100, 15328-15334.	2.9	10
71	Raman Noncoincidence Effect and Intermolecular Interactions in Liquid Dimethyl Sulfoxide: Simulations Based on the Transition Dipole Coupling Mechanism and Liquid Structures Derived by Monte Carlo Method. Bulletin of the Chemical Society of Japan, 1995, 68, 128-134.	3.2	34
72	Vibrational analyses oftransâ€polyacetylene based onabinitiosecondâ€order Mo/llerâ€“Plesset perturbation calculations oftransâ€oligoenes. Journal of Chemical Physics, 1995, 103, 8964-8979.	3.0	63

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73	Vibrational analyses of trans,transâ€1,3,5,7â€octatetraene and allâ€transâ€1,3,5,7,9â€decapentaene based on ab initio molecular orbital calculations and observed infrared and Raman spectra. Journal of Chemical Physics, 1995, 103, 8955-8963.	3.0	39
74	Analysis of the absorption spectrum (1â€‰1Buâ†1â€‰1Ag) and resonance Raman excitation profiles of transâ€1,3,5â€hexatriene based on ab initio molecular orbital calculations. Journal of Chemical Physics, 1994, 101, 4496-4504.	3.0	31
75	Infrared intensities of vibrational modes of an Î±-helical polypeptide: Calculations based on the equilibrium charge/charge flux (ECCF) model. Journal of Molecular Structure, 1993, 300, 171-179.	3.6	25
76	Local order and transition dipole coupling in liquid methanol and acetone as the origin of the Raman noncoincidence effect. Journal of Chemical Physics, 1993, 99, 8459-8465.	3.0	102
77	Correlation between redshifts and widths of the 0â€“0 band in the absorption spectra (1â€‰1Buâ†1â€‰1Ag) ofallâ€transâ€Î²â€carotene in solution. Journal of Chemical Physics, 1993, 98, 3697-3702.	3.0	15
78	Application of the threeâ€dimensional doorwayâ€state theory to analyses of the amideâ€I infrared bands of globular proteins. Journal of Chemical Physics, 1992, 97, 92-98.	3.0	68
79	Model calculations on the amideâ€I infrared bands of globular proteins. Journal of Chemical Physics, 1992, 96, 3379-3387.	3.0	445
80	Threeâ€dimensional doorwayâ€state theory for analyses of absorption bands of manyâ€oscillator systems. Journal of Chemical Physics, 1992, 97, 86-91.	3.0	47
81	Effect of correlation between electronic and vibrational dephasing processes on Raman band shapes. Journal of Raman Spectroscopy, 1991, 22, 601-605.	2.5	3
82	Effects of collisionâ€induced perturbation of atomic motions on the vibrational relaxation of polyatomic molecules. Journal of Chemical Physics, 1990, 93, 1054-1060.	3.0	2