Wei Zhuang

List of Publications by Year
in descending order

90 papers	2,865 citations	159525 30 h-index	175177 52 g-index
93 all docs	93 docs citations	93 times ranked	3488 citing authors

#	Article	IF	Citations
1	Ultrafast formation of interlayer hot excitons in atomically thin MoS2/WS2 heterostructures. Nature Communications, 2016, 7, 12512.	5.8	313
2	Electrostatic DFT Map for the Complete Vibrational Amide Band of NMA. Journal of Physical Chemistry A, 2005, 109, 9747-9759.	1.1	180
3	Significantly Enhanced Overall Water Splitting Performance by Partial Oxidation of Ir through Au Modification in Coreâ€“Shell Alloy Structure. Journal of the American Chemical Society, 2021, 143, 4639-4645.	6.6	160
4	Coherent Multidimensional Vibrational Spectroscopy of Biomolecules: Concepts, Simulations, and Challenges. Angewandte Chemie - International Edition, 2009, 48, 3750-3781.	7.2	152
5	Collective Solvent Coordinates for the Infrared Spectrum of HOD in D2O Based on an ab Initio Electrostatic Map. Journal of Physical Chemistry A, 2005, 109, 64-82.	1.1	142
6	Simulation Protocols for Coherent Femtosecond Vibrational Spectra of Peptides. Journal of Physical Chemistry B, 2006, 110, 3362-3374.	1.2	135
7	Coherent Multidimensional Optical Probes for Electron Correlations and Exciton Dynamics: From NMR to X-rays. Accounts of Chemical Research, 2009, 42, 553-562.	7.6	90
8	Stochastic Liouville equation simulation of multidimensional vibrational line shapes of trialanine. Journal of Chemical Physics, 2004, 121, 10577-10598.	1.2	76
9	Stochastic Liouville equations for hydrogen-bonding fluctuations and their signatures in two-dimensional vibrational spectroscopy of water. Journal of Chemical Physics, 2005, 123, 114504.	1.2	69
10	Simulating the T-Jump-Triggered Unfolding Dynamics of trpzip2 Peptide and Its Time-Resolved IR and Two-Dimensional IR Signals Using the Markov State Model Approach. Journal of Physical Chemistry B, 2011, 115, 5415-5424.	1.2	69
11	High Thermoelectric Performance of New Rhombohedral Phase of GeSe stabilized through Alloying with AgSbSe₂. Angewandte Chemie - International Edition, 2017, 56, 14113-14118.	7.2	68
12	A small molecule activator of SIRT3 promotes deacetylation and activation of manganese superoxide dismutase. Free Radical Biology and Medicine, 2017, 112, 287-297.	1.3	67
13	Dramatically enhanced thermoelectric performance of MoS₂ by introducing MoO₂ nanoinclusions. Journal of Materials Chemistry A, 2017, 5, 2004-2011.	5.2	66
14	Cation Effects on Rotational Dynamics of Anions and Water Molecules in Alkali (Li⁺,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Journal of Physical Chemistry B, 2013, 117, 7972-7984.	1.2	64
15	Ag₁₀Ti₂₈â€Oxo Cluster Containing Singleâ€Atom Silver Sites: Atomic Structure and Synergistic Electronic Properties. Angewandte Chemie - International Edition, 2019, 58, 10932-10935.	7.2	57
16	Highly Active and Stable Water Splitting in Acidic Media Using a Bifunctional Iridium/Cucurbit[6]uril Catalyst. ACS Energy Letters, 2019, 4, 1301-1307.	8.8	54
17	Two-Dimensional Infrared Spectroscopy as a Probe of the Solvent Electrostatic Field for a Twelve Residue Peptide. Journal of Physical Chemistry B, 2008, 112, 5930-5937.	1.2	53
18	Realizing p-Type MoS₂ with Enhanced Thermoelectric Performance by Embedding VMo₂S₄ Nanoinclusions. Journal of Physical Chemistry B, 2018, 122, 713-720.	1.2	44

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19	Sensitivity of 2D IR Spectra to Peptide Helicity: A Concerted Experimental and Simulation Study of an Octapeptide. Journal of Physical Chemistry B, 2009, 113, 12037-12049.	1.2	41
20	Discriminating early stage AÎ²42 monomer structures using chirality-induced 2DIR spectroscopy in a simulation study. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15687-15692.	3.3	40
21	Differentiation between enamines and tautomerizable imines in the oxidation reaction with TEMPO. Nature Communications, 2018, 9, 5002.	5.8	40
22	The opposite effects of sodium and potassium cations on water dynamics. Chemical Science, 2017, 8, 1429-1435.	3.7	39
23	Ion Segregation in Aqueous Solutions. Journal of Physical Chemistry B, 2012, 116, 14426-14432.	1.2	38
24	Molecular mechanism of water reorientational slowing down in concentrated ionic solutions. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10023-10028.	3.3	38
25	Peptide Secondary Structure Determination by Three-Pulse Coherent Vibrational Spectroscopies:Â A Simulation Study. Journal of Physical Chemistry B, 2004, 108, 18034-18045.	1.2	37
26	Mapping Molecular Conformations with Multiple-Mode Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry A, 2011, 115, 3357-3365.	1.1	36
27	Dissecting coherent vibrational spectra of small proteins into secondary structural elements by sensitivity analysis. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 7443-7448.	3.3	35
28	Vibrational Energy Transfer: An Angstrom Molecular Ruler in Studies of Ion Pairing and Clustering in Aqueous Solutions. Journal of Physical Chemistry B, 2015, 119, 4333-4349.	1.2	34
29	Electrostatic interactions in phospholipid membranes revealed by coherent 2D IR spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15323-15327.	3.3	32
30	Frequency Distribution of the Amide-I Vibration Sorted by Residues in Amyloid Fibrils Revealed by 2D-IR Measurements and Simulations. Journal of Physical Chemistry B, 2012, 116, 3322-3330.	1.2	31
31	Two-dimensional vibrational optical probes for peptide fast folding investigation. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 18934-18938.	3.3	30
32	Ultrafast probes of electronâ€“hole transitions between two atomic layers. Nature Communications, 2018, 9, 1859.	5.8	30
33	Simulation of two-dimensional infrared spectroscopy of amyloid fibrils. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14233-14236.	3.3	29
34	Enhancement of anisotropic thermoelectric performance of tungsten disulfide by titanium doping. Journal of Materials Chemistry A, 2016, 4, 10159-10165.	5.2	29
35	Two-dimensional electronic correlation spectroscopy of the nÏ€âˆ— and Ï€Ï€âˆ— protein backbone transitions: A simulation study. Chemical Physics, 2007, 341, 29-36.	0.9	28
36	Microscopic Origin of the Deviation from Stokesâ€“Einstein Behavior Observed in Dynamics of the KSCN Aqueous Solutions: A MD Simulation Study. Journal of Physical Chemistry B, 2013, 117, 2992-3004.	1.2	24

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37	Probing molecular chirality via excitonic nonlinear response. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 5051-5066.	0.6	20
38	Geometry and excitation energy fluctuations of NMA in aqueous solution with CHARMM, AMBER, OPLS, and GROMOS force fields: Implications for protein ultraviolet spectra simulation. Chemical Physics Letters, 2008, 452, 78-83.	1.2	20
39	High Thermoelectric Performance of New Rhombohedral Phase of GeSe stabilized through Alloying with AgSbSe₂. Angewandte Chemie, 2017, 129, 14301-14306.	1.6	19
40	Coherent Two Dimensional Infrared Spectroscopy of a Cyclic Decapeptide Antamanide. A Simulation Study of the Amide-I and A Bands. Journal of Physical Chemistry B, 2008, 112, 12479-12490.	1.2	18
41	Coupling of spin-orbit interaction with phonon anharmonicity leads to significant impact on thermoelectricity in SnSe. Nano Energy, 2019, 60, 673-679.	8.2	17
42	Dissociation of Hydrogen Chloride and Proton Transfer in Liquid Glycerol:Â An Ab Initio Molecular Dynamics Studyâ€. Journal of Physical Chemistry B, 2004, 108, 19647-19656.	1.2	16
43	Effect of Ion Pairing on the Solution Dynamics Investigated by the Simulations of the Optical Kerr Effect and the Dielectric Relaxation Spectra. Journal of Physical Chemistry B, 2013, 117, 15395-15406.	1.2	15
44	Coherent femtosecond multidimensional probes of molecular vibrations. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13717-13718.	3.3	13
45	Modeling Vibrational Spectra of Ester Carbonyl Stretch in Water and DMSO Based on Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2015, 119, 12390-12396.	1.2	13
46	Rational Preparation of Atomically Precise Non-Alkyl Tin-Oxo Clusters with Theoretical to Experimental Insights into Electrocatalytic CO ₂ Reduction Applications. CCS Chemistry, 2021, 3, 2607-2616.	4.6	13
47	Infrared Signature of the Early Stage Microsolvation in the NaSO₄^{â€“}(H₂O)_{1â€“5} Clusters: A Simulation Study. Journal of Physical Chemistry A, 2014, 118, 9157-9162.	1.1	12
48	Low frequency 2D Raman-THz spectroscopy of ionic solution: A simulation study. Journal of Chemical Physics, 2015, 142, 212419.	1.2	12
49	Comparison Studies on Sub-Nanometer-Sized Ion Clusters in Aqueous Solutions: Vibrational Energy Transfers, MD Simulations, and Neutron Scattering. Journal of Physical Chemistry B, 2015, 119, 9893-9904.	1.2	11
50	Ion effect on the dynamics of water hydrogen bonding network: A theoretical and computational spectroscopy point of view. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1373.	6.2	11
51	Investigating the Structural Origin of Trpzip2 Temperature Dependent Unfolding Fluorescence Line Shape Based on a Markov State Model Simulation. Journal of Physical Chemistry B, 2012, 116, 12669-12676.	1.2	10
52	Pairing preferences of the model mono-valence mono-atomic ions investigated by molecular simulation. Journal of Chemical Physics, 2014, 140, 184504.	1.2	10
53	Discriminating trpzip2 and trpzip4 peptidesâ€™ folding landscape using the two-dimensional infrared spectroscopy: A simulation study. Journal of Chemical Physics, 2014, 140, 055101.	1.2	10
54	Cation effect in the ionic solution optical Kerr effect measurements: A simulation study. Journal of Chemical Physics, 2014, 140, 054507.	1.2	9

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55	Electronic Structures and Thermoelectric Properties of Two-Dimensional MoS2/MoSe2 Heterostructures. Chinese Journal of Chemical Physics, 2016, 29, 445-452.	0.6	9
56	Ag 10 Ti 28 â€Oxo Cluster Containing Singleâ€Atom Silver Sites: Atomic Structure and Synergistic Electronic Properties. Angewandte Chemie, 2019, 131, 11048-11051.	1.6	9
57	Detection of Drug Binding to a Target Protein Using EVV 2DIR Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 3598-3606.	1.2	9
58	Binary structure and dynamics of the hydrogen bonds in the hydration shells of ions. Physical Chemistry Chemical Physics, 2021, 23, 11400-11410.	1.3	9
59	Nonresonant Energy Transfers Independent on the Phonon Densities in Polyatomic Liquids. Journal of Physical Chemistry A, 2015, 119, 669-680.	1.1	8
60	Characterizing the Structures, Spectra, and Energy Landscapes Involved in the Excited-State Proton Transfer Process of Red Fluorescent Protein LSSmKate1. Journal of Physical Chemistry B, 2016, 120, 9833-9842.	1.2	8
61	Significant expansion and red-shifting of fluorescent protein chromophore determined through computational design and genetic code expansion. Biophysics Reports, 2018, 4, 273-285.	0.2	8
62	Modeling the Thermal Unfolding 2DIR Spectra of a Î²-Hairpin Peptide Based on the Implicit Solvent MD Simulation. Journal of Physical Chemistry A, 2013, 117, 6256-6263.	1.1	6
63	Differentiation between Enamines and Tautomerizable Imines Oxidation Reaction Mechanism using Electron-Vibration-Vibration Two Dimensional Infrared Spectroscopy. Molecules, 2019, 24, 869.	1.7	6
64	Bridging the Gap Between Optical Spectroscopic Experiments and Computer Simulations for Fast Protein Folding Dynamics. Current Physical Chemistry, 2012, 2, 45-58.	0.1	5
65	Facilitated Diffusion of Methane in Pores with a Higher Aromaticity. Journal of Physical Chemistry C, 2016, 120, 19885-19889.	1.5	5
66	Salting-in/Salting-out Mechanism of Carbon Dioxide in Aqueous Electrolyte Solutions. Chinese Journal of Chemical Physics, 2017, 30, 811-816.	0.6	5
67	Molecular Mechanism of Water Reorientation Dynamics in Dimethyl Sulfoxide Aqueous Mixtures. Journal of Physical Chemistry B, 2020, 124, 1806-1816.	1.2	5
68	Effectively modulating vertical tunneling transport by mechanically twisting bilayer graphene within the all-metallic architecture. Nanoscale, 2020, 12, 8793-8800.	2.8	5
69	Universal dynamical onset in water at distinct material interfaces. Chemical Science, 2022, 13, 4341-4351.	3.7	5
70	Cosolvent effect on the dynamics of water in aqueous binary mixtures. Molecular Physics, 2018, 116, 1014-1025.	0.8	4
71	Iodide-enhanced palladium catalysis via formation of iodide-bridged binuclear palladium complex. Communications Chemistry, 2020, 3, .	2.0	4
72	Quasiparticle effects on the linear and nonlinear susceptibility of ZnGeP₂. RSC Advances, 2019, 9, 35771-35779.	1.7	3

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73	Proteinâ€“Ligand Binding Molecular Details Revealed by Terahertz Optical Kerr Spectroscopy: A Simulation Study. Jacs Au, 2021, 1, 1788-1797.	3.6	3
74	Signatures of Chemical Exchange in 2D Vibrational Spectroscopy; Simulations Based on the Stochastic Liouville Equations. Springer Series in Chemical Physics, 2007, , 401-403.	0.2	3
75	Ion Pairing Kinetics Does not Necessarily Follow the Eigen-Tamm Mechanism. Chinese Journal of Chemical Physics, 2013, 26, 694-700.	0.6	2
76	Simulating ion clustering in potassium thiocyanate aqueous solutions with various ion-water models. Science China Chemistry, 2014, 57, 1723-1730.	4.2	2
77	Rational designing of 8â€hydroxyquinolinâ€imidazolinoneâ€based fluorescent protein mutants with dramatically red shifted emission: A computational study. Journal of Computational Chemistry, 2018, 39, 2307-2315.	1.5	2
78	A Genetically Encoded Twoâ€Dimensional Infrared Probe for Enzyme Activeâ€Site Dynamics. Angewandte Chemie - International Edition, 2021, 60, 11143-11147.	7.2	2
79	The impact of borate on the structure of antifreeze glycoproteins. Chinese Journal of Chemical Physics, 0, , .	0.6	2
80	Modeling the temperature-dependent peptide vibrational spectra based on implicit-solvent model and enhance sampling technique. Chinese Physics B, 2016, 25, 018201.	0.7	1
81	Simulation of the T-jump triggered unfolding and thermal unfolding vibrational spectroscopy related to polypeptides conformation fluctuation. Science China Chemistry, 2017, 60, 1115-1129.	4.2	1
82	Reply to Stirnemann et al.: Frame retardation is the key reason behind the general slowdown of water reorientation dynamics in concentrated electrolytes. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E4955-E4956.	3.3	1
83	Simulating the Peptide Folding Kinetic Related Spectra Based on the Markov State Model. Advances in Experimental Medicine and Biology, 2014, 805, 199-220.	0.8	1
84	Modeling the low frequency vibrational spectroscopy of ionic solutions. International Journal of Quantum Chemistry, 2015, 115, 564-569.	1.0	0
85	Rotational mechanism of ammonium ion in water and methanol. Chinese Journal of Chemical Physics, 2018, 31, 568-574.	0.6	0
86	Theoretical simulation of protein two-dimensional infrared spectroscopy. , 2020, , 89-120.		0
87	A Genetically Encoded Twoâ€Dimensional Infrared Probe for Enzyme Activeâ€Site Dynamics. Angewandte Chemie, 2021, 133, 11243-11247.	1.6	0
88	Coherent Nonlinear Optical Spectroscopy of Proteins: Femtosecond Analogues of Multidimensional NMR. , 2007, , .		0
89	Identification of Trans- and Cis-2-Methylcyclopropanecarboxylic acid using EVV 2DIR spectroscopy: A theoretical study. Chemical Physics Letters, 2022, 788, 139301.	1.2	0
90	Surface hopping dynamics in periodic solid-state materials with a linear vibronic coupling model. Journal of Chemical Physics, 2022, 156, 154116.	1.2	0