# Wei Zhuang

## List of Publications by Year in Descending Order



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| 89 papers | 2,287 citations | 27 h-index | 46 g-index |
| 93 ext. papers | 2,572 ext. citations | 6.2 avg, IF | 4.89 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 89 | Identification of Trans- and Cis-2-Methylcyclopropanecarboxylic acid using EVV 2DIR spectroscopy: A theoretical study. *Chemical Physics Letters*, **2022**, 788, 139301 | 2.5 | |
| 88 | Universal dynamical onset in water at distinct material interfaces.. *Chemical Science*, **2022**, 13, 4341-4351 | 9.4 | 0 |
| 87 | Surface hopping dynamics in periodic solid-state materials with a linear vibronic coupling model.. *Journal of Chemical Physics*, **2022**, 156, 154116 | 3.9 | |
| 86 | A Genetically Encoded Two-Dimensional Infrared Probe for Enzyme Active-Site Dynamics. *Angewandte Chemie - International Edition*, **2021**, 60, 11143-11147 | 16.4 | 2 |
| 85 | A Genetically Encoded Two-Dimensional Infrared Probe for Enzyme Active-Site Dynamics. *Angewandte Chemie*, **2021**, 133, 11243-11247 | 3.6 | |
| 84 | Binary structure and dynamics of the hydrogen bonds in the hydration shells of ions. *Physical Chemistry Chemical Physics*, **2021**, 23, 11400-11410 | 3.6 | 2 |
| 83 | Significantly Enhanced Overall Water Splitting Performance by Partial Oxidation of Ir through Au Modification in Core-Shell Alloy Structure. *Journal of the American Chemical Society*, **2021**, 143, 4639-4645 | 16.4 | 44 |
| 82 | Protein-Ligand Binding Molecular Details Revealed by Terahertz Optical Kerr Spectroscopy: A Simulation Study. *Jacs Au*, **2021**, 1, 1788-1797 | | 1 |
| 81 | Theoretical simulation of protein two-dimensional infrared spectroscopy **2020**, 89-120 | | |
| 80 | Molecular Mechanism of Water Reorientation Dynamics in Dimethyl Sulfoxide Aqueous Mixtures. *Journal of Physical Chemistry B*, **2020**, 124, 1806-1816 | 3.4 | 2 |
| 79 | Iodide-enhanced palladium catalysis via formation of iodide-bridged binuclear palladium complex. *Communications Chemistry*, **2020**, 3, | 6.3 | 2 |
| 78 | Effectively modulating vertical tunneling transport by mechanically twisting bilayer graphene within the all-metallic architecture. *Nanoscale*, **2020**, 12, 8793-8800 | 7.7 | 2 |
| 77 | Ag10Ti28-Oxo Cluster Containing Single-Atom Silver Sites: Atomic Structure and Synergistic Electronic Properties. *Angewandte Chemie*, **2019**, 131, 11048-11051 | 3.6 | 7 |
| 76 | Ag Ti -Oxo Cluster Containing Single-Atom Silver Sites: Atomic Structure and Synergistic Electronic Properties. *Angewandte Chemie - International Edition*, **2019**, 58, 10932-10935 | 16.4 | 33 |
| 75 | Highly Active and Stable Water Splitting in Acidic Media Using a Bifunctional Iridium/Cucurbit[6]uril Catalyst. *ACS Energy Letters*, **2019**, 4, 1301-1307 | 20.1 | 34 |
| 74 | Detection of Drug Binding to a Target Protein Using EVV 2DIR Spectroscopy. *Journal of Physical Chemistry B*, **2019**, 123, 3598-3606 | 3.4 | 6 |
| 73 | Differentiation between Enamines and Tautomerizable Imines Oxidation Reaction Mechanism using Electron-Vibration-Vibration Two Dimensional Infrared Spectroscopy. *Molecules*, **2019**, 24, | 4.8 | 4 |

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| 72 | Coupling of spin-orbit interaction with phonon anharmonicity leads to significant impact on thermoelectricity in SnSe. *Nano Energy*, **2019**, 60, 673-679 | 17.1 | 9 |
| 71 | Quasiparticle effects on the linear and nonlinear susceptibility of ZnGeP.. *RSC Advances*, **2019**, 9, 35771-35779 | 3.7 | 1 |
| 70 | Cosolvent effect on the dynamics of water in aqueous binary mixtures. *Molecular Physics*, **2018**, 116, 1014-1025 | 1.7 | 4 |
| 69 | Realizing p-Type MoS with Enhanced Thermoelectric Performance by Embedding VMoS Nanoinclusions. *Journal of Physical Chemistry B*, **2018**, 122, 713-720 | 3.4 | 25 |
| 68 | Ultrafast probes of electron-hole transitions between two atomic layers. *Nature Communications*, **2018**, 9, 1859 | 17.4 | 23 |
| 67 | 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 | 7.9 | 7 |
| 66 | Rotational mechanism of ammonium ion in water and methanol *Chinese Journal of Chemical Physics*, **2018**, 31, 568-574 | 0.9 | |
| 65 | Differentiation between enamines and tautomerizable imines in the oxidation reaction with TEMPO. *Nature Communications*, **2018**, 9, 5002 | 17.4 | 19 |
| 64 | Significant expansion and red-shifting of fluorescent protein chromophore determined through computational design and genetic code expansion. *Biophysics Reports*, **2018**, 4, 273-285 | 3.5 | 3 |
| 63 | Rational designing of 8-hydroxyquinolin-imidazolinone-based fluorescent protein mutants with dramatically red shifted emission: A computational study. *Journal of Computational Chemistry*, **2018**, 39, 2307-2315 | 3.5 | 1 |
| 62 | 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 | 11.5 | 1 |
| 61 | Dramatically enhanced thermoelectric performance of MoS2 by introducing MoO2 nanoinclusions. *Journal of Materials Chemistry A*, **2017**, 5, 2004-2011 | 13 | 48 |
| 60 | High Thermoelectric Performance of New Rhombohedral Phase of GeSe stabilized through Alloying with AgSbSe2. *Angewandte Chemie*, **2017**, 129, 14301-14306 | 3.6 | 15 |
| 59 | High Thermoelectric Performance of New Rhombohedral Phase of GeSe stabilized through Alloying with AgSbSe. *Angewandte Chemie - International Edition*, **2017**, 56, 14113-14118 | 16.4 | 46 |
| 58 | 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 | 11.5 | 30 |
| 57 | Simulation of the T-jump triggered unfolding and thermal unfolding vibrational spectroscopy related to polypeptides conformation fluctuation. *Science China Chemistry*, **2017**, 60, 1115-1129 | 7.9 | 1 |
| 56 | A small molecule activator of SIRT3 promotes deacetylation and activation of manganese superoxide dismutase. *Free Radical Biology and Medicine*, **2017**, 112, 287-297 | 7.8 | 43 |
| 55 | The opposite effects of sodium and potassium cations on water dynamics. *Chemical Science*, **2017**, 8, 1429-1435 | 9.4 | 26 |

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| 54 | Salting-in/Salting-out Mechanism of Carbon Dioxide in Aqueous Electrolyte Solutions. *Chinese Journal of Chemical Physics*, **2017**, 30, 811-816 | 0.9 | 4 |
| 53 | Ultrafast formation of interlayer hot excitons in atomically thin MoS2/WS2 heterostructures. *Nature Communications*, **2016**, 7, 12512 | 17.4 | 240 |
| 52 | Enhancement of anisotropic thermoelectric performance of tungsten disulfide by titanium doping. *Journal of Materials Chemistry A*, **2016**, 4, 10159-10165 | 13 | 19 |
| 51 | Modeling the temperature-dependent peptide vibrational spectra based on implicit-solvent model and enhance sampling technique. *Chinese Physics B*, **2016**, 25, 018201 | 1.2 | 1 |
| 50 | Electronic Structures and Thermoelectric Properties of Two-Dimensional MoS2/MoSe2 Heterostructures. *Chinese Journal of Chemical Physics*, **2016**, 29, 445-452 | 0.9 | 7 |
| 49 | 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, 9833-42 | 3.4 | 7 |
| 48 | Facilitated Diffusion of Methane in Pores with a Higher Aromaticity. *Journal of Physical Chemistry C*, **2016**, 120, 19885-19889 | 3.8 | 5 |
| 47 | 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, 9893-904 | 3.4 | 10 |
| 46 | Modeling the low frequency vibrational spectroscopy of ionic solutions. *International Journal of Quantum Chemistry*, **2015**, 115, 564-569 | 2.1 | |
| 45 | Low frequency 2D Raman-THz spectroscopy of ionic solution: A simulation study. *Journal of Chemical Physics*, **2015**, 142, 212419 | 3.9 | 12 |
| 44 | Modeling Vibrational Spectra of Ester Carbonyl Stretch in Water and DMSO Based on Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2015**, 119, 12390-6 | 3.4 | 11 |
| 43 | Vibrational energy transfer: an angstrom molecular ruler in studies of ion pairing and clustering in aqueous solutions. *Journal of Physical Chemistry B*, **2015**, 119, 4333-49 | 3.4 | 28 |
| 42 | Nonresonant energy transfers independent on the phonon densities in polyatomic liquids. *Journal of Physical Chemistry A*, **2015**, 119, 669-80 | 2.8 | 8 |
| 41 | Infrared signature of the early stage microsolvation in the NaSO2(H2O)21 clusters: a simulation study. *Journal of Physical Chemistry A*, **2014**, 118, 9157-62 | 2.8 | 11 |
| 40 | Simulating ion clustering in potassium thiocyanate aqueous solutions with various ion-water models. *Science China Chemistry*, **2014**, 57, 1723-1730 | 7.9 | 2 |
| 39 | Cation effect in the ionic solution optical Kerr effect measurements: a simulation study. *Journal of Chemical Physics*, **2014**, 140, 054507 | 3.9 | 8 |
| 38 | Pairing preferences of the model mono-valence mono-atomic ions investigated by molecular simulation. *Journal of Chemical Physics*, **2014**, 140, 184504 | 3.9 | 9 |
| 37 | Discriminating trpzip2 and trpzip4 peptides' folding landscape using the two-dimensional infrared spectroscopy: a simulation study. *Journal of Chemical Physics*, **2014**, 140, 055101 | 3.9 | 10 |

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| 36 | Simulating the peptide folding kinetic related spectra based on the Markov State Model. *Advances in Experimental Medicine and Biology*, **2014**, 805, 199-220 | 3.6 | |
| 35 | Microscopic origin of the deviation from Stokes-Einstein behavior observed in dynamics of the KSCN aqueous solutions: a MD simulation study. *Journal of Physical Chemistry B*, **2013**, 117, 2992-3004 | 3.4 | 24 |
| 34 | Ion Pairing Kinetics Does not Necessarily Follow the Eigen-Tamm Mechanism. *Chinese Journal of Chemical Physics*, **2013**, 26, 694-700 | 0.9 | 2 |
| 33 | Cation effects on rotational dynamics of anions and water molecules in alkali (Li+, Na+, K+, Cs+) thiocyanate (SCN-) aqueous solutions. *Journal of Physical Chemistry B*, **2013**, 117, 7972-84 | 3.4 | 51 |
| 32 | 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, 15395-406 | 3.4 | 14 |
| 31 | Modeling the thermal unfolding 2DIR spectra of a hairpin peptide based on the implicit solvent MD simulation. *Journal of Physical Chemistry A*, **2013**, 117, 6256-63 | 2.8 | 6 |
| 30 | Ion segregation in aqueous solutions. *Journal of Physical Chemistry B*, **2012**, 116, 14426-32 | 3.4 | 35 |
| 29 | 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, 3322-30 | 3.4 | 28 |
| 28 | 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, 12669-76 | 3.4 | 10 |
| 27 | Bridging the Gap Between Optical Spectroscopic Experiments and Computer Simulations for Fast Protein Folding Dynamics. *Current Physical Chemistry*, **2012**, 2, 45-58 | 0.5 | 4 |
| 26 | 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, 5415-24 | 3.4 | 59 |
| 25 | Mapping molecular conformations with multiple-mode two-dimensional infrared spectroscopy. *Journal of Physical Chemistry A*, **2011**, 115, 3357-65 | 2.8 | 35 |
| 24 | Discriminating early stage A{beta}42 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, 15687-92 | 11.5 | 36 |
| 23 | Kohärente mehrdimensionale Schwingungsspektroskopie von Biomolekülen: Konzepte, Simulationen und Herausforderungen. *Angewandte Chemie*, **2009**, 121, 3804-3838 | 3.6 | 9 |
| 22 | Coherent multidimensional vibrational spectroscopy of biomolecules: concepts, simulations, and challenges. *Angewandte Chemie - International Edition*, **2009**, 48, 3750-81 | 16.4 | 138 |
| 21 | Sensitivity of 2D IR spectra to peptide helicity: a concerted experimental and simulation study of an octapeptide. *Journal of Physical Chemistry B*, **2009**, 113, 12037-49 | 3.4 | 39 |
| 20 | Coherent multidimensional optical probes for electron correlations and exciton dynamics: from NMR to X-rays. *Accounts of Chemical Research*, **2009**, 42, 553-62 | 24.3 | 78 |
| 19 | Two-dimensional infrared spectroscopy as a probe of the solvent electrostatic field for a twelve residue peptide. *Journal of Physical Chemistry B*, **2008**, 112, 5930-7 | 3.4 | 52 |

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| 18 | 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, 12479-90 | 3.4 | 14 |
| 17 | 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 | 2.5 | 15 |
| 16 | Two Dimensional Electronic Correlation Spectroscopy of the npi* and pipi* Protein Backbone Transitions: A Simulation Study. *Chemical Physics*, **2007**, 341, 29-36 | 2.3 | 27 |
| 15 | Simulation of two-dimensional infrared spectroscopy of amyloid fibrils. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 14233-6 | 11.5 | 27 |
| 14 | 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, 15323-7 | 11.5 | 27 |
| 13 | Signatures of Chemical Exchange in 2D Vibrational Spectroscopy; Simulations Based on the Stochastic Liouville Equations. *Springer Series in Chemical Physics*, **2007**, 401-403 | 0.3 | 3 |
| 12 | Probing molecular chirality via excitonic nonlinear response. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2006**, 39, 5051-5066 | 1.3 | 19 |
| 11 | 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, 18934-8 | 11.5 | 28 |
| 10 | Simulation protocols for coherent femtosecond vibrational spectra of peptides. *Journal of Physical Chemistry B*, **2006**, 110, 3362-74 | 3.4 | 123 |
| 9 | Electrostatic DFT map for the complete vibrational amide band of NMA. *Journal of Physical Chemistry A*, **2005**, 109, 9747-59 | 2.8 | 169 |
| 8 | 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 | 2.8 | 136 |
| 7 | Stochastic Liouville equations for hydrogen-bonding fluctuations and their signatures in two-dimensional vibrational spectroscopy of water. *Journal of Chemical Physics*, **2005**, 123, 114504 | 3.9 | 68 |
| 6 | 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, 7443-8 | 11.5 | 34 |
| 5 | Coherent femtosecond multidimensional probes of molecular vibrations. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 13717-8 | 11.5 | 13 |
| 4 | Stochastic Liouville equation simulation of multidimensional vibrational line shapes of trialanine. *Journal of Chemical Physics*, **2004**, 121, 10577-98 | 3.9 | 71 |
| 3 | Dissociation of Hydrogen Chloride and Proton Transfer in Liquid Glycerol: An Ab Initio Molecular Dynamics Study *Journal of Physical Chemistry B*, **2004**, 108, 19647-19656 | 3.4 | 15 |
| 2 | Peptide Secondary Structure Determination by Three-Pulse Coherent Vibrational Spectroscopies: A Simulation Study. *Journal of Physical Chemistry B*, **2004**, 108, 18034-18045 | 3.4 | 34 |
| 1 | Rational Preparation of Atomically Precise Non-Alkyl Tin-Oxo Clusters with Theoretical to Experimental Insights into Electrocatalytic CO 2 Reduction Applications. *CCS Chemistry*,2607-2616 | 7.2 | 7 |