

Yu Zhang

List of Publications by Year in descending order

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54
papers

1,718
citations

393982

19
h-index

276539

41
g-index

54
all docs

54
docs citations

54
times ranked

1887
citing authors

#	ARTICLE	IF	CITATIONS
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
2	Multidimensional Attosecond Resonant X-Ray Spectroscopy of Molecules: Lessons from the Optical Regime. <i>Annual Review of Physical Chemistry</i> , 2013, 64, 101-127.	4.8	170
3	Core and valence excitations in resonant X-ray spectroscopy using restricted excitation window time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2012, 137, 194306.	1.2	83
4	Two-dimensional stimulated resonance Raman spectroscopy of molecules with broadband x-ray pulses. <i>Journal of Chemical Physics</i> , 2012, 136, 174117.	1.2	66
5	Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer. <i>Nature Chemistry</i> , 2021, 13, 343-349.	6.6	59
6	First-principles time-dependent quantum transport theory. <i>Physical Review B</i> , 2013, 87, .	1.1	51
7	Simulating Valence-to-Core X-ray Emission Spectroscopy of Transition Metal Complexes with Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5804-5809.	2.3	49
8	Stimulated X-Ray Emission Spectroscopy in Transition Metal Complexes. <i>Physical Review Letters</i> , 2018, 120, 133203.	2.9	48
9	Watching energy transfer in metalloporphyrin heterodimers using stimulated X-ray Raman spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 15597-15601.	3.3	42
10	Comprehensive Experimental and Computational Spectroscopic Study of Hexacyanoferrate Complexes in Water: From Infrared to X-ray Wavelengths. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5075-5086.	1.2	40
11	Monitoring conical intersections in the ring opening of furan by attosecond stimulated X-ray Raman spectroscopy. <i>Structural Dynamics</i> , 2016, 3, 023601.	0.9	38
12	A first-principles molecular dynamics approach for predicting optical phonon lifetimes and far-infrared reflectance of polar materials. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2012, 113, 1683-1688.	1.1	33
13	Nonlinear Spectroscopy of Core and Valence Excitations Using Short X-Ray Pulses: Simulation Challenges. <i>Topics in Current Chemistry</i> , 2014, 368, 273-345.	4.0	30
14	Multidimensional resonant nonlinear spectroscopy with coherent broadband x-ray pulses. <i>Physica Scripta</i> , 2016, T169, 014002.	1.2	30
15	Time-, frequency-, and wavevector-resolved x-ray diffraction from single molecules. <i>Journal of Chemical Physics</i> , 2014, 140, 204311.	1.2	29
16	X-ray circular dichroism signals: a unique probe of local molecular chirality. <i>Chemical Science</i> , 2017, 8, 5969-5978.	3.7	27
17	Entangled Valence Electron-Hole Dynamics Revealed by Stimulated Attosecond X-ray Raman Scattering. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2326-2331.	2.1	25
18	Dissipative time-dependent quantum transport theory. <i>Journal of Chemical Physics</i> , 2013, 138, 164121.	1.2	25

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19	Multidimensional x-ray spectroscopy of valence and core excitations in cysteine. <i>Journal of Chemical Physics</i> , 2013, 138, 144303.	1.2	23
20	Observation of Seeded Mn K α Stimulated X-Ray Emission Using Two-Color X-Ray Free-Electron Laser Pulses. <i>Physical Review Letters</i> , 2020, 125, 037404.	2.9	20
21	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6418-6427.	2.3	20
22	Monitoring Long-Range Electron Transfer Pathways in Proteins by Stimulated Attosecond Broadband X-ray Raman Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3656-3661.	2.1	18
23	Study of double core hole excitations in molecules by X-ray double-quantum-coherence signals: a multi-configuration simulation. <i>Chemical Science</i> , 2016, 7, 5922-5933.	3.7	18
24	X-ray Raman optical activity of chiral molecules. <i>Chemical Science</i> , 2019, 10, 898-908.	3.7	18
25	Double-core excitations in formamide can be probed by X-ray double-quantum-coherence spectroscopy. <i>Journal of Chemical Physics</i> , 2013, 138, 144301.	1.2	17
26	Three-dimensional attosecond resonant stimulated X-ray Raman spectroscopy of electronic excitations in core-ionized glycine. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24323-24331.	1.3	16
27	Time-dependent density functional theory for quantum transport. <i>Frontiers of Physics</i> , 2014, 9, 698-710.	2.4	16
28	π Donation and Its Effects on the Excited-State Lifetimes of Luminescent Platinum(II) Terpyridine Complexes in Solution. <i>Inorganic Chemistry</i> , 2013, 52, 8476-8482.	1.9	14
29	Multiple Core and Vibronic Coupling Effects in Attosecond Stimulated X-Ray Raman Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5479-5489.	2.3	12
30	Coherent (photon) vs incoherent (current) detection of multidimensional optical signals from single molecules in open junctions. <i>Journal of Chemical Physics</i> , 2015, 142, 212445.	1.2	12
31	Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes. <i>Nanoscale</i> , 2016, 8, 13168-13173.	2.8	12
32	Electroluminescence in Molecular Junctions: A Diagrammatic Approach. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4304-4315.	2.3	11
33	Double core hole valence-to-core x-ray emission spectroscopy: A theoretical exploration using time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 144114.	1.2	11
34	Near-Edge X-ray Absorption Fine Structure Spectroscopy of Heteroatomic Core-Hole States as a Probe for Nearly Indistinguishable Chemical Environments. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 556-561.	2.1	11
35	Identifying Cu(II) amyloid peptide binding intermediates in the early stages of aggregation by resonance Raman spectroscopy: a simulation study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31103-31112.	1.3	10
36	Transferability of Atomic Properties in Molecular Partitioning: A Comparison. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3312-3318.	2.3	9

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37	Nonlinear light scattering in molecules triggered by an impulsive x-ray Raman process. <i>Physical Review A</i> , 2013, 87, 53826.	1.0	9
38	Role of the Isolable Hydride Intermediate in the Hydrosilylation of Carbonyl Compounds Catalyzed by the High-Valent Mono-Oxo-Rhenium(V) Complex. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 5714-5723.	1.0	9
39	Femtosecond X-ray Spectroscopy Directly Quantifies Transient Excited-State Mixed Valency. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 378-386.	2.1	9
40	Multidimensional scattering of attosecond x-ray pulses detected by photon-coincidence. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2014, 47, 124037.	0.6	8
41	Understanding excitation energy transfer in metalloporphyrin heterodimers with different linkers, bonding structures, and geometries through stimulated X-ray Raman spectroscopy. <i>Journal of Modern Optics</i> , 2014, 61, 558-567.	0.6	8
42	Coherent control of long-range photoinduced electron transfer by stimulated X-ray Raman processes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 10001-10006.	3.3	8
43	Two-dimensional x-ray correlation spectroscopy of remote core states. <i>Structural Dynamics</i> , 2014, 1, 014101.	0.9	7
44	Resonant Stimulated X-ray Raman Spectroscopy of Mixed-Valence Manganese Complexes. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5925-5931.	2.1	7
45	Characterizing the Intermediates Compound I and II in the Cytochrome P450 Catalytic Cycle with Nonlinear X-ray Spectroscopy: A Simulation Study. <i>ChemPhysChem</i> , 2015, 16, 2006-2014.	1.0	5
46	Monitoring Ultrafast Spin Crossover Intermediates in an Iron(II) Complex by Broad Band Stimulated X-ray Raman Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6524-6531.	1.1	5
47	Photothermally Probing Vibrational Excited-State Absorption with Nanoscale Spatial Resolution through Frequency-Domain Pump-Probe Peak Force Infrared Microscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8333-8338.	1.5	4
48	Generation of intense phase-stable femtosecond hard X-ray pulse pairs. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2119616119.	3.3	4
49	Density-functional derivative discontinuities at the maximum number of bound electrons. <i>Physical Review A</i> , 2012, 85, .	1.0	3
50	Monitoring Excited State Charge Transfer of Transition Metal Mixed-Valence Complexes with Femtosecond X-ray Absorption and Emission Spectroscopy. , 2016, , .		1
51	Dissecting X-Ray Raman Resonances Using Four-Wave Mixing. <i>EPJ Web of Conferences</i> , 2013, 41, 05040.	0.1	0
52	Far Infrared Thermal Radiative Properties of Polar Materials From First-Principle Simulations. , 2011, , .		0
53	Attosecond Stimulated X-ray Raman Probes of Energy and Electron Transfer in Porphyrin Dimers and Proteins. , 2014, , .		0
54	Resonant Stimulated X-Ray Raman Spectroscopy of Molecule Following Core Ionization. <i>Springer Proceedings in Physics</i> , 2015, , 584-586.	0.1	0