

# Yu Zhang

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

52  
papers

1,020  
citations

18  
h-index

30  
g-index

54  
ext. papers

1,319  
ext. citations

5.3  
avg, IF

4.32  
L-index

#	Paper	IF	Citations
52	Femtosecond X-ray Spectroscopy Directly Quantifies Transient Excited-State Mixed Valency.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 378-386	6.4	0
51	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> , <b>2022</b> , 119, e2119616119	11.5	1
50	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> , <b>2021</b> , 125, 8333-8338	3.8	0
49	Resonant Stimulated X-ray Raman Spectroscopy of Mixed-Valence Manganese Complexes. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 5925-5931	6.4	4
48	Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer. <i>Nature Chemistry</i> , <b>2021</b> , 13, 343-349	17.6	21
47	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 084801	3.9	115
46	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> , <b>2020</b> , 11, 556-561	6.4	9
45	Observation of Seeded Mn K $\alpha$ Stimulated X-Ray Emission Using Two-Color X-Ray Free-Electron Laser Pulses. <i>Physical Review Letters</i> , <b>2020</b> , 125, 037404	7.4	7
44	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 6418-6427	6.4	8
43	X-ray Raman optical activity of chiral molecules. <i>Chemical Science</i> , <b>2019</b> , 10, 898-908	9.4	12
42	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> , <b>2019</b> , 151, 144114	3.9	8
41	Comprehensive Experimental and Computational Spectroscopic Study of Hexacyanoferrate Complexes in Water: From Infrared to X-ray Wavelengths. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 5075-5086	3.4	27
40	Stimulated X-Ray Emission Spectroscopy in Transition Metal Complexes. <i>Physical Review Letters</i> , <b>2018</b> , 120, 133203	7.4	29
39	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> , <b>2018</b> , 122, 6524-6531	2.8	4
38	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> , <b>2017</b> , 19, 31103-31112	3.6	17
37	X-ray circular dichroism signals: a unique probe of local molecular chirality. <i>Chemical Science</i> , <b>2017</b> , 8, 5969-5978	9.4	15
36	Multidimensional resonant nonlinear spectroscopy with coherent broadband x-ray pulses. <i>Physica Scripta</i> , <b>2016</b> , T169, 014002	2.6	25

35	Nonlinear Spectroscopy of Core and Valence Excitations Using Short X-Ray Pulses: Simulation Challenges. <i>Topics in Current Chemistry</i> , <b>2016</b> , 368, 273-345		20
34	Monitoring Excited State Charge Transfer of Transition Metal Mixed-Valence Complexes with Femtosecond X-ray Absorption and Emission Spectroscopy <b>2016</b> ,		1
33	Monitoring conical intersections in the ring opening of furan by attosecond stimulated X-ray Raman spectroscopy. <i>Structural Dynamics</i> , <b>2016</b> , 3, 023601	3.2	30
32	Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes. <i>Nanoscale</i> , <b>2016</b> , 8, 13168-73	7.7	8
31	Study of double core hole excitations in molecules by X-ray double-quantum-coherence signals: a multi-configuration simulation. <i>Chemical Science</i> , <b>2016</b> , 7, 5922-5933	9.4	13
30	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> , <b>2016</b> , 113, 10001-6	11.5	7
29	Electroluminescence in Molecular Junctions: A Diagrammatic Approach. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 4304-15	6.4	11
28	Characterizing the Intermediates Compound I and II in the Cytochrome P450 Catalytic Cycle with Nonlinear X-ray Spectroscopy: A Simulation Study. <i>ChemPhysChem</i> , <b>2015</b> , 16, 2006-14	3.2	5
27	Coherent (photon) vs incoherent (current) detection of multidimensional optical signals from single molecules in open junctions. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 212445	3.9	11
26	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> , <b>2015</b> , 11, 5804-9	6.4	37
25	Resonant Stimulated X-Ray Raman Spectroscopy of Molecule Following Core Ionization. <i>Springer Proceedings in Physics</i> , <b>2015</b> , 584-586	0.2	
24	Monitoring Long-Range Electron Transfer Pathways in Proteins by Stimulated Attosecond Broadband X-ray Raman Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 3656-3661	6.4	16
23	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> , <b>2014</b> , 61, 558-567	1.1	8
22	Two-dimensional x-ray correlation spectroscopy of remote core states. <i>Structural Dynamics</i> , <b>2014</b> , 1, 014101	3.2	7
21	Role of the Isolable Hydride Intermediate in the Hydrosilylation of Carbonyl Compounds Catalyzed by the High-Valent Mono-Oxidorehenum(V) Complex. <i>European Journal of Inorganic Chemistry</i> , <b>2014</b> , 2014, 5714-5723	2.3	9
20	Three-dimensional attosecond resonant stimulated X-ray Raman spectroscopy of electronic excitations in core-ionized glycine. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 24323-31	3.6	14
19	Time-, frequency-, and wavevector-resolved x-ray diffraction from single molecules. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 204311	3.9	25
18	Multidimensional scattering of attosecond x-ray pulses detected by photon-coincidence. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , <b>2014</b> , 47, 124037	1.3	8

17	Time-dependent density functional theory for quantum transport. <i>Frontiers of Physics</i> , <b>2014</b> , 9, 698-710	3.7	13
16	Fluorescence quenching and its effects on the excited-state lifetimes of luminescent platinum(II) terpyridine complexes in solution. <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 8476-82	5.1	13
15	First-principles time-dependent quantum transport theory. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	41
14	Multidimensional attosecond resonant X-ray spectroscopy of molecules: lessons from the optical regime. <i>Annual Review of Physical Chemistry</i> , <b>2013</b> , 64, 101-27	15.7	134
13	Multiple Core and Vibronic Coupling Effects in Attosecond Stimulated X-Ray Raman Spectroscopy (SXRS). <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9,	6.4	8
12	Multidimensional x-ray spectroscopy of valence and core excitations in cysteine. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 144303	3.9	21
11	Dissipative time-dependent quantum transport theory. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 164121	3.9	24
10	Nonlinear light scattering in molecules triggered by an impulsive X-ray Raman process. <i>Physical Review A</i> , <b>2013</b> , 87, 53826	2.6	9
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> , <b>2013</b> , 110, 15597-601	11.5	33
8	Double-core excitations in formamide can be probed by X-ray double-quantum-coherence spectroscopy. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 144301	3.9	13
7	Dissecting X-Ray Raman Resonances Using Four-Wave Mixing. <i>EPJ Web of Conferences</i> , <b>2013</b> , 41, 05040	0.3	
6	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> , <b>2012</b> , 113, 1683-1688	2.1	25
5	Entangled Valence Electron-Hole Dynamics Revealed by Stimulated Attosecond X-ray Raman Scattering. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 2326-2331	6.4	22
4	Density-functional derivative discontinuities at the maximum number of bound electrons. <i>Physical Review A</i> , <b>2012</b> , 85,	2.6	3
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> , <b>2012</b> , 137, 194306	3.9	68
2	Two-dimensional stimulated resonance Raman spectroscopy of molecules with broadband x-ray pulses. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 174117	3.9	62
1	Transferability of Atomic Properties in Molecular Partitioning: A Comparison. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 3312-8	6.4	9