Yu Zhang

List of Publications by Year
in descending order

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49 papers	1,743 citations	304368 22 h-index	276539 41 g-index
49 all docs	49 docs citations	49 times ranked	2658 citing authors

#	Article	IF	Citations
1	Hot-Electron-Induced Dissociation of H₂on Gold Nanoparticles Supported on SiO₂. Journal of the American Chemical Society, 2014, 136, 64-67.	6.6	458
2	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. Chemical Reviews, 2020, 120, 2215-2287.	23.0	231
3	Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. ACS Nano, 2018, 12, 8415-8422.	7.3	75
4	Fundamental Limitations to Plasmonic Hot-Carrier Solar Cells. Journal of Physical Chemistry Letters, 2016, 7, 1852-1858.	2.1	64
5	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	2.3	56
6	First-principles time-dependent quantum transport theory. Physical Review B, 2013, 87, .	1.1	51
7	Interlayer-Decoupled Sc-Based Mxene with High Carrier Mobility and Strong Light-Harvesting Ability. Journal of Physical Chemistry Letters, 2018, 9, 6915-6920.	2.1	49
8	Mechanistic Insights into Photocatalyzed H₂ Dissociation on Au Clusters. Journal of the American Chemical Society, 2020, 142, 13090-13101.	6.6	48
9	Supramolecular Double-Helix Formation by Diastereoisomeric Conformations of Configurationally Enantiomeric Macrocycles. Journal of the American Chemical Society, 2016, 138, 14469-14480.	6.6	42
10	Interference and Molecular Transportâ€"A Dynamical View: Time-Dependent Analysis of Disubstituted Benzenes. Journal of Physical Chemistry Letters, 2014, 5, 2748-2752.	2.1	40
11	Conical Nanopores for Efficient Ion Pumping and Desalination. Journal of Physical Chemistry Letters, 2017, 8, 2842-2848.	2.1	39
12	Correlation-Informed Permutation of Qubits for Reducing Ansatz Depth in the Variational Quantum Eigensolver. PRX Quantum, 2021, 2, .	3.5	36
13	Stark control of electrons along nanojunctions. Nature Communications, 2018, 9, 2070.	5.8	32
14	Nonlinear Spectroscopy of Core and Valence Excitations Using Short X-Ray Pulses: Simulation Challenges. Topics in Current Chemistry, 2014, 368, 273-345.	4.0	30
15	Quantum-Mechanical Prediction of Nanoscale Photovoltaics. Journal of Physical Chemistry Letters, 2014, 5, 1272-1277.	2.1	30
16	Multidimensional resonant nonlinear spectroscopy with coherent broadband x-ray pulses. Physica Scripta, 2016, T169, 014002.	1.2	30
17	A multiscale quantum mechanics/electromagnetics method for device simulations. Chemical Society Reviews, 2015, 44, 1763-1776.	18.7	27
18	Supramolecular Gelation of Rigid Triangular Macrocycles through Rings of Multiple Câ€"HÂ·Â·Â·O Interactions Acting Cooperatively. Journal of Organic Chemistry, 2016, 81, 2581-2588.	1.7	27

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19	Dissipative time-dependent quantum transport theory. Journal of Chemical Physics, 2013, 138, 164121.	1.2	25
20	Multiscale Modeling of Plasmon-Enhanced Power Conversion Efficiency in Nanostructured Solar Cells. Journal of Physical Chemistry Letters, 2015, 6, 4410-4416.	2.1	24
21	Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. Journal of Chemical Physics, 2019, 151, 154109.	1.2	24
22	Advantages of Conical Pores for Ion Pumps. Journal of Physical Chemistry C, 2017, 121, 161-168.	1.5	23
23	Quantum transport through an array of quantum dots. Nanoscale, 2013, 5, 169-173.	2.8	22
24	Timeâ€dependent quantum transport theory and its applications to graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2013, 250, 2481-2494.	0.7	22
25	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2020, 16, 6418-6427.	2.3	20
26	Multiscale Study of Plasmonic Scattering and Light Trapping Effect in Silicon Nanowire Array Solar Cells. Journal of Physical Chemistry Letters, 2017, 8, 571-575.	2.1	19
27	Mixed-Valence Superstructure Assembled from a Mixed-Valence Hostâ€“Guest Complex. Journal of the American Chemical Society, 2018, 140, 9387-9391.	6.6	18
28	Time-dependent density functional theory for quantum transport. Frontiers of Physics, 2014, 9, 698-710.	2.4	16
29	Computing molecular excited states on a D-Wave quantum annealer. Scientific Reports, 2021, 11, 18796.	1.6	16
30	Dissipative time-dependent quantum transport theory: Quantum interference and phonon induced decoherence dynamics. Journal of Chemical Physics, 2015, 142, 164101.	1.2	15
31	An Ab Initio Multiple Cloning Method for Non-Adiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2021, 17, 3629-3643.	2.3	15
32	Coherent (photon) vs incoherent (current) detection of multidimensional optical signals from single molecules in open junctions. Journal of Chemical Physics, 2015, 142, 212445.	1.2	12
33	Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes. Nanoscale, 2016, 8, 13168-13173.	2.8	12
34	Investigating Single-Molecule Fluorescence Spectral Heterogeneity of Rhodamines Using High-Throughput Single-Molecule Spectroscopy. Journal of Physical Chemistry Letters, 2021, 12, 3914-3921.	2.1	12
35	Electroluminescence in Molecular Junctions: A Diagrammatic Approach. Journal of Chemical Theory and Computation, 2015, 11, 4304-4315.	2.3	11
36	Reduction of the molecular hamiltonian matrix using quantum community detection. Scientific Reports, 2021, 11, 4099.	1.6	11

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37	Theory of Plasmonic Hot-Carrier Generation and Relaxation. Journal of Physical Chemistry A, 2021, 125, 9201-9208.	1.1	11
38	Nonadiabatic Excited-State Molecular Dynamics for Open-Shell Systems. Journal of Chemical Theory and Computation, 2020, 16, 2053-2064.	2.3	10
39	Site-Specific Photodecomposition in Conjugated Energetic Materials. Journal of Physical Chemistry A, 2018, 122, 6055-6061.	1.1	8
40	Controllable Single-Molecule Light Emission by Selective Charge Injection in Scanning Tunneling Microscopy. Journal of Physical Chemistry C, 2019, 123, 15761-15768.	1.5	8
41	Kinetic Master Equation Modeling of an Artificial Protein Pump. Journal of Physical Chemistry C, 2016, 120, 14495-14501.	1.5	6
42	A variational approach for dissipative quantum transport in a wide parameter space. Journal of Chemical Physics, 2015, 143, 104112.	1.2	4
43	Light-Driven Ca²⁺ Ion Pump: How Does It Work?. Journal of Physical Chemistry B, 2015, 119, 15110-15117.	1.2	4
44	An approximate framework for quantum transport calculation with model order reduction. Journal of Computational Physics, 2015, 286, 49-61.	1.9	3
45	QUANTUM MECHANICAL MODELING OF ELECTRON-PHOTON INTERACTIONS IN NANOSCALE DEVICES (Invited) Tj ETQq1 1 0.784314	1.6	2
46	Atomistic Simulations of Plasmon Mediated Photochemistry. ACS Symposium Series, 2019, , 239-256.	0.5	2
47	Toward a QUBO-Based Density Matrix Electronic Structure Method. Journal of Chemical Theory and Computation, 2022, 18, 4177-4185.	2.3	2
48	Charge separation and dissipation in molecular wires under a light radiation. Organic Electronics, 2018, 58, 94-104.	1.4	1
49	Preferred states of open electronic systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2878-2882.	0.9	0