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	Toward a QUBO-Based Density Matrix Electronic Structure Method. Journal of Chemical Theory and Computation, 2022, 18, 4177-4185.	2.3	2
2	Reduction of the molecular hamiltonian matrix using quantum community detection. Scientific Reports, 2021, 11, 4099.	1.6	11
3	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
4	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
5	Correlation-Informed Permutation of Qubits for Reducing Ansatz Depth in the Variational Quantum Eigensolver. PRX Quantum, 2021, 2, .	3.5	36
6	Computing molecular excited states on a D-Wave quantum annealer. Scientific Reports, 2021, 11, 18796.	1.6	16
7	Theory of Plasmonic Hot-Carrier Generation and Relaxation. Journal of Physical Chemistry A, 2021, 125, 9201-9208.	1.1	11
8	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2020, 16, 6418-6427.	2.3	20
9	Nonadiabatic Excited-State Molecular Dynamics for Open-Shell Systems. Journal of Chemical Theory and Computation, 2020, 16, 2053-2064.	2.3	10
10	Mechanistic Insights into Photocatalyzed H₂ Dissociation on Au Clusters. Journal of the American Chemical Society, 2020, 142, 13090-13101.	6.6	48
11	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	2.3	56
12	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
13	Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. Journal of Chemical Physics, 2019, 151, 154109.	1.2	24
14	Preferred states of open electronic systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2878-2882.	0.9	0
15	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
16	Atomistic Simulations of Plasmon Mediated Photochemistry. ACS Symposium Series, 2019, , 239-256.	0.5	2
17	Charge separation and dissipation in molecular wires under a light radiation. Organic Electronics, 2018, 58, 94-104.	1.4	1
18	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

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19	Stark control of electrons along nanojunctions. Nature Communications, 2018, 9, 2070.	5.8	32
20	Site-Specific Photodecomposition in Conjugated Energetic Materials. Journal of Physical Chemistry A, 2018, 122, 6055-6061.	1.1	8
21	Mixed-Valence Superstructure Assembled from a Mixed-Valence Hostâ€“Guest Complex. Journal of the American Chemical Society, 2018, 140, 9387-9391.	6.6	18
22	Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. ACS Nano, 2018, 12, 8415-8422.	7.3	75
23	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
24	Conical Nanopores for Efficient Ion Pumping and Desalination. Journal of Physical Chemistry Letters, 2017, 8, 2842-2848.	2.1	39
25	Advantages of Conical Pores for Ion Pumps. Journal of Physical Chemistry C, 2017, 121, 161-168.	1.5	23
26	Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes. Nanoscale, 2016, 8, 13168-13173.	2.8	12
27	Fundamental Limitations to Plasmonic Hot-Carrier Solar Cells. Journal of Physical Chemistry Letters, 2016, 7, 1852-1858.	2.1	64
28	Supramolecular Double-Helix Formation by Diastereoisomeric Conformations of Configurationally Enantiomeric Macrocycles. Journal of the American Chemical Society, 2016, 138, 14469-14480.	6.6	42
29	Kinetic Master Equation Modeling of an Artificial Protein Pump. Journal of Physical Chemistry C, 2016, 120, 14495-14501.	1.5	6
30	Multidimensional resonant nonlinear spectroscopy with coherent broadband x-ray pulses. Physica Scripta, 2016, T169, 014002.	1.2	30
31	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
32	A variational approach for dissipative quantum transport in a wide parameter space. Journal of Chemical Physics, 2015, 143, 104112.	1.2	4
33	QUANTUM MECHANICAL MODELING OF ELECTRON-PHOTON INTERACTIONS IN NANOSCALE DEVICES (Invited) Tj ETQq1 1 0.784314 rg	1.6	2
34	An approximate framework for quantum transport calculation with model order reduction. Journal of Computational Physics, 2015, 286, 49-61.	1.9	3
35	Electroluminescence in Molecular Junctions: A Diagrammatic Approach. Journal of Chemical Theory and Computation, 2015, 11, 4304-4315.	2.3	11
36	Dissipative time-dependent quantum transport theory: Quantum interference and phonon induced decoherence dynamics. Journal of Chemical Physics, 2015, 142, 164101.	1.2	15

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37	A multiscale quantum mechanics/electromagnetics method for device simulations. Chemical Society Reviews, 2015, 44, 1763-1776.	18.7	27
38	Multiscale Modeling of Plasmon-Enhanced Power Conversion Efficiency in Nanostructured Solar Cells. Journal of Physical Chemistry Letters, 2015, 6, 4410-4416.	2.1	24
39	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
40	Light-Driven Ca²⁺ Ion Pump: How Does It Work?. Journal of Physical Chemistry B, 2015, 119, 15110-15117.	1.2	4
41	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
42	Time-dependent density functional theory for quantum transport. Frontiers of Physics, 2014, 9, 698-710.	2.4	16
43	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
44	Quantum-Mechanical Prediction of Nanoscale Photovoltaics. Journal of Physical Chemistry Letters, 2014, 5, 1272-1277.	2.1	30
45	Hot-Electron-Induced Dissociation of H₂on Gold Nanoparticles Supported on SiO₂. Journal of the American Chemical Society, 2014, 136, 64-67.	6.6	458
46	Quantum transport through an array of quantum dots. Nanoscale, 2013, 5, 169-173.	2.8	22
47	Timeâ€dependent quantum transport theory and its applications to graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2013, 250, 2481-2494.	0.7	22
48	First-principles time-dependent quantum transport theory. Physical Review B, 2013, 87, .	1.1	51
49	Dissipative time-dependent quantum transport theory. Journal of Chemical Physics, 2013, 138, 164121.	1.2	25