

Yu Zhang

List of Publications by Year in descending order

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49
papers

1,743
citations

304743

22
h-index

276875

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. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4177-4185.	5.3	2
2	Reduction of the molecular hamiltonian matrix using quantum community detection. <i>Scientific Reports</i> , 2021, 11, 4099.	3.3	11
3	Investigating Single-Molecule Fluorescence Spectral Heterogeneity of Rhodamines Using High-Throughput Single-Molecule Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3914-3921.	4.6	12
4	An Ab Initio Multiple Cloning Method for Non-Adiabatic Excited-State Molecular Dynamics in NWChem. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3629-3643.	5.3	15
5	Correlation-Informed Permutation of Qubits for Reducing Ansatz Depth in the Variational Quantum Eigensolver. <i>PRX Quantum</i> , 2021, 2, .	9.2	36
6	Computing molecular excited states on a D-Wave quantum annealer. <i>Scientific Reports</i> , 2021, 11, 18796.	3.3	16
7	Theory of Plasmonic Hot-Carrier Generation and Relaxation. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9201-9208.	2.5	11
8	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6418-6427.	5.3	20
9	Nonadiabatic Excited-State Molecular Dynamics for Open-Shell Systems. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2053-2064.	5.3	10
10	Mechanistic Insights into Photocatalyzed H ₂ Dissociation on Au Clusters. <i>Journal of the American Chemical Society</i> , 2020, 142, 13090-13101.	13.7	48
11	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5771-5783.	5.3	56
12	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. <i>Chemical Reviews</i> , 2020, 120, 2215-2287.	47.7	231
13	Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. <i>Journal of Chemical Physics</i> , 2019, 151, 154109.	3.0	24
14	Preferred states of open electronic systems. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 2878-2882.	2.1	0
15	Controllable Single-Molecule Light Emission by Selective Charge Injection in Scanning Tunneling Microscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15761-15768.	3.1	8
16	Atomistic Simulations of Plasmon Mediated Photochemistry. <i>ACS Symposium Series</i> , 2019, , 239-256.	0.5	2
17	Charge separation and dissipation in molecular wires under a light radiation. <i>Organic Electronics</i> , 2018, 58, 94-104.	2.6	1
18	Interlayer-Decoupled Sc-Based Mxene with High Carrier Mobility and Strong Light-Harvesting Ability. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6915-6920.	4.6	49

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19	Stark control of electrons along nanojunctions. <i>Nature Communications</i> , 2018, 9, 2070.	12.8	32
20	Site-Specific Photodecomposition in Conjugated Energetic Materials. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6055-6061.	2.5	8
21	Mixed-Valence Superstructure Assembled from a Mixed-Valence Host-Guest Complex. <i>Journal of the American Chemical Society</i> , 2018, 140, 9387-9391.	13.7	18
22	Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. <i>ACS Nano</i> , 2018, 12, 8415-8422.	14.6	75
23	Multiscale Study of Plasmonic Scattering and Light Trapping Effect in Silicon Nanowire Array Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 571-575.	4.6	19
24	Conical Nanopores for Efficient Ion Pumping and Desalination. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2842-2848.	4.6	39
25	Advantages of Conical Pores for Ion Pumps. <i>Journal of Physical Chemistry C</i> , 2017, 121, 161-168.	3.1	23
26	Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes. <i>Nanoscale</i> , 2016, 8, 13168-13173.	5.6	12
27	Fundamental Limitations to Plasmonic Hot-Carrier Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1852-1858.	4.6	64
28	Supramolecular Double-Helix Formation by Diastereoisomeric Conformations of Configurationally Enantiomeric Macrocycles. <i>Journal of the American Chemical Society</i> , 2016, 138, 14469-14480.	13.7	42
29	Kinetic Master Equation Modeling of an Artificial Protein Pump. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14495-14501.	3.1	6
30	Multidimensional resonant nonlinear spectroscopy with coherent broadband x-ray pulses. <i>Physica Scripta</i> , 2016, T169, 014002.	2.5	30
31	Supramolecular Gelation of Rigid Triangular Macrocycles through Rings of Multiple H ₂ O Interactions Acting Cooperatively. <i>Journal of Organic Chemistry</i> , 2016, 81, 2581-2588.	3.2	27
32	A variational approach for dissipative quantum transport in a wide parameter space. <i>Journal of Chemical Physics</i> , 2015, 143, 104112.	3.0	4
33	QUANTUM MECHANICAL MODELING OF ELECTRON-PHOTON INTERACTIONS IN NANOSCALE DEVICES (Invited) Tj ETQq1 1 0,784314	4.4	2
34	An approximate framework for quantum transport calculation with model order reduction. <i>Journal of Computational Physics</i> , 2015, 286, 49-61.	3.8	3
35	Electroluminescence in Molecular Junctions: A Diagrammatic Approach. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4304-4315.	5.3	11
36	Dissipative time-dependent quantum transport theory: Quantum interference and phonon induced decoherence dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 164101.	3.0	15

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37	A multiscale quantum mechanics/electromagnetics method for device simulations. <i>Chemical Society Reviews</i> , 2015, 44, 1763-1776.	38.1	27
38	Multiscale Modeling of Plasmon-Enhanced Power Conversion Efficiency in Nanostructured Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4410-4416.	4.6	24
39	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.	3.0	12
40	Light-Driven Ca ²⁺ Ion Pump: How Does It Work?. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15110-15117.	2.6	4
41	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
42	Time-dependent density functional theory for quantum transport. <i>Frontiers of Physics</i> , 2014, 9, 698-710.	5.0	16
43	Interference and Molecular Transport—A Dynamical View: Time-Dependent Analysis of Disubstituted Benzenes. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2748-2752.	4.6	40
44	Quantum-Mechanical Prediction of Nanoscale Photovoltaics. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1272-1277.	4.6	30
45	Hot-Electron-Induced Dissociation of H ₂ on Gold Nanoparticles Supported on SiO ₂ . <i>Journal of the American Chemical Society</i> , 2014, 136, 64-67.	13.7	458
46	Quantum transport through an array of quantum dots. <i>Nanoscale</i> , 2013, 5, 169-173.	5.6	22
47	Time-dependent quantum transport theory and its applications to graphene nanoribbons. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 2481-2494.	1.5	22
48	First-principles time-dependent quantum transport theory. <i>Physical Review B</i> , 2013, 87, .	3.2	51
49	Dissipative time-dependent quantum transport theory. <i>Journal of Chemical Physics</i> , 2013, 138, 164121.	3.0	25