Xiao Zheng

List of Publications by Year
in descending order

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134	4,890	94433 37	106344 65
papers	citations	h-index	g-index

140	140	140	3911
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improving Density Functional Prediction of Molecular Thermochemical Properties with a Machine-Learning-Corrected Generalized Gradient Approximation. Journal of Physical Chemistry A, 2022, 126, 970-978.	2.5	4
2	Computational characterization of nanosystems. Chinese Journal of Chemical Physics, 2022, 35, 1-15.	1.3	2
3	Origin of Asymmetric Splitting of Kondo Peak in Spin-Polarized Scanning Tunneling Spectroscopy: Insights from First-Principles-Based Simulations. Journal of Physical Chemistry Letters, 2022, 13, 2094-2100.	4.6	6
4	Competition between Spin Excitation and Kondo Correlation in Magnetic Molecular Junctions: Theoretical Insight from First-principles-based Simulations. Current Chinese Science, 2022, 2, 310-324.	0.5	0
5	Study the mixed valence problem in asymmetric Anderson model: Fanoâ€“Kondo resonance around Fermi level. Journal of Physics Condensed Matter, 2022, 34, 255601.	1.8	1
6	Bio-inspired synthesis of transition-metal oxide hybrid ultrathin nanosheets for enhancing the cycling stability in lithium-ion batteries. Nano Research, 2022, 15, 5064-5071.	10.4	8
7	Identification of Cu(100)/Cu(111) Interfaces as Superior Active Sites for CO Dimerization During CO₂ Electroreduction. Journal of the American Chemical Society, 2022, 144, 259-269.	13.7	171
8	A General Strategy to Immobilize Singleâ€Atom Catalysts in Metalâ€“Organic Frameworks for Enhanced Photocatalysis. Advanced Materials, 2022, 34, e2109203.	21.0	80
9	Reduction-Controlled Atomic Migration for Single Atom Alloy Library. Nano Letters, 2022, 22, 4232-4239.	9.1	20
10	Universal time-domain Prony fitting decomposition for optimized hierarchical quantum master equations. Journal of Chemical Physics, 2022, 156, .	3.0	23
11	A statistical quasi-particles thermofield theory with Gaussian environments: Systemâ€“bath entanglement theorem for nonequilibrium correlation functions. Journal of Chemical Physics, 2022, 157, 044102.	3.0	7
12	Quantum Mechanical Simulation of Electron Dynamics on Surfaces of Materials. Springer Series in Materials Science, 2021, , 115-136.	0.6	0
13	Effect of quantum resonances on local temperature in nonequilibrium open systems. Physical Review B, 2021, 103, .	3.2	5
14	An Efficient Turingâ€Type Ag₂Seâ€CoSe₂ Multiâ€Interfacial Oxygenâ€Evolving Electrocatalyst**. Angewandte Chemie - International Edition, 2021, 60, 6553-6560.	13.8	45
15	An Efficient Turingâ€Type Ag 2 Seâ€CoSe 2 Multiâ€Interfacial Oxygenâ€Evolving Electrocatalyst**. Angewandte Chemie, 2021, 133, 6627-6634.	2.0	7
16	RÃ¼cktitelbild: An Efficient Turingâ€Type Ag₂Seâ€CoSe₂ Multiâ€Interfacial Oxygenâ€Evolving Electrocatalyst (Angew. Chem. 12/2021). Angewandte Chemie, 2021, 133, 6904-6904.	2.0	0
17	Enhancing Circular Dichroism Signals with Vector Beams. Physical Review Letters, 2021, 126, 123001.	7.8	12
18	Understanding the Sub-meV Precision-Tuning of Magnetic Anisotropy of Single-Molecule Junction. Journal of Physical Chemistry C, 2021, 125, 6990-6997.	3.1	8

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19	Unveiling the High Catalytic Activity of a Dinuclear Iron Complex for the Oxygen Evolution Reaction. Inorganic Chemistry, 2021, 60, 7297-7305.	4.0	6
20	Boosting the oxygen evolution activity over cobalt nitride nanosheets through optimizing the electronic configuration. Applied Catalysis B: Environmental, 2021, 286, 119894.	20.2	56
21	Tracking Electron Dynamics of Single Molecules in Scanning Tunneling Microscopy Junctions with Laser Pulses. Journal of Physical Chemistry Letters, 2021, 12, 6398-6404.	4.6	3
22	Marcusâ€™ electron transfer rate revisited via a Rice-Ramsperger-Kassel-Marcus analogue: A unified formalism for linear and nonlinear solvation scenarios. Chinese Journal of Chemical Physics, 2021, 34, 462-470.	1.3	3
23	Phase-Controlled 1T Transition-Metal Dichalcogenide-Based Multidimensional Hybrid Nanostructures. CCS Chemistry, 2021, 3, 58-68.	7.8	6
24	Adiabatic terminator for fermionic hierarchical equations of motion. Chinese Journal of Chemical Physics, 2021, 34, 905-914.	1.3	6
25	Highâ€Curvature Transitionâ€Metal Chalcogenide Nanostructures with a Pronounced Proximity Effect Enable Fast and Selective CO₂ Electroreduction. Angewandte Chemie - International Edition, 2020, 59, 8706-8712.	13.8	145
26	Highâ€Curvature Transitionâ€Metal Chalcogenide Nanostructures with a Pronounced Proximity Effect Enable Fast and Selective CO₂ Electroreduction. Angewandte Chemie, 2020, 132, 8784-8790.	2.0	37
27	Equilibrium and transient thermodynamics: A unified dissipaton-space approach. Journal of Chemical Physics, 2020, 153, 154111.	3.0	14
28	Thermodynamic free-energy spectrum theory for open quantum systems. Journal of Chemical Physics, 2020, 153, 214115.	3.0	10
29	Stochastic equation of motion approach to fermionic dissipative dynamics. I. Formalism. Journal of Chemical Physics, 2020, 152, 204105.	3.0	13
30	Stochastic equation of motion approach to fermionic dissipative dynamics. II. Numerical implementation. Journal of Chemical Physics, 2020, 152, 204106.	3.0	12
31	Enhanced photocurrent in heterostructures formed between CH₃NH₃PbI₃perovskite films and graphdiyne. Physical Chemistry Chemical Physics, 2020, 22, 6239-6246.	2.8	10
32	Unit cell consistency of maximally localized Wannier functions. Electronic Structure, 2020, 2, 014001.	2.8	4
33	Hierarchical equations of motion method based on Fano spectrum decomposition for low temperature environments. Journal of Chemical Physics, 2020, 152, 064107.	3.0	42
34	Molecular molds for regularizing Kondo states at atom/metal interfaces. Nature Communications, 2020, 11, 2566.	12.8	19
35	Density Functional Prediction of Quasiparticle, Excitation, and Resonance Energies of Molecules With a Global Scaling Correction Approach. Frontiers in Chemistry, 2020, 8, 588808.	3.6	4
36	Scaledâ€Up Synthesis of Amorphous NiFeMo Oxides and Their Rapid Surface Reconstruction for Superior Oxygen Evolution Catalysis. Angewandte Chemie - International Edition, 2019, 58, 15772-15777.	13.8	426

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37	Scaledâ€Up Synthesis of Amorphous NiFeMo Oxides and Their Rapid Surface Reconstruction for Superior Oxygen Evolution Catalysis. Angewandte Chemie, 2019, 131, 15919-15924.	2.0	62
38	Stochastic Representation of Non-Markovian Fermionic Quantum Dissipation. Physical Review Letters, 2019, 123, 050601.	7.8	14
39	Highly efficient and accurate sum-over-poles expansion of Fermi and Bose functions at near zero temperatures: Fano spectrum decomposition scheme. Journal of Chemical Physics, 2019, 151, 024110.	3.0	42
40	Local temperatures out of equilibrium. Physics Reports, 2019, 830, 1-66.	25.6	22
41	Theoretical investigation of real-time charge dynamics in open systems coupled to bulk materials. Journal of Chemical Physics, 2019, 150, 174119.	3.0	4
42	Equilibria between the K+ binding and cation vacancy conformations of potassium channels. Protein and Cell, 2019, 10, 533-537.	11.0	1
43	Polymorphic cobalt diselenide as extremely stable electrocatalyst in acidic media via a phase-mixing strategy. Nature Communications, 2019, 10, 5338.	12.8	65
44	Evolution of Magnetic Anisotropy of an Organometallic Molecule in a Mechanically Controlled Break Junction: The Roles of Connecting Electrodes. Journal of Physical Chemistry C, 2019, 123, 30754-30764.	3.1	8
45	First-Principles Study of Mixed Cation Methylammonium-Formamidinium Hybrid Perovskite. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2019, 35, 69-75.	4.9	7
46	Precise Control of Local Spin States in an Adsorbed Magnetic Molecule with an STM Tip: Theoretical Insights from First-Principles-Based Simulation. Journal of Physical Chemistry Letters, 2018, 9, 2418-2425.	4.6	32
47	Synthesis of Subâ€2â€…nm Ironâ€Doped NiSe₂ Nanowires and Their Surfaceâ€Confined Oxidation for Oxygen Evolution Catalysis. Angewandte Chemie, 2018, 130, 4084-4088.	2.0	33
48	Synthesis of Subâ€2â€…nm Ironâ€Doped NiSe₂ Nanowires and Their Surfaceâ€Confined Oxidation for Oxygen Evolution Catalysis. Angewandte Chemie - International Edition, 2018, 57, 4020-4024.	13.8	133
49	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. National Science Review, 2018, 5, 203-215.	9.5	110
50	Theoretical insights into the reactivity of Fe-based catalysts for water oxidation: the role of electron-withdrawing groups. Physical Chemistry Chemical Physics, 2018, 20, 14919-14926.	2.8	5
51	Statistical quasi-particle theory for open quantum systems. Molecular Physics, 2018, 116, 780-812.	1.7	20
52	Accurate density functional prediction of molecular electron affinity with the scaling corrected Kohnâ€“Sham frontier orbital energies. Molecular Physics, 2018, 116, 927-934.	1.7	10
53	Manipulation of spin and magnetic anisotropy in bilayer magnetic molecular junctions. Physical Chemistry Chemical Physics, 2018, 20, 26396-26404.	2.8	18
54	Quantum entanglement of parallel-coupled double quantum dots: A theoretical study using the hierarchical equations of motion approach. Chinese Journal of Chemical Physics, 2018, 31, 510-516.	1.3	5

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55	Kondo-peak splitting and resonance enhancement caused by interdot tunneling in coupled double quantum dots. Physical Review B, 2018, 98, .	3.2	18
56	On the exact truncation tier of fermionic hierarchical equations of motion. Journal of Chemical Physics, 2018, 148, 234108.	3.0	25
57	Temperature-dependent ESR and computational studies on antiferromagnetic electron transfer in the yeast NADH dehydrogenase Ndi1. Physical Chemistry Chemical Physics, 2017, 19, 4849-4854.	2.8	8
58	Fokkerâ€“Planck quantum master equation for mixed quantumâ€“semiclassical dynamics. Journal of Chemical Physics, 2017, 146, 024104.	3.0	12
59	Corrected Kondo temperature beyond the conventional Kondo scaling limit. Journal of Physics Condensed Matter, 2017, 29, 175601.	1.8	8
60	Enhanced Photovoltaic Properties Induced by Ferroelectric Domain Structures in Organometallic Halide Perovskites. Journal of Physical Chemistry C, 2017, 121, 11151-11158.	3.1	44
61	Spin switch in iron phthalocyanine on Au(111) surface by hydrogen adsorption. Journal of Chemical Physics, 2017, 147, 134701.	3.0	17
62	Low-frequency logarithmic discretization of the reservoir spectrum for improving the efficiency of hierarchical equations of motion approach. Journal of Chemical Physics, 2017, 147, 074111.	3.0	23
63	Improving the Performance of Long-Range-Corrected Exchange-Correlation Functional with an Embedded Neural Network. Journal of Physical Chemistry A, 2017, 121, 7273-7281.	2.5	37
64	Efficient steady-state solver for hierarchical quantum master equations. Journal of Chemical Physics, 2017, 147, 044105.	3.0	22
65	Davydov Collective Vibrational Modes and Infrared Spectrum Features in Aniline Crystal: Influence of Geometry Change Induced by van der Waals Interactions. Journal of Physical Chemistry C, 2017, 121, 18867-18875.	3.1	1
66	Electronic Structures and Thermoelectric Properties of Two-Dimensional MoS2/MoSe2 Heterostructures. Chinese Journal of Chemical Physics, 2016, 29, 445-452.	1.3	9
67	HEOM-QUICK: a program for accurate, efficient, and universal characterization of strongly correlated quantum impurity systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 608-638.	14.6	87
68	Thermodynamic meaning of local temperature of nonequilibrium open quantum systems. Physical Review B, 2016, 94, .	3.2	15
69	Generating giant and tunable nonlinearity in a macroscopic mechanical resonator from a single chemical bond. Nature Communications, 2016, 7, 11517.	12.8	21
70	Minimum-exponents ansatz for molecular dynamics and quantum dissipation. Journal of Chemical Physics, 2016, 145, 204110.	3.0	11
71	Rational Ligand Design for an Efficient Biomimetic Water Splitting Complex. Journal of Physical Chemistry A, 2016, 120, 10033-10042.	2.5	6
72	Anisotropy induced Kondo splitting in a mechanically stretched molecular junction: A first-principles based study. Journal of Chemical Physics, 2016, 144, 034101.	3.0	27

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73	Dissipation equation of motion approach to open quantum systems. Frontiers of Physics, 2016, 11, 1.	5.0	58
74	Environment-modulated Kondo phenomena in FePc/Au(111) adsorption systems. Physical Review B, 2016, 93, .	3.2	37
75	Kondo screening and spin excitation in few-layer CoPc molecular assembly stacking on Pb(111) surface: A DFT+HEOM study. Journal of Chemical Physics, 2016, 145, 154301.	3.0	21
76	Local temperatures of strongly-correlated quantum dots out of equilibrium. Physical Review B, 2015, 91, .	3.2	29
77	Orbital relaxation effects on Kohnâ€“Sham frontier orbital energies in density functional theory. Journal of Chemical Physics, 2015, 142, 154113.	3.0	18
78	Heavy Metal Detection: Facet-Dependent Stripping Behavior of Cu₂ O Microcrystals Toward Lead Ions: A Rational Design for the Determination of Lead Ions (Small 21/2015). Small, 2015, 11, 2584-2584.	10.0	1
79	Local Scaling Correction for Reducing Delocalization Error in Density Functional Approximations. Physical Review Letters, 2015, 114, 053001.	7.8	69
80	Facet-Dependent Stripping Behavior of Cu₂O Microcrystals Toward Lead Ions: A Rational Design for the Determination of Lead Ions. Small, 2015, 11, 2493-2498.	10.0	47
81	Current noise spectra and mechanisms with dissipaton equation of motion theory. Journal of Chemical Physics, 2015, 142, 234108.	3.0	35
82	Improving the efficiency of hierarchical equations of motion approach and application to coherent dynamics in Aharonovâ€“Bohm interferometers. Journal of Chemical Physics, 2015, 142, 104112.	3.0	40
83	Dissipaton equation of motion for system-and-bath interference dynamics. Science China Chemistry, 2015, 58, 1816-1824.	8.2	17
84	Nonperturbative spinâ€“boson and spinâ€“spin dynamics and nonlinear Fano interferences: A unified dissipaton theory based study. Journal of Chemical Physics, 2015, 142, 024112.	3.0	38
85	Time-dependent density functional theory for open systems with a positivity-preserving decomposition scheme for environment spectral functions. Journal of Chemical Physics, 2015, 142, 144112.	3.0	8
86	Scaling correction approaches for reducing delocalization error in density functional approximations. Science China Chemistry, 2015, 58, 1825-1844.	8.2	12
87	Thermopower of few-electron quantum dots with Kondo correlations. Physical Review B, 2014, 90, .	3.2	35
88	Understanding the Kondo resonance in the d-CoPc/Au(111) adsorption system. Journal of Chemical Physics, 2014, 141, 084713.	3.0	38
89	Complex absorbing potential based Lorentzian fitting scheme and time dependent quantum transport. Journal of Chemical Physics, 2014, 141, 164122.	3.0	21
90	Hierarchical equations of motion for an impurity solver in dynamical mean-field theory. Physical Review B, 2014, 90, .	3.2	39

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91	Time-dependent density-functional theory for open electronic systems. Science China Chemistry, 2014, 57, 26-35.	8.2	6
92	First-Principles Study on Structural and Chemical Asymmetry of a Biomimetic Water-Splitting Dimanganese Complex. Journal of Chemical Theory and Computation, 2013, 9, 1073-1080.	5.3	8
93	Structural Stability of La₂Ce₂O₇ as a Proton Conductor: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 20379-20386.	3.1	26
94	Time-dependent density-functional theory for real-time electronic dynamics on material surfaces. Physical Review B, 2013, 88, .	3.2	27
95	Gauge-invariant and current-continuous microscopic ac quantum transport theory. European Physical Journal B, 2013, 86, 1.	1.5	5
96	A nonempirical scaling correction approach for density functional methods involving substantial amount of Hartreeâ€“Fock exchange. Journal of Chemical Physics, 2013, 138, 174105.	3.0	23
97	Timeâ€dependent quantum transport theory and its applications to graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2013, 250, 2481-2494.	1.5	22
98	Electrochemical and Density Functional Theory Investigation on High Selectivity and Sensitivity of Exfoliated Nano-Zirconium Phosphate toward Lead(II). Analytical Chemistry, 2013, 85, 3984-3990.	6.5	66
99	Time-dependent density functional theory quantum transport simulation in non-orthogonal basis. Journal of Chemical Physics, 2013, 139, 224111.	3.0	23
100	Kondo Memory in Driven Strongly Correlated Quantum Dots. Physical Review Letters, 2013, 111, 086601.	7.8	68
101	Hierarchical Liouville-space approach to nonequilibrium dynamical properties of quantum impurity systems. Physical Review B, 2013, 88, .	3.2	39
102	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66
103	Hierarchical Liouville-Space Approach for Accurate and Universal Characterization of Quantum Impurity Systems. Physical Review Letters, 2012, 109, 266403.	7.8	136
104	Time-dependent quantum transport: An efficient method based on Liouville-von-Neumann equation for single-electron density matrix. Journal of Chemical Physics, 2012, 137, 044113.	3.0	46
105	Firstâ€principles Liouvilleâ€“von Neumann equation for open systems and its applications. Physica Status Solidi (B): Basic Research, 2012, 249, 270-275.	1.5	9
106	Existence of time-dependent density-functional theory for open electronic systems: Time-dependent holographic electron density theorem. Physical Chemistry Chemical Physics, 2011, 13, 14358.	2.8	20
107	Single-Molecule Conductance of Pyridine-Terminated Dithienylethene Switch Molecules. ACS Nano, 2011, 5, 5115-5123.	14.6	95
108	Improving Band Gap Prediction in Density Functional Theory from Molecules to Solids. Physical Review Letters, 2011, 107, 026403.	7.8	161

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109	Time-dependent versus static quantum transport simulations beyond linear response. Physical Review B, 2011, 83, .	3.2	47
110	Time-Dependent Current Distributions of a Two-Terminal Carbon Nanotube-Based Electronic Device. Journal of Physical Chemistry B, 2011, 115, 5519-5525.	2.6	14
111	Computer simulation of Feynmanâ€™s ratchet and pawl system. Physical Review E, 2010, 81, 061104.	2.1	5
112	Conductive junctions with parallel graphene sheets. Journal of Chemical Physics, 2010, 132, 114703.	3.0	11
113	Time-dependent density functional theory for quantum transport. Journal of Chemical Physics, 2010, 133, 114101.	3.0	96
114	Numerical approach to time-dependent quantum transport and dynamical Kondo transition. Journal of Chemical Physics, 2009, 130, 164708.	3.0	104
115	Transient electronic dynamics of noninteracting open systems beyond linear response. Journal of Physics Condensed Matter, 2009, 21, 355301.	1.8	14
116	Complex non-Markovian effect on time-dependent quantum transport. Journal of Chemical Physics, 2009, 130, 124508.	3.0	44
117	The roles of apex dipoles and field penetration in the physics of charged, field emitting, single-walled carbon nanotubes. Journal of Applied Physics, 2008, 104, 014310.	2.5	33
118	Exact dynamics of dissipative electronic systems and quantum transport: Hierarchical equations of motion approach. Journal of Chemical Physics, 2008, 128, 234703.	3.0	336
119	Dynamic electronic response of a quantum dot driven by time-dependent voltage. Journal of Chemical Physics, 2008, 129, 184112.	3.0	61
120	Dynamic Coulomb blockade in single-lead quantum dots. New Journal of Physics, 2008, 10, 093016.	2.9	56
121	Dynamic admittance of carbon nanotube-based molecular electronic devices and their equivalent electric circuit. Nanotechnology, 2008, 19, 495203.	2.6	42
122	Dissipative dynamic theory for open many-electron systems: Hierarchical equations-of-motion approach. , 2008, , .		1
123	First-Principles Method for Open Electronic Systems. , 2008, , 235-243.		1
124	Maxwellâ€™s demon and Smoluchowskiâ€™s trap door. Physical Review E, 2007, 75, 041109.	2.1	6
125	Atomic Decoration for Improving the Efficiency of Field Electron Emission of Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 4939-4945.	3.1	17
126	Time-dependent density-functional theory for open systems. Physical Review B, 2007, 75, .	3.2	163

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127	Effect of temperature on field emission from a micrometer-long single-walled carbon nanotube. Physical Review B, 2006, 73, .	3.2	4
128	Some Recent Progresses in Density-Functional Theory: Efficiency, Accuracy, and Applicability. Journal of Computational and Theoretical Nanoscience, 2006, 3, 857-863.	0.4	8
129	Quantum mechanical understanding of field dependence of the apex barrier of a single-wall carbon nanotube. Physical Review B, 2005, 72, .	3.2	26
130	Quantum-Mechanical Investigation of Field-Emission Mechanism of a Micrometer-Long Single-Walled Carbon Nanotube. Physical Review Letters, 2004, 92, 106803.	7.8	148
131	A generalized exchange-correlation functional: the Neural-Networks approach. Chemical Physics Letters, 2004, 390, 186-192.	2.6	42
132	Reaction on a Rink: Kondo-Enhanced Heterogeneous Single-Atom Catalysis. Journal of Physical Chemistry C, 0, , .	3.1	0
133	Magnetic Field Dependent Kondo Transport through Double Quantum Dots System. Annalen Der Physik, 0, , 2100439.	2.4	0
134	Nonequilibrium work distributions in quantum impurity system-bath mixing processes. Journal of Chemical Physics, 0, , .	3.0	5