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	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
2	Exact dynamics of dissipative electronic systems and quantum transport: Hierarchical equations of motion approach. Journal of Chemical Physics, 2008, 128, 234703.	3.0	336
3	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
4	Time-dependent density-functional theory for open systems. Physical Review B, 2007, 75, .	3.2	163
5	Improving Band Gap Prediction in Density Functional Theory from Molecules to Solids. Physical Review Letters, 2011, 107, 026403.	7.8	161
6	Quantum-Mechanical Investigation of Field-Emission Mechanism of a Micrometer-Long Single-Walled Carbon Nanotube. Physical Review Letters, 2004, 92, 106803.	7.8	148
7	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
8	Hierarchical Liouville-Space Approach for Accurate and Universal Characterization of Quantum Impurity Systems. Physical Review Letters, 2012, 109, 266403.	7.8	136
9	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
10	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. National Science Review, 2018, 5, 203-215.	9.5	110
11	Numerical approach to time-dependent quantum transport and dynamical Kondo transition. Journal of Chemical Physics, 2009, 130, 164708.	3.0	104
12	Time-dependent density functional theory for quantum transport. Journal of Chemical Physics, 2010, 133, 114101.	3.0	96
13	Single-Molecule Conductance of Pyridine-Terminated Dithienylethene Switch Molecules. ACS Nano, 2011, 5, 5115-5123.	14.6	95
14	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
15	A General Strategy to Immobilize Singleâ€Atom Catalysts in Metalâ€“Organic Frameworks for Enhanced Photocatalysis. Advanced Materials, 2022, 34, e2109203.	21.0	80
16	Local Scaling Correction for Reducing Delocalization Error in Density Functional Approximations. Physical Review Letters, 2015, 114, 053001.	7.8	69
17	Kondo Memory in Driven Strongly Correlated Quantum Dots. Physical Review Letters, 2013, 111, 086601.	7.8	68
18	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66

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19	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
20	Polymorphic cobalt diselenide as extremely stable electrocatalyst in acidic media via a phase-mixing strategy. Nature Communications, 2019, 10, 5338.	12.8	65
21	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
22	Dynamic electronic response of a quantum dot driven by time-dependent voltage. Journal of Chemical Physics, 2008, 129, 184112.	3.0	61
23	Dissipation equation of motion approach to open quantum systems. Frontiers of Physics, 2016, 11, 1.	5.0	58
24	Dynamic Coulomb blockade in single-lead quantum dots. New Journal of Physics, 2008, 10, 093016.	2.9	56
25	Boosting the oxygen evolution activity over cobalt nitride nanosheets through optimizing the electronic configuration. Applied Catalysis B: Environmental, 2021, 286, 119894.	20.2	56
26	Time-dependent versus static quantum transport simulations beyond linear response. Physical Review B, 2011, 83, .	3.2	47
27	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
28	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
29	An Efficient Turingâ€Type Ag₂Seâ€CoSe₂ Multiâ€Interfacial Oxygenâ€Evolving Electrocatalyst**. Angewandte Chemie - International Edition, 2021, 60, 6553-6560.	13.8	45
30	Complex non-Markovian effect on time-dependent quantum transport. Journal of Chemical Physics, 2009, 130, 124508.	3.0	44
31	Enhanced Photovoltaic Properties Induced by Ferroelectric Domain Structures in Organometallic Halide Perovskites. Journal of Physical Chemistry C, 2017, 121, 11151-11158.	3.1	44
32	A generalized exchange-correlation functional: the Neural-Networks approach. Chemical Physics Letters, 2004, 390, 186-192.	2.6	42
33	Dynamic admittance of carbon nanotube-based molecular electronic devices and their equivalent electric circuit. Nanotechnology, 2008, 19, 495203.	2.6	42
34	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
35	Hierarchical equations of motion method based on Fano spectrum decomposition for low temperature environments. Journal of Chemical Physics, 2020, 152, 064107.	3.0	42
36	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

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37	Hierarchical Liouville-space approach to nonequilibrium dynamical properties of quantum impurity systems. Physical Review B, 2013, 88, .	3.2	39
38	Hierarchical equations of motion for an impurity solver in dynamical mean-field theory. Physical Review B, 2014, 90, .	3.2	39
39	Understanding the Kondo resonance in the d-CoPc/Au(111) adsorption system. Journal of Chemical Physics, 2014, 141, 084713.	3.0	38
40	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
41	Environment-modulated Kondo phenomena in FePc/Au(111) adsorption systems. Physical Review B, 2016, 93, .	3.2	37
42	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
43	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
44	Thermopower of few-electron quantum dots with Kondo correlations. Physical Review B, 2014, 90, .	3.2	35
45	Current noise spectra and mechanisms with dissipaton equation of motion theory. Journal of Chemical Physics, 2015, 142, 234108.	3.0	35
46	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
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	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
49	Local temperatures of strongly-correlated quantum dots out of equilibrium. Physical Review B, 2015, 91, .	3.2	29
50	Time-dependent density-functional theory for real-time electronic dynamics on material surfaces. Physical Review B, 2013, 88, .	3.2	27
51	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
52	Quantum mechanical understanding of field dependence of the apex barrier of a single-wall carbon nanotube. Physical Review B, 2005, 72, .	3.2	26
53	Structural Stability of La₂Ce₂O₇ as a Proton Conductor: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 20379-20386.	3.1	26
54	On the exact truncation tier of fermionic hierarchical equations of motion. Journal of Chemical Physics, 2018, 148, 234108.	3.0	25

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55	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
56	Time-dependent density functional theory quantum transport simulation in non-orthogonal basis. Journal of Chemical Physics, 2013, 139, 224111.	3.0	23
57	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
58	Universal time-domain Prony fitting decomposition for optimized hierarchical quantum master equations. Journal of Chemical Physics, 2022, 156, .	3.0	23
59	Timeâ€dependent quantum transport theory and its applications to graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2013, 250, 2481-2494.	1.5	22
60	Efficient steady-state solver for hierarchical quantum master equations. Journal of Chemical Physics, 2017, 147, 044105.	3.0	22
61	Local temperatures out of equilibrium. Physics Reports, 2019, 830, 1-66.	25.6	22
62	Complex absorbing potential based Lorentzian fitting scheme and time dependent quantum transport. Journal of Chemical Physics, 2014, 141, 164122.	3.0	21
63	Generating giant and tunable nonlinearity in a macroscopic mechanical resonator from a single chemical bond. Nature Communications, 2016, 7, 11517.	12.8	21
64	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
65	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
66	Statistical quasi-particle theory for open quantum systems. Molecular Physics, 2018, 116, 780-812.	1.7	20
67	Reduction-Controlled Atomic Migration for Single Atom Alloy Library. Nano Letters, 2022, 22, 4232-4239.	9.1	20
68	Molecular molds for regularizing Kondo states at atom/metal interfaces. Nature Communications, 2020, 11, 2566.	12.8	19
69	Orbital relaxation effects on Kohnâ€“Sham frontier orbital energies in density functional theory. Journal of Chemical Physics, 2015, 142, 154113.	3.0	18
70	Manipulation of spin and magnetic anisotropy in bilayer magnetic molecular junctions. Physical Chemistry Chemical Physics, 2018, 20, 26396-26404.	2.8	18
71	Kondo-peak splitting and resonance enhancement caused by interdot tunneling in coupled double quantum dots. Physical Review B, 2018, 98, .	3.2	18
72	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

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73	Dissipaton equation of motion for system-and-bath interference dynamics. Science China Chemistry, 2015, 58, 1816-1824.	8.2	17
74	Spin switch in iron phthalocyanine on Au(111) surface by hydrogen adsorption. Journal of Chemical Physics, 2017, 147, 134701.	3.0	17
75	Thermodynamic meaning of local temperature of nonequilibrium open quantum systems. Physical Review B, 2016, 94, .	3.2	15
76	Transient electronic dynamics of noninteracting open systems beyond linear response. Journal of Physics Condensed Matter, 2009, 21, 355301.	1.8	14
77	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
78	Stochastic Representation of Non-Markovian Fermionic Quantum Dissipation. Physical Review Letters, 2019, 123, 050601.	7.8	14
79	Equilibrium and transient thermodynamics: A unified dissipaton-space approach. Journal of Chemical Physics, 2020, 153, 154111.	3.0	14
80	Stochastic equation of motion approach to fermionic dissipative dynamics. I. Formalism. Journal of Chemical Physics, 2020, 152, 204105.	3.0	13
81	Scaling correction approaches for reducing delocalization error in density functional approximations. Science China Chemistry, 2015, 58, 1825-1844.	8.2	12
82	Fokkerâ€“Planck quantum master equation for mixed quantumâ€“semiclassical dynamics. Journal of Chemical Physics, 2017, 146, 024104.	3.0	12
83	Stochastic equation of motion approach to fermionic dissipative dynamics. II. Numerical implementation. Journal of Chemical Physics, 2020, 152, 204106.	3.0	12
84	Enhancing Circular Dichroism Signals with Vector Beams. Physical Review Letters, 2021, 126, 123001.	7.8	12
85	Conductive junctions with parallel graphene sheets. Journal of Chemical Physics, 2010, 132, 114703.	3.0	11
86	Minimum-exponents ansatz for molecular dynamics and quantum dissipation. Journal of Chemical Physics, 2016, 145, 204110.	3.0	11
87	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
88	Thermodynamic free-energy spectrum theory for open quantum systems. Journal of Chemical Physics, 2020, 153, 214115.	3.0	10
89	Enhanced photocurrent in heterostructures formed between CH₃NH₃PbI₃perovskite films and graphdiyne. Physical Chemistry Chemical Physics, 2020, 22, 6239-6246.	2.8	10
90	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

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91	Electronic Structures and Thermoelectric Properties of Two-Dimensional MoS2/MoSe2 Heterostructures. Chinese Journal of Chemical Physics, 2016, 29, 445-452.	1.3	9
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	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
94	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
95	Corrected Kondo temperature beyond the conventional Kondo scaling limit. Journal of Physics Condensed Matter, 2017, 29, 175601.	1.8	8
96	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
97	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
98	Some Recent Progresses in Density-Functional Theory: Efficiency, Accuracy, and Applicability. Journal of Computational and Theoretical Nanoscience, 2006, 3, 857-863.	0.4	8
99	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
100	An Efficient Turingâ€Type Ag 2 Seâ€CoSe 2 Multiâ€Interfacial Oxygenâ€Evolving Electrocatalyst**. Angewandte Chemie, 2021, 133, 6627-6634.	2.0	7
101	First-Principles Study of Mixed Cation Methylammonium-Formamidinium Hybrid Perovskite. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2019, 35, 69-75.	4.9	7
102	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
103	Maxwellâ€™s demon and Smoluchowskiâ€™s trap door. Physical Review E, 2007, 75, 041109.	2.1	6
104	Time-dependent density-functional theory for open electronic systems. Science China Chemistry, 2014, 57, 26-35.	8.2	6
105	Rational Ligand Design for an Efficient Biomimetic Water Splitting Complex. Journal of Physical Chemistry A, 2016, 120, 10033-10042.	2.5	6
106	Unveiling the High Catalytic Activity of a Dinuclear Iron Complex for the Oxygen Evolution Reaction. Inorganic Chemistry, 2021, 60, 7297-7305.	4.0	6
107	Phase-Controlled 1T Transition-Metal Dichalcogenide-Based Multidimensional Hybrid Nanostructures. CCS Chemistry, 2021, 3, 58-68.	7.8	6
108	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

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109	Adiabatic terminator for fermionic hierarchical equations of motion. Chinese Journal of Chemical Physics, 2021, 34, 905-914.	1.3	6
110	Computer simulation of Feynmanâ€™s ratchet and pawl system. Physical Review E, 2010, 81, 061104.	2.1	5
111	Gauge-invariant and current-continuous microscopic ac quantum transport theory. European Physical Journal B, 2013, 86, 1.	1.5	5
112	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
113	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
114	Effect of quantum resonances on local temperature in nonequilibrium open systems. Physical Review B, 2021, 103, .	3.2	5
115	Nonequilibrium work distributions in quantum impurity system-bath mixing processes. Journal of Chemical Physics, 0, , .	3.0	5
116	Effect of temperature on field emission from a micrometer-long single-walled carbon nanotube. Physical Review B, 2006, 73, .	3.2	4
117	Theoretical investigation of real-time charge dynamics in open systems coupled to bulk materials. Journal of Chemical Physics, 2019, 150, 174119.	3.0	4
118	Unit cell consistency of maximally localized Wannier functions. Electronic Structure, 2020, 2, 014001.	2.8	4
119	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
120	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
121	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
122	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
123	Computational characterization of nanosystems. Chinese Journal of Chemical Physics, 2022, 35, 1-15.	1.3	2
124	Dissipative dynamic theory for open many-electron systems: Hierarchical equations-of-motion approach. , 2008, , .		1
125	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
126	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

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127	Equilibria between the K+ binding and cation vacancy conformations of potassium channels. Protein and Cell, 2019, 10, 533-537.	11.0	1
128	First-Principles Method for Open Electronic Systems. , 2008, , 235-243.		1
129	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
130	Quantum Mechanical Simulation of Electron Dynamics on Surfaces of Materials. Springer Series in Materials Science, 2021, , 115-136.	0.6	0
131	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
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	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