Tao Zeng

List of Publications by Year
in descending order

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58	2,130	304743 22	233421 45
papers	citations	h-index	g-index

68	68	68	2296
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Do Diradicals Behave Like Radicals?. Chemical Reviews, 2019, 119, 11291-11351.	47.7	228
2	The Low-Lying Electronic States of Pentacene and Their Roles in Singlet Fission. Journal of the American Chemical Society, 2014, 136, 5755-5764.	13.7	197
3	A Direct Mechanism of Ultrafast Intramolecular Singlet Fission in Pentacene Dimers. ACS Central Science, 2016, 2, 316-324.	11.3	176
4	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. Chemical Reviews, 2016, 116, 8173-8192.	47.7	155
5	Electronegativity Seen as the Ground-State Average Valence Electron Binding Energy. Journal of the American Chemical Society, 2019, 141, 342-351.	13.7	139
6	Seeking Small Molecules for Singlet Fission: A Heteroatom Substitution Strategy. Journal of the American Chemical Society, 2014, 136, 12638-12647.	13.7	121
7	Direct mapping of curve-crossing dynamics in IBr by attosecond transient absorption spectroscopy. Science, 2019, 365, 79-83.	12.6	98
8	Theoretical Studies of Singlet Fission: Searching for Materials and Exploring Mechanisms. ChemPlusChem, 2018, 83, 146-182.	2.8	85
9	Design of Small Intramolecular Singlet Fission Chromophores: An Azaborine Candidate and General Small Size Effects. Journal of Physical Chemistry Letters, 2016, 7, 1351-1358.	4.6	66
10	Diradical Character as a Guiding Principle for the Insightful Design of Molecular Nanowires with an Increasing Conductance with Length. Nano Letters, 2018, 18, 7298-7304.	9.1	51
11	Through-Linker Intramolecular Singlet Fission: General Mechanism and Designing Small Chromophores. Journal of Physical Chemistry Letters, 2016, 7, 4405-4412.	4.6	48
12	Two-component natural spinors from two-step spin-orbit coupled wave functions. Journal of Chemical Physics, 2011, 134, 214107.	3.0	44
13	Structure-function relationships of hydroxyl radical scavenging and chromium-VI reducing cysteine-tripeptides derived from rye secalin. Food Chemistry, 2018, 254, 165-169.	8.2	43
14	Li-Filled, B-Substituted Carbon Clathrates. Journal of the American Chemical Society, 2015, 137, 12639-12652.	13.7	42
15	Effects of Spinâ€“Orbit Coupling on Covalent Bonding and the Jahnâ€“Teller Effect Are Revealed with the Natural Language of Spinors. Journal of Chemical Theory and Computation, 2011, 7, 2864-2875.	5.3	37
16	Thiophene Cation Intercalation to Improve Bandâ€Edge Integrity in Reducedâ€Dimensional Perovskites. Angewandte Chemie - International Edition, 2020, 59, 13977-13983.	13.8	36
17	Design of singlet fission chromophores with cyclic (alkyl)(amino) carbene building blocks. Journal of Chemical Physics, 2019, 150, 234306.	3.0	35
18	Captodative Substitution: A Strategy for Enhancing the Conductivity of Molecular Electronic Devices. Journal of Physical Chemistry C, 2018, 122, 3194-3200.	3.1	32

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19	Multireference study of spin-orbit coupling in the hydrides of the 6p-block elements using the model core potential method. Journal of Chemical Physics, 2010, 132, 074102.	3.0	30
20	A diabatization protocol that includes spin-orbit coupling. Journal of Chemical Physics, 2017, 146, 144103.	3.0	30
21	Identifying (BN)‹sub›2‹/sub›-pyrenes as a New Class of Singlet Fission Chromophores: Significance of Azaborine Substitution. Journal of Physical Chemistry Letters, 2018, 9, 2919-2927.	4.6	28
22	Model core potentials for studies of scalar-relativistic effects and spin-orbit coupling at Douglasâ€“Kroll level. I. Theory and applications to Pb and Bi. Journal of Chemical Physics, 2009, 131, 124109.	3.0	25
23	Diboron- and Diaza-Doped Anthracenes and Phenanthrenes: Their Electronic Structures for Being Singlet Fission Chromophores. Journal of Physical Chemistry A, 2020, 124, 8159-8172.	2.5	24
24	Relativistic Model Core Potential Study of the Au+Xe System. Journal of Physical Chemistry A, 2008, 112, 5236-5242.	2.5	23
25	Model core potentials of p-block elements generated considering the Douglasâ€“Kroll relativistic effects, suitable for accurate spin-orbit coupling calculations. Journal of Chemical Physics, 2010, 133, 114107.	3.0	21
26	Performance of dynamically weighted multiconfiguration self-consistent field and spin-orbit coupling calculations of diatomic molecules of Group 14 elements. Journal of Chemical Physics, 2011, 134, 024108.	3.0	20
27	Coherent electronic-vibrational dynamics in deuterium bromide probed via attosecond transient-absorption spectroscopy. Physical Review A, 2020, 101, .	2.5	20
28	General Formalism of Vibronic Hamiltonians for Tetrahedral and Octahedral Systems: Problems That Involve T, E States and t, e Vibrations. Journal of Chemical Theory and Computation, 2017, 13, 5004-5018.	5.3	18
29	Revisiting the (E + A) âŠ— (e + a) problems of polyatomic systems with trigonal symmetry: general expansions of their vibronic Hamiltonians. Physical Chemistry Chemical Physics, 2017, 19, 11098-11110.	2.8	18
30	New model core potentials for gold. Journal of Chemical Physics, 2009, 130, 204107.	3.0	17
31	Analytical Morse/long-Range model potential and predicted infrared and microwave spectra for a symmetric top-atom dimer: A case study of CH3Fâ€“He. Journal of Chemical Physics, 2014, 140, 214309.	3.0	16
32	Thiophene Cation Intercalation to Improve Bandâ€Edge Integrity in Reducedâ€Dimensional Perovskites. Angewandte Chemie, 2020, 132, 14081-14087.	2.0	16
33	General formalism for vibronic Hamiltonians in tetragonal symmetry and beyond. Physical Chemistry Chemical Physics, 2018, 20, 12312-12322.	2.8	13
34	Natural Spinors Reveal How the Spinâ€“Orbit Coupling Affects the Jahnâ€“Teller Distortions in the Hexafluorotungstate(V) Anion. Journal of Chemical Theory and Computation, 2012, 8, 3061-3071.	5.3	12
35	Designs of Singlet Fission Chromophores with a Diazadiborinine Framework**. ChemPhotoChem, 2020, 4, 5279-5287.	3.0	12
36	Tuning Spin-States of Carbynes and Silylynes: A Long Jump with One Leg. Journal of the American Chemical Society, 2014, 136, 13388-13398.	13.7	11

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37	Vibronic interaction in CO₃^{â˜} photo-detachment: Jahnâ€“Teller effects beyond structural distortion and general formalisms for vibronic Hamiltonians in trigonal symmetries. Physical Chemistry Chemical Physics, 2019, 21, 8679-8690.	2.8	11
38	Controlling the Thermal Stability and Volatility of Organogold(I) Compounds for Vapor Deposition with Complementary Ligand Design. European Journal of Inorganic Chemistry, 2019, 2019, 4927-4938.	2.0	11
39	An Iodabenzene Story. Journal of the American Chemical Society, 2017, 139, 7124-7129.	13.7	10
40	General formalism of vibronic Hamiltonians for tetrahedral and octahedral systems: Problems that involve A-type states and a-type vibrations. Chemical Physics, 2018, 515, 36-45.	1.9	9
41	Ab initio investigation of Br-3d core-excited states in HBr and HBr+ toward XUV probing of photochemical dynamics. Structural Dynamics, 2019, 6, 014101.	2.3	9
42	Structure-reactivity studies on hypervalent square-pyramidal dithieno[3,2-b:2â€²,3â€²-d]phospholes. Dalton Transactions, 2021, 50, 2243-2252.	3.3	9
43	Hamiltonian formalism of spinâ€“orbit Jahnâ€“Teller and pseudo-Jahnâ€“Teller problems in trigonal and tetragonal symmetries. Physical Chemistry Chemical Physics, 2019, 21, 18939-18957.	2.8	8
44	Unified Hamiltonian Formalism of Jahnâ€“Teller and Pseudo-Jahnâ€“Teller Problems in Axial Symmetries. Journal of Chemical Theory and Computation, 2021, 17, 4392-4402.	5.3	8
45	Zintl Ions within Framework Channels: The Complex Structure and Low-Temperature Transport Properties of Na4Ge13. Inorganic Chemistry, 2018, 57, 2002-2012.	4.0	7
46	Dicarbonyl anthracenes and phenanthrenes as singlet fission chromophores. Canadian Journal of Chemistry, 2022, 100, 520-529.	1.1	7
47	Design of singlet fission chromophores by the introduction of N-oxyl fragments. Journal of Chemical Physics, 2022, 156, 034303.	3.0	7
48	NaI revisited: Theoretical investigation of predissociation via ultrafast XUV transient absorption spectroscopy. Journal of Chemical Physics, 2019, 151, 204103.	3.0	6
49	VHEGEN: A vibronic Hamiltonian expansion generator for trigonal and tetragonal polyatomic systems. Computer Physics Communications, 2020, 247, 106946.	7.5	6
50	Bis(pentafluorophenyl)phenothiazylborane â€“ an intramolecular frustrated Lewis pair catalyst for stannane dehydrocoupling. Dalton Transactions, 2020, 49, 16054-16058.	3.3	6
51	Tuning the Ground State Symmetry of Acetylenyl Radicals. ACS Central Science, 2015, 1, 270-278.	11.3	5
52	Calibration of new model core potentials for main group elements. International Journal of Quantum Chemistry, 2009, 109, 3235-3245.	2.0	4
53	Potential generation and pathâ€integral <scp>M</scp>onte <scp>C</scp>arlo in study of microscopic superfluidity. International Journal of Quantum Chemistry, 2015, 115, 535-540.	2.0	4
54	Unified one-electron Hamiltonian formalism of spinâ€“orbit Jahnâ€“Teller and pseudo-Jahnâ€“Teller problems in axial symmetries. Journal of Chemical Physics, 2021, 155, 224108.	3.0	4

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55	A Computational Study of the Protoisomerization of Indigo and Its Imine Derivatives. Journal of Physical Chemistry A, 2016, 120, 7569-7576.	2.5	3
56	The synthesis, properties, and reactivity of Lewis acidic aminoboranes. Organic and Biomolecular Chemistry, 2021, 19, 4796-4802.	2.8	3
57	Unified one-electron Hamiltonian formalism of spinâ€“orbit Jahnâ€“Teller and pseudo-Jahnâ€“Teller problems in tetrahedral and octahedral symmetries. Journal of Chemical Physics, 2022, 157, .	3.0	2
58	Difficulty of the evaluation of the barrier height of an open-shell transition state between closed shell minima: the case of small C_{4n} rings. Journal of Chemical Physics, 0, , .	3.0	2