Tao Zeng

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3139349/publications.pdf

Version: 2024-02-01

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	Dicarbonyl anthracenes and phenanthrenes as singlet fission chromophores. Canadian Journal of Chemistry, 2022, 100, 520-529.	1.1	7
2	Design of singlet fission chromophores by the introduction of N-oxyl fragments. Journal of Chemical Physics, 2022, 156, 034303.	3.0	7
3	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
4	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
5	The synthesis, properties, and reactivity of Lewis acidic aminoboranes. Organic and Biomolecular Chemistry, 2021, 19, 4796-4802.	2.8	3
6	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
7	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
8	VHEGEN: A vibronic Hamiltonian expansion generator for trigonal and tetragonal polyatomic systems. Computer Physics Communications, 2020, 247, 106946.	7.5	6
9	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
10	Thiophene Cation Intercalation to Improve Bandâ€Edge Integrity in Reducedâ€Dimensional Perovskites. Angewandte Chemie - International Edition, 2020, 59, 13977-13983.	13.8	36
11	Thiophene Cation Intercalation to Improve Bandâ€Edge Integrity in Reducedâ€Dimensional Perovskites. Angewandte Chemie, 2020, 132, 14081-14087.	2.0	16
12	Coherent electronic-vibrational dynamics in deuterium bromide probed via attosecond transient-absorption spectroscopy. Physical Review A, 2020, 101, .	2.5	20
13	Designs of Singlet Fission Chromophores with a Diazadiborinine Framework**. ChemPhotoChem, 2020, 4, 5279-5287.	3.0	12
14	Bis(pentafluorophenyl)phenothiazylborane â€“ an intramolecular frustrated Lewis pair catalyst for stannane dehydrocoupling. Dalton Transactions, 2020, 49, 16054-16058.	3.3	6
15	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
16	Direct mapping of curve-crossing dynamics in IBr by attosecond transient absorption spectroscopy. Science, 2019, 365, 79-83.	12.6	98
17	Do Diradicals Behave Like Radicals?. Chemical Reviews, 2019, 119, 11291-11351.	47.7	228
18	Design of singlet fission chromophores with cyclic (alkyl)(amino) carbene building blocks. Journal of Chemical Physics, 2019, 150, 234306.	3.0	35

#	Article	IF	Citations
19	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
20	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
21	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
22	NaI revisited: Theoretical investigation of predissociation via ultrafast XUV transient absorption spectroscopy. Journal of Chemical Physics, 2019, 151, 204103.	3.0	6
23	Electronegativity Seen as the Ground-State Average Valence Electron Binding Energy. Journal of the American Chemical Society, 2019, 141, 342-351.	13.7	139
24	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
25	Zintl Ions within Framework Channels: The Complex Structure and Low-Temperature Transport Properties of Na4Ge13. Inorganic Chemistry, 2018, 57, 2002-2012.	4.0	7
26	Theoretical Studies of Singlet Fission: Searching for Materials and Exploring Mechanisms. ChemPlusChem, 2018, 83, 146-182.	2.8	85
27	Captodative Substitution: A Strategy for Enhancing the Conductivity of Molecular Electronic Devices. Journal of Physical Chemistry C, 2018, 122, 3194-3200.	3.1	32
28	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
29	Identifying (BN)₂-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
30	General formalism for vibronic Hamiltonians in tetragonal symmetry and beyond. Physical Chemistry Chemical Physics, 2018, 20, 12312-12322.	2.8	13
31	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
32	A diabatization protocol that includes spin-orbit coupling. Journal of Chemical Physics, 2017, 146, 144103.	3.0	30
33	An Iodabenzene Story. Journal of the American Chemical Society, 2017, 139, 7124-7129.	13.7	10
34	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
35	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
36	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. Chemical Reviews, 2016, 116, 8173-8192.	47.7	155

#	Article	IF	Citations
37	A Direct Mechanism of Ultrafast Intramolecular Singlet Fission in Pentacene Dimers. ACS Central Science, 2016, 2, 316-324.	11.3	176
38	A Computational Study of the Protoisomerization of Indigo and Its Imine Derivatives. Journal of Physical Chemistry A, 2016, 120, 7569-7576.	2.5	3
39	Through-Linker Intramolecular Singlet Fission: General Mechanism and Designing Small Chromophores. Journal of Physical Chemistry Letters, 2016, 7, 4405-4412.	4.6	48
40	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
41	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
42	Li-Filled, B-Substituted Carbon Clathrates. Journal of the American Chemical Society, 2015, 137, 12639-12652.	13.7	42
43	Tuning the Ground State Symmetry of Acetylenyl Radicals. ACS Central Science, 2015, 1, 270-278.	11.3	5
44	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
45	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
46	Seeking Small Molecules for Singlet Fission: A Heteroatom Substitution Strategy. Journal of the American Chemical Society, 2014, 136, 12638-12647.	13.7	121
47	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
48	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
49	Two-component natural spinors from two-step spin-orbit coupled wave functions. Journal of Chemical Physics, 2011, 134, 214107.	3.0	44
50	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
51	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
52	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
53	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
54	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

#	Article	IF	Citations
55	New model core potentials for gold. Journal of Chemical Physics, 2009, 130, 204107.	3.0	17
56	Calibration of new model core potentials for main group elements. International Journal of Quantum Chemistry, 2009, 109, 3235-3245.	2.0	4
57	Relativistic Model Core Potential Study of the Au+Xe System. Journal of Physical Chemistry A, 2008, 112, 5236-5242.	2.5	23
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