Ze-xing Qu

List of Publications by Year
in descending order

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Version: 2024-02-01

29	369	1163117 8	794594 19
papers	citations	h-index	g-index

31	31	31	426
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Surface molecule induced effective light absorption and charge transfer for H2 production photocatalysis in a carbonized polymer dots-carbon nitride system. Applied Catalysis B: Environmental, 2022, 305, 121064.	20.2	14
2	Lacking of ESIPT Band of Aromatic ortho-Aminoaldehyde Derivatives Triggered by the N-H Vibration. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
3	Community Reaction Network Reduction for Constructing a Coarse-Grained Representation of Combustion Reaction Mechanisms. Journal of Chemical Information and Modeling, 2022, 62, 2352-2364.	5.4	6
4	Top-Down Rational Engineering of Heteroatom-Doped Graphene Quantum Dots for Laser Desorption/Ionization Mass Spectrometry Detection and Imaging of Small Biomolecules. Analytical Chemistry, 2022, 94, 7609-7618.	6.5	8
5	Generation of singlet oxygen catalyzed by the room-temperature-stable anthraquinone anion radical. Physical Chemistry Chemical Physics, 2022, 24, 14165-14171.	2.8	2
6	Minimal Active Space for Diradicals Using Multistate Density Functional Theory. Molecules, 2022, 27, 3466.	3.8	1
7	Dearomatization of Benzenoid Arenes Triggered by Triplet Excited State Intramolecular Proton Transfer. Journal of Physical Chemistry A, 2022, 126, 4424-4431.	2.5	1
8	Impact of Î”E_{ST} on Delayed Fluorescence Rate, Lifetime, and Intensity Ratio of Tetrahedral Cu(I) Complexes: Theoretical Simulation in Solution and Solid Phases. Journal of Physical Chemistry Letters, 2021, 12, 2232-2244.	4.6	6
9	Theoretical Study of a Two-Photon Fluorescent Probe Based on Nile Red Derivatives with Controllable Fluorescence Wavelength and Water Solubility. Journal of Chemical Information and Modeling, 2021, 61, 5082-5097.	5.4	8
10	A new permutation-symmetry-adapted machine learning diabatization procedure and its application in MgH₂ system. Journal of Chemical Physics, 2021, 155, 214102.	3.0	5
11	Coupled electron and proton transfer in the piperidine drug metabolism pathway by the active species of cytochromes P450. Dalton Transactions, 2020, 49, 11099-11107.	3.3	4
12	Variational Multistate Density Functional Theory for a Balanced Treatment of Static and Dynamic Correlations. Journal of Chemical Theory and Computation, 2020, 16, 4912-4922.	5.3	7
13	A selfâ€consistent coulomb bath model using density fitting. Journal of Computational Chemistry, 2020, 41, 1698-1708.	3.3	6
14	Reactivities of singlet oxygen: open-shell or closed-shell?. Physical Chemistry Chemical Physics, 2020, 22, 13373-13377.	2.8	6
15	The Câ€“H bond activation by non-heme oxidant [(N4Py)FeIV(O)]2+ with external electric field. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	1
16	Theoretical study of the photochemical isomerization process of perfluoroaryltetrahedrane to perfluoroarylcyclobutadiene mediated by 9,10-dicyanoanthracene. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	0
17	Bond-breakage-dependent dissociative ionization of an asymmetric molecule in an intense femtosecond laser field. Physical Review A, 2019, 99, .	2.5	6
18	The charger transfer electronic coupling in diabatic perspective: A multi-state density functional theory study. Chemical Physics Letters, 2018, 691, 91-97.	2.6	11

#	Article	IF	Citations
19	Combined Multistate and Kohn-Sham Density Functional Theory Studies of the Elusive Mechanism of N-Dealkylation of N,N-Dimethylanilines Mediated by the Biomimetic Nonheme Oxidant FeIV(O)(N4Py)(ClO4)2. Frontiers in Chemistry, 2018, 6, 406.	3.6	7
20	Diabatic-At-Construction Method for Diabatic and Adiabatic Ground and Excited States Based on Multistate Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 1176-1187.	5.3	49
21	Theoretical investigation on the effect of ancillary ligand modification for highly efficient phosphorescent platinum(<scp>ii</scp>) complex design. RSC Advances, 2017, 7, 17368-17376.	3.6	25
22	Accurate potential surfaces for the ground state of H+C2 reaction. European Physical Journal D, 2017, 71, 1.	1.3	7
23	Perturbation Approach for Computing Infrared Spectra of the Local Mode of Probe Molecules. Journal of Chemical Theory and Computation, 2017, 13, 191-201.	5.3	10
24	Why HSâ^' and CNâ^' can be detected by different chemosensors with similar structures: a quantum mechanics and molecular dynamics study. RSC Advances, 2016, 6, 63548-63558.	3.6	2
25	Multistate Density Functional Theory for Effective Diabatic Electronic Coupling. Journal of Physical Chemistry Letters, 2016, 7, 2286-2293.	4.6	59
26	Photoisomerization of Silyl-Substituted Cyclobutadiene Induced by ÏƒÂâ†' Ï€* Excitation: A Computational Study. Journal of Physical Chemistry A, 2015, 119, 442-451.	2.5	1
27	A non-adiabatic dynamics study of octatetraene: The radiationless conversion from S2 to S1. Journal of Chemical Physics, 2013, 139, 244304.	3.0	5
28	Communication: A dramatic transition from nonferromagnet to ferromagnet in finite fused-azulene chain. Journal of Chemical Physics, 2011, 134, 021101.	3.0	12
29	Open-Shell Ground State of Polyacenes: A Valence Bond Study. Journal of Physical Chemistry A, 2009, 113, 7909-7914.	2.5	98