

Ze-xing Qu

List of Publications by Year in descending order

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29
papers

369
citations

1163117

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19
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31
all docs

31
docs citations

31
times ranked

426
citing authors

#	ARTICLE	IF	CITATIONS
1	Open-Shell Ground State of Polyacenes: A Valence Bond Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7909-7914.	2.5	98
2	Multistate Density Functional Theory for Effective Diabatic Electronic Coupling. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2286-2293.	4.6	59
3	Diabatic-At-Construction Method for Diabatic and Adiabatic Ground and Excited States Based on Multistate Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1176-1187.	5.3	49
4	Theoretical investigation on the effect of ancillary ligand modification for highly efficient phosphorescent platinum($\text{Pt}(\text{II})$) complex design. <i>RSC Advances</i> , 2017, 7, 17368-17376.	3.6	25
5	Surface molecule induced effective light absorption and charge transfer for H ₂ production photocatalysis in a carbonized polymer dots-carbon nitride system. <i>Applied Catalysis B: Environmental</i> , 2022, 305, 121064.	20.2	14
6	Communication: A dramatic transition from nonferromagnet to ferromagnet in finite fused-azulene chain. <i>Journal of Chemical Physics</i> , 2011, 134, 021101.	3.0	12
7	The charger transfer electronic coupling in diabatic perspective: A multi-state density functional theory study. <i>Chemical Physics Letters</i> , 2018, 691, 91-97.	2.6	11
8	Perturbation Approach for Computing Infrared Spectra of the Local Mode of Probe Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 191-201.	5.3	10
9	Theoretical Study of a Two-Photon Fluorescent Probe Based on Nile Red Derivatives with Controllable Fluorescence Wavelength and Water Solubility. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5082-5097.	5.4	8
10	Top-Down Rational Engineering of Heteroatom-Doped Graphene Quantum Dots for Laser Desorption/Ionization Mass Spectrometry Detection and Imaging of Small Biomolecules. <i>Analytical Chemistry</i> , 2022, 94, 7609-7618.	6.5	8
11	Accurate potential surfaces for the ground state of H+C ₂ reaction. <i>European Physical Journal D</i> , 2017, 71, 1.	1.3	7
12	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)(N ₄ P _y)(ClO ₄) ₂ . <i>Frontiers in Chemistry</i> , 2018, 6, 406.	3.6	7
13	Variational Multistate Density Functional Theory for a Balanced Treatment of Static and Dynamic Correlations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4912-4922.	5.3	7
14	Bond-breakage-dependent dissociative ionization of an asymmetric molecule in an intense femtosecond laser field. <i>Physical Review A</i> , 2019, 99, .	2.5	6
15	A self-consistent coulomb bath model using density fitting. <i>Journal of Computational Chemistry</i> , 2020, 41, 1698-1708.	3.3	6
16	Reactivities of singlet oxygen: open-shell or closed-shell?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13373-13377.	2.8	6
17	Impact of \hat{T}^{ST} on Delayed Fluorescence Rate, Lifetime, and Intensity Ratio of Tetrahedral Cu(I) Complexes: Theoretical Simulation in Solution and Solid Phases. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2232-2244.	4.6	6
18	Community Reaction Network Reduction for Constructing a Coarse-Grained Representation of Combustion Reaction Mechanisms. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2352-2364.	5.4	6

#	ARTICLE	IF	CITATIONS
19	A non-adiabatic dynamics study of octatetraene: The radiationless conversion from S ₂ to S ₁ . Journal of Chemical Physics, 2013, 139, 244304.	3.0	5
20	A new permutation-symmetry-adapted machine learning diabaticization procedure and its application in MgH ₂ system. Journal of Chemical Physics, 2021, 155, 214102.	3.0	5
21	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
22	Why HS ⁻ and CN ⁻ 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
23	Generation of singlet oxygen catalyzed by the room-temperature-stable anthraquinone anion radical. Physical Chemistry Chemical Physics, 2022, 24, 14165-14171.	2.8	2
24	Photoisomerization of Silyl-Substituted Cyclobutadiene Induced by $\pi\pi^*$ Excitation: A Computational Study. Journal of Physical Chemistry A, 2015, 119, 442-451.	2.5	1
25	The C-H bond activation by non-heme oxidant [(N4Py)FeIV(O)] ²⁺ with external electric field. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	1
26	Minimal Active Space for Diradicals Using Multistate Density Functional Theory. Molecules, 2022, 27, 3466.	3.8	1
27	Dearomatization of Benzenoid Arenes Triggered by Triplet Excited State Intramolecular Proton Transfer. Journal of Physical Chemistry A, 2022, 126, 4424-4431.	2.5	1
28	Theoretical study of the photochemical isomerization process of perfluoroaryltetrahydro to perfluoroarylcyclobutadiene mediated by 9,10-dicyanoanthracene. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	0
29	Lacking of ESIPT Band of Aromatic ortho-Aminoaldehyde Derivatives Triggered by the N-H Vibration. Physical Chemistry Chemical Physics, 2022, , .	2.8	0