Xintian Feng

List of Publications by Year
in descending order

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17	4,465	567281 15	888059 17
papers	citations	h-index	g-index

17	17	17	4816
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
3	Singlet Fission in a Covalently Linked Cofacial Alkynyltetracene Dimer. Journal of the American Chemical Society, 2016, 138, 617-627.	13.7	248
4	Fission of Entangled Spins: An Electronic Structure Perspective. Journal of Physical Chemistry Letters, 2013, 4, 3845-3852.	4.6	170
5	New and Efficient Equation-of-Motion Coupled-Cluster Framework for Core-Excited and Core-Ionized States. Journal of Chemical Theory and Computation, 2019, 15, 3117-3133.	5.3	139
6	Linker-Dependent Singlet Fission in Tetracene Dimers. Journal of the American Chemical Society, 2018, 140, 10179-10190.	13.7	129
7	General implementation of the resolution-of-the-identity and Cholesky representations of electron repulsion integrals within coupled-cluster and equation-of-motion methods: Theory and benchmarks. Journal of Chemical Physics, 2013, 139, 134105.	3.0	117
8	A Simple Kinetic Model for Singlet Fission: A Role of Electronic and Entropic Contributions to Macroscopic Rates. Journal of Physical Chemistry C, 2014, 118, 5188-5195.	3.1	116
9	On couplings and excimers: lessons from studies of singlet fission in covalently linked tetracene dimers. Physical Chemistry Chemical Physics, 2016, 18, 7751-7761.	2.8	92
10	Dissecting the Effect of Morphology on the Rates of Singlet Fission: Insights from Theory. Journal of Physical Chemistry C, 2014, 118, 19608-19617.	3.1	80
11	What We Can Learn from the Norms of One-Particle Density Matrices, and What We Canâ€™t: Some Results for Interstate Properties in Model Singlet Fission Systems. Journal of Physical Chemistry A, 2014, 118, 11943-11955.	2.5	80
12	Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four. Journal of Chemical Theory and Computation, 2022, 18, 3460-3473.	5.3	61
13	Intra- and Intermolecular Singlet Fission in Covalently Linked Dimers. Journal of Physical Chemistry C, 2016, 120, 19070-19077.	3.1	56
14	Quantifying charge resonance and multiexciton character in coupled chromophores by charge and spin cumulant analysis. Journal of Chemical Physics, 2015, 142, 224104.	3.0	46
15	Implementation of analytic gradients for CCSD and EOM-CCSD using Cholesky decomposition of the electron-repulsion integrals and their derivatives: Theory and benchmarks. Journal of Chemical Physics, 2019, 151, 014110.	3.0	27
16	Approaching the basis set limit in Gaussian-orbital-based periodic calculations with transferability: Performance of pure density functionals for simple semiconductors. Journal of Chemical Physics, 2021, 155, 164102.	3.0	14
17	Transition states, reaction paths, and thermochemistry using the nuclearâ€“electronic orbital analytic Hessian. Journal of Chemical Physics, 2021, 154, 054108.	3.0	11