

Xing Zhang

List of Publications by Year in descending order

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Version: 2024-02-01

12
papers

3,874
citations

840776

11
h-index

1199594

12
g-index

12
all docs

12
docs citations

12
times ranked

4396
citing authors

#	ARTICLE	IF	CITATIONS
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
2	Nonadiabatic dynamics with spin-flip vs linear-response time-dependent density functional theory: A case study for the protonated Schiff base C ₅ H ₆ NH ₂ ⁺ . <i>Journal of Chemical Physics</i> , 2021, 155, 124111.	3.0	14
3	Benchmarking an Embedded Adaptive Sampling Configuration Interaction Method for Surface Reactions: H ₂ Desorption from and CH ₄ Dissociation on Cu(111). <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7078-7088.	5.3	23
4	Recent developments in the PySCF program package. <i>Journal of Chemical Physics</i> , 2020, 153, 024109.	3.0	388
5	Subspace Density Matrix Functional Embedding Theory: Theory, Implementation, and Applications to Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 949-960.	5.3	19
6	Kohn-Sham potentials from electron densities using a matrix representation within finite atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2018, 148, 034105.	3.0	23
7	Beyond Time-Dependent Density Functional Theory Using Only Single Excitations: Methods for Computational Studies of Excited States in Complex Systems. <i>Accounts of Chemical Research</i> , 2016, 49, 931-941.	15.6	75
8	Spin-flip, tensor equation-of-motion configuration interaction with a density-functional correction: A spin-complete method for exploring excited-state potential energy surfaces. <i>Journal of Chemical Physics</i> , 2015, 143, 234107.	3.0	57
9	Analytic derivative couplings in time-dependent density functional theory: Quadratic response theory versus pseudo-wavefunction approach. <i>Journal of Chemical Physics</i> , 2015, 142, 064109.	3.0	60
10	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	1.7	2,561
11	Analytic derivative couplings for spin-flip configuration interaction singles and spin-flip time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2014, 141, 064104.	3.0	89
12	Excited-State Deactivation Pathways in Uracil versus Hydrated Uracil: Solvatochromatic Shift in the ¹ ππ* State is the Key. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7806-7817.	2.6	47