Xing Zhang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3301581/publications.pdf

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12	3,874	840776 11	1199594 12
papers	citations	h-index	g-index

12	12	12	4396
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	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
4	Analytic derivative couplings for spin-flip configuration interaction singles and spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2014, 141, 064104.	3.0	89
5	Beyond Time-Dependent Density Functional Theory Using Only Single Excitations: Methods for Computational Studies of Excited States in Complex Systems. Accounts of Chemical Research, 2016, 49, 931-941.	15.6	75
6	Analytic derivative couplings in time-dependent density functional theory: Quadratic response theory versus pseudo-wavefunction approach. Journal of Chemical Physics, 2015, 142, 064109.	3.0	60
7	Spin-flip, tensor equation-of-motion configuration interaction with a density-functional correction: A spin-complete method for exploring excited-state potential energy surfaces. Journal of Chemical Physics, 2015, 143, 234107.	3.0	57
8	Excited-State Deactivation Pathways in Uracil versus Hydrated Uracil: Solvatochromatic Shift in the ¹nÏ€* State is the Key. Journal of Physical Chemistry B, 2014, 118, 7806-7817.	2.6	47
9	Kohn-Sham potentials from electron densities using a matrix representation within finite atomic orbital basis sets. Journal of Chemical Physics, 2018, 148, 034105.	3.0	23
10	Benchmarking an Embedded Adaptive Sampling Configuration Interaction Method for Surface Reactions: H₂ Desorption from and CH₄ Dissociation on Cu(111). Journal of Chemical Theory and Computation, 2020, 16, 7078-7088.	5.3	23
11	Subspace Density Matrix Functional Embedding Theory: Theory, Implementation, and Applications to Molecular Systems. Journal of Chemical Theory and Computation, 2019, 15, 949-960.	5.3	19
12	Nonadiabatic dynamics with spin-flip vs linear-response time-dependent density functional theory: A case study for the protonated SchiffÂbase C5H6NH2+. Journal of Chemical Physics, 2021, 155, 124111.	3.0	14