Joseph M Kasper

List of Publications by Year
in descending order

16	400	759233 12	940533 16
papers	citations	h-index	g-index

17	17	17	494
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Relativistic Effects in Modeling the Ligand K-Edge X-ray Absorption Near-Edge Structure of Uranium Complexes. Journal of Chemical Theory and Computation, 2022, , .	5.3	3
2	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
3	Theoretical investigation of quantum confinement on the Rashba effect in ZnO semiconductor nanocrystals. Journal of Chemical Physics, 2020, 152, 014308.	3.0	8
4	Perspective on Kramers symmetry breaking and restoration in relativistic electronic structure methods for open-shell systems. Journal of Chemical Physics, 2020, 153, 090903.	3.0	7
5	Localized relativistic two-component methods for ground and excited state calculations. Annual Reports in Computational Chemistry, 2020, 16, 17-37.	1.7	6
6	Natural transition orbitals for complex <scp>twoâ€component</scp> excited state calculations. Journal of Computational Chemistry, 2020, 41, 1557-1563.	3.3	15
7	Relativistic Two-Component Multireference Configuration Interaction Method with Tunable Correlation Space. Journal of Chemical Theory and Computation, 2020, 16, 2975-2984.	5.3	30
8	Ab initio methods for L-edge x-ray absorption spectroscopy. Chemical Physics Reviews, 2020, 1, .	5.7	25
9	Modeling L2,3-edge X-ray absorption spectroscopy with linear response exact two-component relativistic time-dependent density functional theory. Journal of Chemical Physics, 2019, 150, 234103.	3.0	28
10	Variational Relativistic Two-Component Complete-Active-Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2019, 15, 2974-2982.	5.3	28
11	Effect of Surface Passivation on Nanodiamond Crystallinity. Journal of Physical Chemistry C, 2018, 122, 8573-8580.	3.1	24
12	A Well-Tempered Hybrid Method for Solving Challenging Time-Dependent Density Functional Theory (TDDFT) Systems. Journal of Chemical Theory and Computation, 2018, 14, 2034-2041.	5.3	15
13	Modeling L_{2,3}-Edge X-ray Absorption Spectroscopy with Real-Time Exact Two-Component Relativistic Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 1998-2006.	5.3	44
14	Electronic structures and spectroscopic signatures of silicon-vacancy containing nanodiamonds. Physical Review B, 2018, 98, .	3.2	16
15	Model Order Reduction Algorithm for Estimating the Absorption Spectrum. Journal of Chemical Theory and Computation, 2017, 13, 4950-4961.	5.3	14
16	Real time propagation of the exact two component time-dependent density functional theory. Journal of Chemical Physics, 2016, 145, 104107.	3.0	71