Katherine J Oosterbaan

List of Publications by Year
in descending order

8	685	1307594 7	1474206 9
papers	citations	h-index	g-index

11	11	11	586
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. Journal of Chemical Physics, 2018, 149, 044116.	3.0	44
3	Non-Orthogonal Configuration Interaction with Single Substitutions for Core-Excited States: An Extension to Doublet Radicals. Journal of Chemical Theory and Computation, 2019, 15, 2966-2973.	5.3	39
4	Accurate prediction of core-level spectra of radicals at density functional theory cost via square gradient minimization and recoupling of mixed configurations. Journal of Chemical Physics, 2020, 153, 134108.	3.0	31
5	Tracing the 267 nm-Induced Radical Formation in Dimethyl Disulfide Using Time-Resolved X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 1382-1387.	4.6	24
6	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. Physical Chemistry Chemical Physics, 2020, 22, 8182-8192.	2.8	16
7	Computing x-ray absorption spectra from linear-response particles atop optimized holes. Journal of Chemical Physics, 2022, 156, .	3.0	7
8	Revisiting the Ï€Ââ†'ÂÏ€* transition of the nitrite ion at the air/water interface: A combined experimental and theoretical study. Chemical Physics Letters, 2020, 751, 137516.	2.6	3