J Patrick Zobel

List of Publications by Year
in descending order

17	1,173	840776 11	839539 18
papers	citations	h-index	g-index

21	21	21	1412
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Benchmarking ANO-R basis set for multiconfigurational calculations. Electronic Structure, 2022, 4, 014009.	2.8	2
2	Rydberg states of ZnAr complex. Molecular Physics, 2022, 120, .	1.7	2
3	Ultrafast and long-time excited state kinetics of an NIR-emissive vanadium(<scp>iii</scp>) complex II. Elucidating triplet-to-singlet excited-state dynamics. Chemical Science, 2021, 12, 10791-10801.	7.4	24
4	The Quest to Simulate Excited-State Dynamics of Transition Metal Complexes. Jacs Au, 2021, 1, 1116-1140.	7.9	30
5	Surface Hopping Dynamics on Vibronic Coupling Models. Accounts of Chemical Research, 2021, 54, 3760-3771.	15.6	32
6	The ANO-R Basis Set. Journal of Chemical Theory and Computation, 2020, 16, 278-294.	5.3	31
7	Intersystem Crossing and Triplet Dynamics in an Iron(II) N-Heterocyclic Carbene Photosensitizer. Inorganic Chemistry, 2020, 59, 14666-14678.	4.0	23
8	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
9	Nonadiabatic Dynamics Simulation Predict Intersystem Crossing in Nitroaromatic Molecules on a Picosecond Time Scale. ChemPhotoChem, 2019, 3, 833-845.	3.0	12
10	Finite-temperature Wigner phase-space sampling and temperature effects on the excited-state dynamics of 2-nitronaphthalene. Physical Chemistry Chemical Physics, 2019, 21, 13906-13915.	2.8	29
11	Vibrational Sampling and Solvent Effects on the Electronic Structure of the Absorption Spectrum of 2-Nitronaphthalene. Journal of Chemical Theory and Computation, 2018, 14, 3205-3217.	5.3	21
12	Mechanism of Ultrafast Intersystem Crossing in 2â€Nitronaphthalene. Chemistry - A European Journal, 2018, 24, 5379-5387.	3.3	50
13	New compact density matrix averaged ANO basis sets for relativistic calculations. Journal of Chemical Physics, 2018, 149, 194102.	3.0	9
14	The IPEA dilemma in CASPT2. Chemical Science, 2017, 8, 1482-1499.	7.4	194
15	Quenching of Charge Transfer in Nitrobenzene Induced by Vibrational Motion. Journal of Physical Chemistry Letters, 2015, 6, 3006-3011.	4.6	24
16	Communication: Electron transfer mediated decay enabled by spin-orbit interaction in small krypton/xenon clusters. Journal of Chemical Physics, 2014, 140, 161103.	3.0	4
17	Spinâ€“orbit effects, electronic decay and breakdown phenomena in the photoelectron spectra of iodomethane. Chemical Physics, 2012, 407, 39-45.	1.9	10