Pavel Pokhilko

List of Publications by Year in descending order

16 papers	889 citations	759233 12 h-index	940533 16 g-index
21 all docs	21 docs citations	21 times ranked	710 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	A Combined Experimental and Theoretical Study on the Formation of Interstellar Propylene Oxide (CH₃CHCH₂O)â€"A Chiral Molecule. Astrophysical Journal, 2018, 860, 108.	4.5	54
3	Equation-of-Motion Coupled-Cluster Theory to Model L-Edge X-ray Absorption and Photoelectron Spectra. Journal of Physical Chemistry Letters, 2020, 11, 8314-8321.	4.6	46
4	Quantitative El-Sayed Rules for Many-Body Wave Functions from Spinless Transition Density Matrices. Journal of Physical Chemistry Letters, 2019, 10, 4857-4862.	4.6	41
5	General framework for calculating spinâ€"orbit couplings using spinless one-particle density matrices: Theory and application to the equation-of-motion coupled-cluster wave functions. Journal of Chemical Physics, 2019, 151, 034106.	3.0	41
6	Double Precision Is Not Needed for Many-Body Calculations: Emergent Conventional Wisdom. Journal of Chemical Theory and Computation, 2018, 14, 4088-4096.	5.3	38
7	Extension of frozen natural orbital approximation to open-shell references: Theory, implementation, and application to single-molecule magnets. Journal of Chemical Physics, 2020, 152, 034105.	3.0	27
8	Spin-Forbidden Channels in Reactions of Unsaturated Hydrocarbons with O(³P). Journal of Physical Chemistry A, 2019, 123, 482-491.	2.5	20
9	Calculation of spinâ€"orbit couplings using RASCI spinless one-particle density matrices: Theory and applications. Journal of Chemical Physics, 2020, 153, 214107.	3.0	18
10	Interpretation of multiple solutions in fully iterative GF2 and GW schemes using local analysis of two-particle density matrices. Journal of Chemical Physics, 2021, 155, 024101.	3.0	17
11	Evaluation of two-particle properties within finite-temperature self-consistent one-particle Greenâ€™s function methods: Theory and application to GW and GF2. Journal of Chemical Physics, 2021, 155, 024119.	3.0	16
12	Effective Hamiltonians derived from equation-of-motion coupled-cluster wave functions: Theory and application to the Hubbard and Heisenberg Hamiltonians. Journal of Chemical Physics, 2020, 152, 094108.	3.0	14
13	Is Solid Copper Oxalate a Spin Chain or a Mixture of Entangled Spin Pairs?. Journal of Physical Chemistry C, 2021, 125, 7502-7510.	3.1	11
14	Iterative subspace algorithms for finite-temperature solution of Dyson equation. Journal of Chemical Physics, 2022, 156, 094101.	3.0	11
15	Solvent Thermodynamic Driving Force Controls Stacking Interactions between Polyaromatics. Journal of Physical Chemistry C, 2016, 120, 23858-23869.	3.1	10
16	The elusive dynamics of aqueous permanganate photochemistry. Physical Chemistry Chemical Physics, 2020, 22, 10043-10055.	2.8	7