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	Iterative subspace algorithms for finite-temperature solution of Dyson equation. Journal of Chemical Physics, 2022, 156, 094101.	3.0	11
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	The elusive dynamics of aqueous permanganate photochemistry. Physical Chemistry Chemical Physics, 2020, 22, 10043-10055.	2.8	7
11	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
12	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
13	Spin-Forbidden Channels in Reactions of Unsaturated Hydrocarbons with O(³P). Journal of Physical Chemistry A, 2019, 123, 482-491.	2.5	20
14	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
15	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
16	Solvent Thermodynamic Driving Force Controls Stacking Interactions between Polyaromatics. Journal of Physical Chemistry C, 2016, 120, 23858-23869.	3.1	10