Sebastian Wouters

List of Publications by Year
in descending order

22	2,957	567281 15	677142 22
papers	citations	h-index	g-index

23	23	23	2430
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	14.6	894
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
3	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
4	The density matrix renormalization group for ab initio quantum chemistry. European Physical Journal D, 2014, 68, 1.	1.3	198
5	A Practical Guide to Density Matrix Embedding Theory in Quantum Chemistry. Journal of Chemical Theory and Computation, 2016, 12, 2706-2719.	5.3	147
6	CheMPS2: A free open-source spin-adapted implementation of the density matrix renormalization group for ab initio quantum chemistry. Computer Physics Communications, 2014, 185, 1501-1514.	7.5	143
7	Cumulant Approximated Second-Order Perturbation Theory Based on the Density Matrix Renormalization Group for Transition Metal Complexes: A Benchmark Study. Journal of Chemical Theory and Computation, 2016, 12, 4352-4361.	5.3	93
8	Communication: DMRG-SCF study of the singlet, triplet, and quintet states of oxo-Mn(Salen). Journal of Chemical Physics, 2014, 140, 241103.	3.0	82
9	DMRG-CASPT2 study of the longitudinal static second hyperpolarizability of all-trans polyenes. Journal of Chemical Physics, 2016, 145, 054120.	3.0	58
10	Longitudinal static optical properties of hydrogen chains: Finite field extrapolations of matrix product state calculations. Journal of Chemical Physics, 2012, 136, 134110.	3.0	56
11	Linear response theory for the density matrix renormalization group: Efficient algorithms for strongly correlated excited states. Journal of Chemical Physics, 2014, 140, 024108.	3.0	46
12	Thouless theorem for matrix product states and subsequent post density matrix renormalization group methods. Physical Review B, 2013, 88, .	3.2	38
13	T3NS: Three-Legged Tree Tensor Network States. Journal of Chemical Theory and Computation, 2018, 14, 2026-2033.	5.3	36
14	Block product density matrix embedding theory for strongly correlated spin systems. Physical Review B, 2017, 95, .	3.2	20
15	Projector quantum Monte Carlo with matrix product states. Physical Review B, 2014, 90, .	3.2	16
16	CheMPS2 : Improved DMRG-SCF routine and correlation functions. Computer Physics Communications, 2015, 191, 235-237.	7.5	15
17	Possibility of [1,5] Sigmatropic Shifts in Bicyclo[4.2.0]octa-2,4-dienes. Journal of Organic Chemistry, 2015, 80, 2609-2620.	3.2	13
18	Extensive v2DM study of the one-dimensional Hubbard model for large lattice sizes: Exploiting translational invariance and parity. Computational and Theoretical Chemistry, 2013, 1003, 12-21.	2.5	10

#	Article	IF	Citations
19	Mechanistic Investigation on Oxygen Transfer with the Manganeseâ€Salen Complex. ChemCatChem, 2015, 7, 2711-2719.	3.7	10
20	PPV Polymerization through the Gilch Route: Diradical Character of Monomers. Chemistry - A European Journal, 2015, 21, 19176-19185.	3.3	9
21	The enantioselectivity of the manganese-salen complex in the epoxidation of unfunctionalized olefins and the influence of grafting. Journal of Molecular Catalysis A, 2015, 406, 106-113.	4.8	7
22	Variational optimization of the 2DM: approaching three-index accuracy using extended cluster constraints. European Physical Journal B, 2014, 87, 1.	1.5	2