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	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
3	T3NS: Three-Legged Tree Tensor Network States. Journal of Chemical Theory and Computation, 2018, 14, 2026-2033.	5.3	36
4	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	14.6	894
5	Block product density matrix embedding theory for strongly correlated spin systems. Physical Review B, 2017, 95, .	3.2	20
6	A Practical Guide to Density Matrix Embedding Theory in Quantum Chemistry. Journal of Chemical Theory and Computation, 2016, 12, 2706-2719.	5.3	147
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	DMRG-CASPT2 study of the longitudinal static second hyperpolarizability of all-trans polyenes. Journal of Chemical Physics, 2016, 145, 054120.	3.0	58
9	Mechanistic Investigation on Oxygen Transfer with the Manganeseâ€Salen Complex. ChemCatChem, 2015, 7, 2711-2719.	3.7	10
10	PPV Polymerization through the Gilch Route: Diradical Character of Monomers. Chemistry - A European Journal, 2015, 21, 19176-19185.	3.3	9
11	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
12	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
13	CheMPS2 : Improved DMRG-SCF routine and correlation functions. Computer Physics Communications, 2015, 191, 235-237.	7.5	15
14	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
15	Projector quantum Monte Carlo with matrix product states. Physical Review B, 2014, 90, .	3.2	16
16	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
17	Variational optimization of the 2DM: approaching three-index accuracy using extended cluster constraints. European Physical Journal B, 2014, 87, 1.	1.5	2
18	The density matrix renormalization group for ab initio quantum chemistry. European Physical Journal D, 2014, 68, 1.	1.3	198

#	Article	IF	Citations
19	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
20	Thouless theorem for matrix product states and subsequent post density matrix renormalization group methods. Physical Review B, 2013, 88, .	3.2	38
21	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
22	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