Gunnar Schmitz

List of Publications by Year
in descending order

19	1,201	687363 13	794594 19
papers	citations	h-index	g-index

19	19	19	1370
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
2	Explicitly correlated PNO-MP2 and PNO-CCSD and their application to the S66 set and large molecular systems. Physical Chemistry Chemical Physics, 2014, 16, 22167-22178.	2.8	92
3	Perturbative triples correction for local pair natural orbital based explicitly correlated CCSD(F12*) using Laplace transformation techniques. Journal of Chemical Physics, 2016, 145, 234107.	3.0	72
4	A scaling PNOâ€“MP2 method using a hybrid OSVâ€“PNO approach with an iterative direct generation of OSVs^{â€}. Molecular Physics, 2013, 111, 2463-2476.	1.7	60
5	Gaussian process regression to accelerate geometry optimizations relying on numerical differentiation. Journal of Chemical Physics, 2018, 148, 241704.	3.0	54
6	Auxiliary basis sets for density-fitted correlated wavefunction calculations: weighted core-valence and ECP basis sets for post-d elements. Physical Chemistry Chemical Physics, 2012, 14, 6549.	2.8	53
7	Machine learning for potential energy surfaces: An extensive database and assessment of methods. Journal of Chemical Physics, 2019, 150, 244113.	3.0	42
8	Assessment of the DLPNO Binding Energies of Strongly Noncovalent Bonded Atmospheric Molecular Clusters. ACS Omega, 2020, 5, 7601-7612.	3.5	38
9	Accuracy of Explicitly Correlated Local PNO-CCSD(T). Journal of Chemical Theory and Computation, 2017, 13, 2623-2633.	5.3	37
10	Approximate high mode coupling potentials using Gaussian process regression and adaptive density guided sampling. Journal of Chemical Physics, 2019, 150, 131102.	3.0	36
11	The PNOâ€“MP2 gradient and its application to molecular geometry optimisations. Molecular Physics, 2017, 115, 343-356.	1.7	32
12	A Gaussian process regression adaptive density guided approach for potential energy surface construction. Journal of Chemical Physics, 2020, 153, 064105.	3.0	17
13	Combining Accuracy and Efficiency: An Incremental Focal-Point Method Based on Pair Natural Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 6023-6042.	5.3	14
14	Atomic-batched tensor decomposed two-electron repulsion integrals. Journal of Chemical Physics, 2017, 146, 134112.	3.0	9
15	Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics. Journal of Physical Chemistry A, 2020, 124, 9626-9637.	2.5	8
16	Accuracy of Frequencies Obtained with the Aid of Explicitly Correlated Wave Function Based Methods. Journal of Chemical Theory and Computation, 2017, 13, 3602-3613.	5.3	6
17	Implementation of the iterative triples model CC3 for excitation energies using pair natural orbitals and Laplace transformation techniques. Journal of Chemical Physics, 2020, 153, 034109.	3.0	6
18	An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. Journal of Computational Chemistry, 2021, 42, 2264-2282.	3.3	6

#	Article	IF	Citations
19	Assessment of the overlap metric in the context of RI-MP2 and atomic batched tensor decomposed MP2. Chemical Physics Letters, 2018, 701, 7-14.	2.6	3