JÃ©rÃ´me F Gonthier

List of Publications by Year
in descending order

22 papers	1,836 citations	623734 14 h-index	642732 23 g-index
24 all docs	24 docs citations	24 times ranked	2776 citing authors

#	Article	IF	Citations
1	Adaptive pruning-based optimization of parameterized quantum circuits. Quantum Science and Technology, 2021, 6, 025019.	5.8	30
2	Approaching the basis set limit in Gaussian-orbital-based periodic calculations with transferability: Performance of pure density functionals for simple semiconductors. Journal of Chemical Physics, 2021, 155, 164102.	3.0	14
3	Compressed intramolecular dispersion interactions. Journal of Chemical Physics, 2020, 152, 024112.	3.0	2
4	Assessing Electronic Structure Methods for Long-Range Three-Body Dispersion Interactions: Analysis and Calculations on Well-Separated Metal Atom Trimers. Journal of Chemical Theory and Computation, 2019, 15, 4351-4361.	5.3	7
5	Water Bridges Conduct Sequential Proton Transfer in Photosynthetic Oxygen Evolution. Journal of Physical Chemistry B, 2019, 123, 4487-4496.	2.6	5
6	Understanding Non-Covalent Interactions: Correlated Energy Decomposition Analysis and Applications to Halogen Bonding. Chimia, 2018, 72, 193.	0.6	7
7	Quantum algorithms for electronic structure calculations: Particle-hole Hamiltonian and optimized wave-function expansions. Physical Review A, 2018, 98, .	2.5	214
8	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	5.3	961
9	Compressed representation of dispersion interactions and long-range electronic correlations. Journal of Chemical Physics, 2017, 147, 144110.	3.0	7
10	Chloride Maintains a Protonated Internal Water Network in the Photosynthetic Oxygen Evolving Complex. Journal of Physical Chemistry B, 2017, 121, 10327-10337.	2.6	14
11	Density-fitted open-shell symmetry-adapted perturbation theory and application to Ï€-stacking in benzene dimer cation and ionized DNA base pair steps. Journal of Chemical Physics, 2016, 145, 134106.	3.0	40
12	Intramolecular symmetry-adapted perturbation theory with a single-determinant wavefunction. Journal of Chemical Physics, 2015, 143, 224107.	3.0	19
13	Communication: Practical intramolecular symmetry adapted perturbation theory via Hartree-Fock embedding. Journal of Chemical Physics, 2015, 143, 051103.	3.0	62
14	Exploration of zeroth-order wavefunctions and energies as a first step toward intramolecular symmetry-adapted perturbation theory. Journal of Chemical Physics, 2014, 140, 154107.	3.0	15
15	Quantification and Analysis of Intramolecular Interactions. Chimia, 2014, 68, 221.	0.6	7
16	Adjusting the Local Arrangement of Ï€-Stacked Oligothiophenes through Hydrogen Bonds: A Viable Route to Promote Charge Transfer. Journal of Physical Chemistry Letters, 2014, 5, 2320-2324.	4.6	22
17	Ligandâ€Controlled Regiodivergent Pathways of Rhodium(III)â€Catalyzed Dihydroisoquinolone Synthesis: Experimental and Computational Studies of Different Cyclopentadienyl Ligands. Chemistry - A European Journal, 2014, 20, 15409-15418.	3.3	120
18	Ï€-Depletion as a criterion to predict Ï€-stacking ability. Chemical Communications, 2012, 48, 9239.	4.1	68

#	Article	IF	Citations
19	Quantification of â€œfuzzyâ€•chemical concepts: a computational perspective. Chemical Society Reviews, 2012, 41, 4671.	38.1	108
20	Four-Electron Oxygen Reduction by Tetrathiafulvalene. Journal of the American Chemical Society, 2011, 133, 12115-12123.	13.7	56
21	Branched Alkanes Have Contrasting Stabilities. Organic Letters, 2010, 12, 3070-3073.	4.6	34
22	How Strained are Carbomeric-Cycloalkanes?. Journal of Physical Chemistry A, 2010, 114, 6705-6712.	2.5	22