Anthony Scemama

List of Publications by Year
in descending order

23	824	567281 15	642732 23
papers	citations	h-index	g-index

23	23	23	583
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reference Excitation Energies of Increasingly Large Molecules: A QMC Study of Cyanine Dyes. Journal of Chemical Theory and Computation, 2022, 18, 1089-1095.	5.3	7
2	The effect of uncertainty on building blocks in molecules. Journal of Chemical Physics, 2022, 156, .	3.0	2
3	Reference Energies for Cyclobutadiene: Automerization and Excited States. Journal of Physical Chemistry A, 2022, 126, 4664-4679.	2.5	11
4	<scp>QUESTDB</scp>: A database of highly accurate excitation energies for the electronic structure community. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1517.	14.6	84
5	Tailoring CIPSI Expansions for QMC Calculations of Electronic Excitations: The Case Study of Thiophene. Journal of Chemical Theory and Computation, 2021, 17, 3426-3434.	5.3	17
6	Excited States from State-Specific Orbital-Optimized Pair Coupled Cluster. Journal of Chemical Theory and Computation, 2021, 17, 4756-4768.	5.3	29
7	Accurate full configuration interaction correlation energy estimates for five- and six-membered rings. Journal of Chemical Physics, 2021, 155, 134104.	3.0	14
8	The performance of CIPSI on the ground state electronic energy of benzene. Journal of Chemical Physics, 2020, 153, 176101.	3.0	26
9	A basis-set error correction based on density-functional theory for strongly correlated molecular systems. Journal of Chemical Physics, 2020, 152, 174104.	3.0	16
10	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solidsâ€"A case study in diamond. Journal of Chemical Physics, 2020, 153, 184111.	3.0	16
11	Taming the fixed-node error in diffusion Monte Carlo via range separation. Journal of Chemical Physics, 2020, 153, 174107.	3.0	11
12	Excited States with Selected Configuration Interaction-Quantum Monte Carlo: Chemically Accurate Excitation Energies and Geometries. Journal of Chemical Theory and Computation, 2019, 15, 4896-4906.	5.3	34
13	Chemically accurate excitation energies with small basis sets. Journal of Chemical Physics, 2019, 151, 144118.	3.0	30
14	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. Journal of Chemical Theory and Computation, 2019, 15, 3591-3609.	5.3	108
15	Deterministic Construction of Nodal Surfaces within Quantum Monte Carlo: The Case of FeS. Journal of Chemical Theory and Computation, 2018, 14, 1395-1402.	5.3	48
16	Selected configuration interaction dressed by perturbation. Journal of Chemical Physics, 2018, 149, 064103.	3.0	92
17	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. Journal of Chemical Physics, 2018, 149, 034108.	3.0	50
18	Alternative definition of excitation amplitudes in multi-reference state-specific coupled cluster. Journal of Chemical Physics, 2017, 146, 154107.	3.0	8

#	Article	IF	Citations
19	Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory. Journal of Chemical Physics, 2017, 147, 034101.	3.0	106
20	A Jeziorski-Monkhorst fully uncontracted multi-reference perturbative treatment. I. Principles, second-order versions, and tests on ground state potential energy curves. Journal of Chemical Physics, 2017, 146, 224108.	3.0	25
21	A simple approach to the state-specific MR-CC using the intermediate Hamiltonian formalism. Journal of Chemical Physics, 2016, 144, 064101.	3.0	14
22	Communication: Toward an improved control of the fixed-node error in quantum Monte Carlo: The case of the water molecule. Journal of Chemical Physics, 2016, 144, 151103.	3.0	48
23	Quantum Monte Carlo for large chemical systems: Implementing efficient strategies for petascale platforms and beyond. Journal of Computational Chemistry, 2013, 34, 938-951.	3.3	28