Nicholas Bauman

List of Publications by Year
in descending order

19	780	840585 11	752573 20
papers	citations	h-index	g-index

20	20	20	1015
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
2	Downfolding of many-body Hamiltonians using active-space models: Extension of the sub-system embedding sub-algebras approach to unitary coupled cluster formalisms. Journal of Chemical Physics, 2019, 151, 014107.	1.2	57
3	Resource-Efficient Chemistry on Quantum Computers with the Variational Quantum Eigensolver and the Double Unitary Coupled-Cluster Approach. Journal of Chemical Theory and Computation, 2020, 16, 6165-6175.	2.3	50
4	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	23.0	39
5	Combining active-space coupled-cluster approaches with moment energy corrections via the CC(P;Q) methodology: connected quadruple excitations. Molecular Physics, 2017, 115, 2860-2891.	0.8	35
6	Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Beryllium Dimer. Journal of Physical Chemistry A, 2018, 122, 1350-1368.	1.1	27
7	Quantum simulations of excited states with active-space downfolded Hamiltonians. Journal of Chemical Physics, 2019, 151, 234114.	1.2	25
8	Sub-system quantum dynamics using coupled cluster downfolding techniques. Journal of Chemical Physics, 2020, 152, 244127.	1.2	25
9	Index of multi-determinantal and multi-reference character in coupled-cluster theory. Journal of Chemical Physics, 2020, 153, 234103.	1.2	17
10	Toward Quantum Computing for High-Energy Excited States in Molecular Systems: Quantum Phase Estimations of Core-Level States. Journal of Chemical Theory and Computation, 2021, 17, 201-210.	2.3	16
11	Improving the accuracy and efficiency of quantum connected moments expansions *. Quantum Science and Technology, 2021, 6, 034012.	2.6	11
12	Coupled Cluster Downfolding Theory: towards universal many-body algorithms for dimensionality reduction of composite quantum systems in chemistry and materials science. Materials Theory, 2022, 6, .	2.2	11
13	Quantum Solvers for Plane-Wave Hamiltonians: Abridging Virtual Spaces Through the Optimization of Pairwise Correlations. Frontiers in Chemistry, 2021, 9, 603019.	1.8	10
14	Coupled Cluster Downfolding Methods: the effect of double commutator terms on the accuracy of ground-state energies. Journal of Chemical Physics, 2022, 156, 094106.	1.2	9
15	Communication: Coupled-cluster interpretation of the photoelectron spectrum of ${m Au}_{3}^{-}$ Au 3â^'. Journal of Chemical Physics, 2014, 141, 101102.	1.2	6
16	Coupled Cluster Green's function formulations based on the effective Hamiltonians. Molecular Physics, 2020, 118, e1725669.	0.8	5
17	Real-time equation-of-motion CC cumulant and CC Greenâ€™s function simulations of photoemission spectra of water and water dimer. Journal of Chemical Physics, 2022, 157, .	1.2	4
18	Coupled-cluster interpretation of the photoelectron spectrum of Ag3â^'. Journal of Chemical Physics, 2016, 145, 084306.	1.2	3

#	Article	IF	Citations
19	Ab initio coupled-cluster and multi-reference configuration interaction studies of the low-lying electronic states of 1,2,3,4-cyclobutanetetraone. Molecular Physics, 2016, 114, 695-708.	0.8	3