Bo Peng

List of Publications by Year
in descending order

27 papers	947 citations	687363 13 h-index	610901 24 g-index
27 all docs	27 docs citations	27 times ranked	1086 citing authors

#	Article	IF	Citations
1	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
2	Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-edge X-ray Absorption Spectroscopy. Journal of Chemical Theory and Computation, 2015, 11, 4146-4153.	5.3	92
3	VQE method: a short survey and recent developments. Materials Theory, 2022, 6, .	4.3	70
4	Highly Efficient and Scalable Compound Decomposition of Two-Electron Integral Tensor and Its Application in Coupled Cluster Calculations. Journal of Chemical Theory and Computation, 2017, 13, 4179-4192.	5.3	41
5	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
6	Greenâ€™s Function Coupled-Cluster Approach: Simulating Photoelectron Spectra for Realistic Molecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 4335-4352.	5.3	32
7	Coupled-cluster Green's function: Analysis of properties originating in the exponential parametrization of the ground-state wave function. Physical Review A, 2016, 94, .	2.5	25
8	Equation of motion coupled-cluster cumulant approach for intrinsic losses in x-ray spectra. Journal of Chemical Physics, 2020, 152, 174113.	3.0	25
9	Real-Time Coupled-Cluster Approach for the Cumulant Greenâ€™s Function. Journal of Chemical Theory and Computation, 2020, 16, 6983-6992.	5.3	19
10	Approximate Greenâ€™s Function Coupled Cluster Method Employing Effective Dimension Reduction. Journal of Chemical Theory and Computation, 2019, 15, 3185-3196.	5.3	17
11	Quantum simulations employing connected moments expansions. Journal of Chemical Physics, 2020, 153, 201102.	3.0	17
12	Properties of advanced coupled-cluster Green's function. Molecular Physics, 2018, 116, 561-569.	1.7	16
13	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.	5.3	16
14	State preparation and evolution in quantum computing: A perspective from Hamiltonian moments. International Journal of Quantum Chemistry, 2022, 122, e26853.	2.0	15
15	Greenâ€™s function coupled cluster formulations utilizing extended inner excitations. Journal of Chemical Physics, 2018, 149, 214102.	3.0	11
16	Variational quantum solver employing the PDS energy functional. Quantum - the Open Journal for Quantum Science, 0, 5, 473.	0.0	11
17	Improving the accuracy and efficiency of quantum connected moments expansions *. Quantum Science and Technology, 2021, 6, 034012.	5.8	11
18	Real-Time Equation-of-Motion CCSD Cumulant Greenâ€™s Function. Journal of Chemical Theory and Computation, 2022, 18, 1799-1807.	5.3	10

#	Article	IF	Citations
19	Coupled Cluster Studies of Ionization Potentials and Electron Affinities of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2017, 121, 1328-1335.	2.5	9
20	GFCCLib: Scalable and efficient coupled-cluster Green's function library for accurately tackling many-body electronic structure problems. Computer Physics Communications, 2021, 265, 108000.	7.5	8
21	Equation-of-Motion Coupled-Cluster Cumulant Greenâ€™s Function for Excited States and X-Ray Spectra. Frontiers in Chemistry, 2021, 9, 734945.	3.6	8
22	Low-rank factorization of electron integral tensors and its application in electronic structure theory. Chemical Physics Letters, 2017, 672, 47-53.	2.6	7
23	Greenâ€™s function coupled cluster simulation of the near-valence ionizations of DNA-fragments. Journal of Chemical Physics, 2020, 152, 011101.	3.0	6
24	Coupled cluster Green's function: Past, present, and future. Annual Reports in Computational Chemistry, 2021, , 23-53.	1.7	6
25	Coupled Cluster Green's function formulations based on the effective Hamiltonians. Molecular Physics, 2020, 118, e1725669.	1.7	5
26	Scalable Heterogeneous Execution of a Coupled-Cluster Model with Perturbative Triples. , 2020, , .		3
27	Hybrid quantum-classical approach for coupled-cluster Green's function theory. Quantum - the Open Journal for Quantum Science, 0, 6, 675.	0.0	3