George H Booth

List of Publications by Year
in descending order

62 papers	5,055 citations	117625 34 h-index	118850 62 g-index
62 all docs	62 docs citations	62 times ranked	2419 citing authors

#	Article	IF	Citations
1	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	14.6	894
2	Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space. Journal of Chemical Physics, 2009, 131, 054106.	3.0	567
3	Towards an exact description of electronic wavefunctions in real solids. Nature, 2013, 493, 365-370.	27.8	440
4	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
5	Communications: Survival of the fittest: Accelerating convergence in full configuration-interaction quantum Monte Carlo. Journal of Chemical Physics, 2010, 132, 041103.	3.0	308
6	Breaking the carbon dimer: The challenges of multiple bond dissociation with full configuration interaction quantum Monte Carlo methods. Journal of Chemical Physics, 2011, 135, 084104.	3.0	134
7	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. Journal of Chemical Theory and Computation, 2011, 7, 2780-2785.	5.3	117
8	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: A study of ionization potentials. Journal of Chemical Physics, 2010, 132, 174104.	3.0	110
9	Convergence of many-body wave-function expansions using a plane-wave basis: From homogeneous electron gas to solid state systems. Physical Review B, 2012, 86, .	3.2	101
10	Full configuration interaction perspective on the homogeneous electron gas. Physical Review B, 2012, 85, .	3.2	99
11	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. Molecular Physics, 2014, 112, 1855-1869.	1.7	92
12	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2014, 141, 244117.	3.0	90
13	A study of electron affinities using the initiator approach to full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2011, 134, 024112.	3.0	89
14	Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models. Journal of Chemical Physics, 2012, 136, 244101.	3.0	86
15	Stochastic Multiconfigurational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2015, 11, 5316-5325.	5.3	86
16	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. Journal of Chemical Physics, 2015, 142, 184107.	3.0	83
17	Taming the First-Row Diatomics: A Full Configuration Interaction Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2012, 8, 4138-4152.	5.3	77
18	An excited-state approach within full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 134117.	3.0	77

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19	Spectroscopic accuracy directly from quantum chemistry: Application to ground and excited states of beryllium dimer. Journal of Chemical Physics, 2014, 140, 104112.	3.0	75
20	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. Physical Review X, 2020, 10, .	8.9	68
21	Explicitly correlated plane waves: Accelerating convergence in periodic wavefunction expansions. Journal of Chemical Physics, 2013, 139, 084112.	3.0	62
22	Full Configuration Interaction Excitations of Ethene and Butadiene: Resolution of an Ancient Question. Journal of Chemical Theory and Computation, 2012, 8, 4441-4451.	5.3	57
23	From plane waves to local Gaussians for the simulation of correlated periodic systems. Journal of Chemical Physics, 2016, 145, 084111.	3.0	56
24	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. Journal of Chemical Physics, 2020, 153, 034107.	3.0	55
25	Krylov-Projected Quantum MonteÂCarlo Method. Physical Review Letters, 2015, 115, 050603.	7.8	53
26	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2012, 137, 164112.	3.0	49
27	Communication: Excited states, dynamic correlation functions and spectral properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2012, 137, 191102.	3.0	47
28	Intermediate and spin-liquid phase of the half-filled honeycomb Hubbard model. Physical Review B, 2014, 89, .	3.2	47
29	Spectral functions of strongly correlated extended systems via an exact quantum embedding. Physical Review B, 2015, 91, .	3.2	47
30	Density matrices in full configuration interaction quantum Monte Carlo: Excited states, transition dipole moments, and parallel distribution. Journal of Chemical Physics, 2017, 146, 244105.	3.0	47
31	On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. Journal of Chemical Physics, 2015, 142, 194114.	3.0	44
32	AccurateAbÂInitioCalculation of Ionization Potentials of the First-Row Transition Metals with the Configuration-Interaction Quantum MonteÂCarlo Technique. Physical Review Letters, 2015, 114, 033001.	7.8	42
33	Rigorous wave function embedding with dynamical fluctuations. Physical Review B, 2018, 98, .	3.2	36
34	A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. Journal of Chemical Physics, 2017, 146, 204108.	3.0	35
35	Energy-weighted density matrix embedding of open correlated chemical fragments. Journal of Chemical Physics, 2019, 151, 014115.	3.0	28
36	Projector Quantum MonteÂCarlo Method for Nonlinear Wave Functions. Physical Review Letters, 2017, 118, 176403.	7.8	25

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37	Efficient and stochastic multireference perturbation theory for large active spaces within a full configuration interaction quantum Monte Carlo framework. Journal of Chemical Physics, 2020, 152, 054101.	3.0	25
38	Reduced density matrix sampling: Self-consistent embedding and multiscale electronic structure on current generation quantum computers. Physical Review Research, 2021, 3, .	3.6	25
39	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 054108.	3.0	24
40	Assessment of multireference approaches to explicitly correlated full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2016, 145, 054117.	3.0	20
41	Driven Imposters: Controlling Expectations in Many-Body Systems. Physical Review Letters, 2020, 124, 183201.	7.8	20
42	Fully algebraic and self-consistent effective dynamics in a static quantum embedding. Physical Review B, 2021, 103, .	3.2	20
43	Variational quantum eigensolver for dynamic correlation functions. Physical Review A, 2021, 104, .	2.5	19
44	High harmonic generation in two-dimensional Mott insulators. Npj Quantum Materials, 2021, 6, .	5.2	18
45	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. Physical Review B, 2018, 98, .	3.2	16
46	Symmetry Breaking and Broken Ergodicity in Full Configuration Interaction Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2014, 10, 1915-1922.	5.3	15
47	Controlling arbitrary observables in correlated many-body systems. Physical Review A, 2020, 101, .	2.5	15
48	Insights into the structure of many-electron wave functions of Mott-insulating antiferromagnets: The three-band Hubbard model in full configuration interaction quantum Monte Carlo. Physical Review B, 2015, 91, .	3.2	14
49	Systematic Improvability in Quantum Embedding for Real Materials. Physical Review X, 2022, 12, .	8.9	14
50	Wave Function Perspective and Efficient Truncation of Renormalized Second-Order Perturbation Theory. Journal of Chemical Theory and Computation, 2020, 16, 1090-1104.	5.3	12
51	Efficient Excitations and Spectra within a Perturbative Renormalization Approach. Journal of Chemical Theory and Computation, 2020, 16, 6294-6304.	5.3	11
52	Response Formalism within Full Configuration Interaction Quantum Monte Carlo: Static Properties and Electrical Response. Journal of Chemical Theory and Computation, 2018, 14, 3532-3546.	5.3	9
53	Scalable and Predictive Spectra of Correlated Molecules with Moment Truncated Iterated Perturbation Theory. Journal of Physical Chemistry Letters, 2021, 12, 7650-7658.	4.6	9
54	Four-component full configuration interaction quantum Monte Carlo for relativistic correlated electron problems. Journal of Chemical Physics, 2020, 153, 184103.	3.0	9

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55	A Bayesian inference framework for compression and prediction of quantum states. Journal of Chemical Physics, 2020, 153, 124108.	3.0	8
56	Extending density matrix embedding: A static two-particle theory. Physical Review B, 2021, 104, .	3.2	8
57	Improved stochastic multireference perturbation theory for correlated systems with large active spaces. Molecular Physics, 2020, 118, e1802072.	1.7	7
58	Gaussian Process States: A Data-Driven Representation of Quantum Many-Body Physics. Physical Review X, 2020, 10, .	8.9	6
59	Frequency-dependent and algebraic bath states for a dynamical mean-field theory with compact support. Physical Review B, 2020, 101, .	3.2	6
60	Efficient compression of the environment of an open quantum system. Physical Review B, 2020, 102, .	3.2	5
61	Equation of state of atomic solid hydrogen by stochastic many-body wave function methods. Journal of Chemical Physics, 2020, 153, 204107.	3.0	5
62	Quantum Gaussian process state: A kernel-inspired state with quantum support data. Physical Review Research, 2022, 4, .	3.6	4