George H Booth

List of Publications by Year in Descending Order

57 papers	3,622 citations	31 h-index	60 g-index
62 ext. papers	4,294 ext. citations	5.2 avg, IF	5.72 L-index

#	Paper	IF	Citations
57	Fully algebraic and self-consistent effective dynamics in a static quantum embedding. *Physical Review B*, **2021**, 103,	3.3	10
56	Scalable and Predictive Spectra of Correlated Molecules with Moment Truncated Iterated Perturbation Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 7650-7658	6.4	3
55	Reduced density matrix sampling: Self-consistent embedding and multiscale electronic structure on current generation quantum computers. *Physical Review Research*, **2021**, 3,	3.9	2
54	High harmonic generation in two-dimensional Mott insulators. *Npj Quantum Materials*, **2021**, 6,	5	2
53	A Bayesian inference framework for compression and prediction of quantum states. *Journal of Chemical Physics*, **2020**, 153, 124108	3.9	1
52	Controlling arbitrary observables in correlated many-body systems. *Physical Review A*, **2020**, 101,	2.6	4
51	Driven Imposters: Controlling Expectations in Many-Body Systems. *Physical Review Letters*, **2020**, 124, 183201	7.4	6
50	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	3.9	16
49	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. *Physical Review X*, **2020**, 10,	9.1	46
48	Wave Function Perspective and Efficient Truncation of Renormalized Second-Order Perturbation Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 1090-1104	6.4	6
47	Frequency-dependent and algebraic bath states for a dynamical mean-field theory with compact support. *Physical Review B*, **2020**, 101,	3.3	4
46	Equation of state of atomic solid hydrogen by stochastic many-body wave function methods. *Journal of Chemical Physics*, **2020**, 153, 204107	3.9	1
45	Four-component full configuration interaction quantum Monte Carlo for relativistic correlated electron problems. *Journal of Chemical Physics*, **2020**, 153, 184103	3.9	2
44	Efficient compression of the environment of an open quantum system. *Physical Review B*, **2020**, 102,	3.3	2
43	Recent developments in the PySCF program package. *Journal of Chemical Physics*, **2020**, 153, 024109	3.9	121
42	Improved stochastic multireference perturbation theory for correlated systems with large active spaces. *Molecular Physics*, **2020**, 118, e1802072	1.7	4
41	Efficient Excitations and Spectra within a Perturbative Renormalization Approach. *Journal of Chemical Theory and Computation*, **2020**, 16, 6294-6304	6.4	3

40	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. *Journal of Chemical Physics*, **2020**, 153, 034107	3.9	28
39	Energy-weighted density matrix embedding of open correlated chemical fragments. *Journal of Chemical Physics*, **2019**, 151, 014115	3.9	17
38	PySCF: the Python-based simulations of chemistry framework. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1340	7.9	482
37	Rigorous wave function embedding with dynamical fluctuations. *Physical Review B*, **2018**, 98,	3.3	24
36	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. *Physical Review B*, **2018**, 98,	3.3	10
35	Response Formalism within Full Configuration Interaction Quantum Monte Carlo: Static Properties and Electrical Response. *Journal of Chemical Theory and Computation*, **2018**, 14, 3532-3546	6.4	7
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	3.9	31
33	Density matrices in full configuration interaction quantum Monte Carlo: Excited states, transition dipole moments, and parallel distribution. *Journal of Chemical Physics*, **2017**, 146, 244105	3.9	34
32	Projector Quantum Monte Carlo Method for Nonlinear Wave Functions. *Physical Review Letters*, **2017**, 118, 176403	7.4	19
31	From plane waves to local Gaussians for the simulation of correlated periodic systems. *Journal of Chemical Physics*, **2016**, 145, 084111	3.9	45
30	Assessment of multireference approaches to explicitly correlated full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2016**, 145, 054117	3.9	14
29	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. *Journal of Chemical Physics*, **2015**, 142, 184107	3.9	71
28	Krylov-Projected Quantum Monte Carlo Method. *Physical Review Letters*, **2015**, 115, 050603	7.4	44
27	Stochastic Multiconfigurational Self-Consistent Field Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 5316-25	6.4	78
26	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2015**, 143, 054108	3.9	18
25	Spectral functions of strongly correlated extended systems via an exact quantum embedding. *Physical Review B*, **2015**, 91,	3.3	42
24	An excited-state approach within full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2015**, 143, 134117	3.9	60
23	On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. *Journal of Chemical Physics*, **2015**, 142, 194114	3.9	35

22	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,	3.3	13
21	Accurate Ab initio calculation of ionization potentials of the first-row transition metals with the configuration-interaction quantum Monte Carlo technique. *Physical Review Letters*, **2015**, 114, 033001	7.4	37
20	Intermediate and spin-liquid phase of the half-filled honeycomb Hubbard model. *Physical Review B*, **2014**, 89,	3.3	41
19	Spectroscopic accuracy directly from quantum chemistry: application to ground and excited states of beryllium dimer. *Journal of Chemical Physics*, **2014**, 140, 104112	3.9	65
18	Symmetry Breaking and Broken Ergodicity in Full Configuration Interaction Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2014**, 10, 1915-22	6.4	15
17	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2014**, 141, 244117	3.9	74
16	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. *Molecular Physics*, **2014**, 112, 1855-1869	1.7	82
15	Explicitly correlated plane waves: accelerating convergence in periodic wavefunction expansions. *Journal of Chemical Physics*, **2013**, 139, 084112	3.9	55
14	Towards an exact description of electronic wavefunctions in real solids. *Nature*, **2013**, 493, 365-70	50.4	375
13	Taming the First-Row Diatomics: A Full Configuration Interaction Quantum Monte Carlo Study. *Journal of Chemical Theory and Computation*, **2012**, 8, 4138-52	6.4	68
12	Full Configuration Interaction Excitations of Ethene and Butadiene: Resolution of an Ancient Question. *Journal of Chemical Theory and Computation*, **2012**, 8, 4441-51	6.4	56
11	Communication: Excited states, dynamic correlation functions and spectral properties from full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2012**, 137, 191102	3.9	41
10	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,	3.3	87
9	Full configuration interaction perspective on the homogeneous electron gas. *Physical Review B*, **2012**, 85,	3.3	86
8	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2012**, 137, 164112	3.9	44
7	Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models. *Journal of Chemical Physics*, **2012**, 136, 244101	3.9	73
6	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. *Journal of Chemical Theory and Computation*, **2011**, 7, 2780-5	6.4	95
5	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	3.9	120

4	A study of electron affinities using the initiator approach to full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2011**, 134, 024112	3.9	75
3	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: a study of ionization potentials. *Journal of Chemical Physics*, **2010**, 132, 174104	3.9	98
2	Communications: Survival of the fittest: accelerating convergence in full configuration-interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2010**, 132, 041103	3.9	256
1	Fermion Monte Carlo without fixed nodes: a game of life, death, and annihilation in Slater determinant space. *Journal of Chemical Physics*, **2009**, 131, 054106	3.9	469