

George H Booth

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	PySCF: the Python-based simulations of chemistry framework. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018 , 8, e1340	7.9	482
56	Fermion Monte Carlo without fixed nodes: a game of life, death, and annihilation in Slater determinant space. <i>Journal of Chemical Physics</i> , 2009 , 131, 054106	3.9	469
55	Towards an exact description of electronic wavefunctions in real solids. <i>Nature</i> , 2013 , 493, 365-70	50.4	375
54	Communications: Survival of the fittest: accelerating convergence in full configuration-interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2010 , 132, 041103	3.9	256
53	Recent developments in the PySCF program package. <i>Journal of Chemical Physics</i> , 2020 , 153, 024109	3.9	121
52	Breaking the carbon dimer: the challenges of multiple bond dissociation with full configuration interaction quantum Monte Carlo methods. <i>Journal of Chemical Physics</i> , 2011 , 135, 084104	3.9	120
51	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: a study of ionization potentials. <i>Journal of Chemical Physics</i> , 2010 , 132, 174104	3.9	98
50	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2780-5	6.4	95
49	Convergence of many-body wave-function expansions using a plane-wave basis: From homogeneous electron gas to solid state systems. <i>Physical Review B</i> , 2012 , 86,	3.3	87
48	Full configuration interaction perspective on the homogeneous electron gas. <i>Physical Review B</i> , 2012 , 85,	3.3	86
47	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. <i>Molecular Physics</i> , 2014 , 112, 1855-1869	1.7	82
46	Stochastic Multiconfigurational Self-Consistent Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5316-25	6.4	78
45	A study of electron affinities using the initiator approach to full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2011 , 134, 024112	3.9	75
44	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2014 , 141, 244117	3.9	74
43	Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models. <i>Journal of Chemical Physics</i> , 2012 , 136, 244101	3.9	73
42	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. <i>Journal of Chemical Physics</i> , 2015 , 142, 184107	3.9	71
41	Taming the First-Row Diatomics: A Full Configuration Interaction Quantum Monte Carlo Study. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4138-52	6.4	68

40	Spectroscopic accuracy directly from quantum chemistry: application to ground and excited states of beryllium dimer. <i>Journal of Chemical Physics</i> , 2014 , 140, 104112	3.9	65
39	An excited-state approach within full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2015 , 143, 134117	3.9	60
38	Full Configuration Interaction Excitations of Ethene and Butadiene: Resolution of an Ancient Question. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4441-51	6.4	56
37	Explicitly correlated plane waves: accelerating convergence in periodic wavefunction expansions. <i>Journal of Chemical Physics</i> , 2013 , 139, 084112	3.9	55
36	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. <i>Physical Review X</i> , 2020 , 10,	9.1	46
35	From plane waves to local Gaussians for the simulation of correlated periodic systems. <i>Journal of Chemical Physics</i> , 2016 , 145, 084111	3.9	45
34	Krylov-Projected Quantum Monte Carlo Method. <i>Physical Review Letters</i> , 2015 , 115, 050603	7.4	44
33	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2012 , 137, 164112	3.9	44
32	Spectral functions of strongly correlated extended systems via an exact quantum embedding. <i>Physical Review B</i> , 2015 , 91,	3.3	42
31	Intermediate and spin-liquid phase of the half-filled honeycomb Hubbard model. <i>Physical Review B</i> , 2014 , 89,	3.3	41
30	Communication: Excited states, dynamic correlation functions and spectral properties from full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2012 , 137, 191102	3.9	41
29	Accurate Ab initio calculation of ionization potentials of the first-row transition metals with the configuration-interaction quantum Monte Carlo technique. <i>Physical Review Letters</i> , 2015 , 114, 033001	7.4	37
28	On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. <i>Journal of Chemical Physics</i> , 2015 , 142, 194114	3.9	35
27	Density matrices in full configuration interaction quantum Monte Carlo: Excited states, transition dipole moments, and parallel distribution. <i>Journal of Chemical Physics</i> , 2017 , 146, 244105	3.9	34
26	A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. <i>Journal of Chemical Physics</i> , 2017 , 146, 204108	3.9	31
25	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. <i>Journal of Chemical Physics</i> , 2020 , 153, 034107	3.9	28
24	Rigorous wave function embedding with dynamical fluctuations. <i>Physical Review B</i> , 2018 , 98,	3.3	24
23	Projector Quantum Monte Carlo Method for Nonlinear Wave Functions. <i>Physical Review Letters</i> , 2017 , 118, 176403	7.4	19

22	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2015 , 143, 054108	3.9	18
21	Energy-weighted density matrix embedding of open correlated chemical fragments. <i>Journal of Chemical Physics</i> , 2019 , 151, 014115	3.9	17
20	Efficient and stochastic multireference perturbation theory for large active spaces within a full configuration interaction quantum Monte Carlo framework. <i>Journal of Chemical Physics</i> , 2020 , 152, 054101	3.9	16
19	Symmetry Breaking and Broken Ergodicity in Full Configuration Interaction Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1915-22	6.4	15
18	Assessment of multireference approaches to explicitly correlated full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2016 , 145, 054117	3.9	14
17	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. <i>Physical Review B</i> , 2015 , 91,	3.3	13
16	Fully algebraic and self-consistent effective dynamics in a static quantum embedding. <i>Physical Review B</i> , 2021 , 103,	3.3	10
15	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. <i>Physical Review B</i> , 2018 , 98,	3.3	10
14	Response Formalism within Full Configuration Interaction Quantum Monte Carlo: Static Properties and Electrical Response. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3532-3546	6.4	7
13	Driven Imposters: Controlling Expectations in Many-Body Systems. <i>Physical Review Letters</i> , 2020 , 124, 183201	7.4	6
12	Wave Function Perspective and Efficient Truncation of Renormalized Second-Order Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1090-1104	6.4	6
11	Controlling arbitrary observables in correlated many-body systems. <i>Physical Review A</i> , 2020 , 101,	2.6	4
10	Frequency-dependent and algebraic bath states for a dynamical mean-field theory with compact support. <i>Physical Review B</i> , 2020 , 101,	3.3	4
9	Improved stochastic multireference perturbation theory for correlated systems with large active spaces. <i>Molecular Physics</i> , 2020 , 118, e1802072	1.7	4
8	Efficient Excitations and Spectra within a Perturbative Renormalization Approach. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6294-6304	6.4	3
7	Scalable and Predictive Spectra of Correlated Molecules with Moment Truncated Iterated Perturbation Theory. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 7650-7658	6.4	3
6	Four-component full configuration interaction quantum Monte Carlo for relativistic correlated electron problems. <i>Journal of Chemical Physics</i> , 2020 , 153, 184103	3.9	2
5	Efficient compression of the environment of an open quantum system. <i>Physical Review B</i> , 2020 , 102,	3.3	2

4	Reduced density matrix sampling: Self-consistent embedding and multiscale electronic structure on current generation quantum computers. <i>Physical Review Research</i> , 2021 , 3,	3.9	2
3	High harmonic generation in two-dimensional Mott insulators. <i>Npj Quantum Materials</i> , 2021 , 6,	5	2
2	A Bayesian inference framework for compression and prediction of quantum states. <i>Journal of Chemical Physics</i> , 2020 , 153, 124108	3.9	1
1	Equation of state of atomic solid hydrogen by stochastic many-body wave function methods. <i>Journal of Chemical Physics</i> , 2020 , 153, 204107	3.9	1