

George H Booth

List of Publications by Year in descending order

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62
papers

5,055
citations

117453

34
h-index

118652

62
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all docs

62
docs citations

62
times ranked

2419
citing authors

#	ARTICLE	IF	CITATIONS
1	Systematic Improvability in Quantum Embedding for Real Materials. <i>Physical Review X</i> , 2022, 12, .	2.8	14
2	Quantum Gaussian process state: A kernel-inspired state with quantum support data. <i>Physical Review Research</i> , 2022, 4, .	1.3	4
3	Fully algebraic and self-consistent effective dynamics in a static quantum embedding. <i>Physical Review B</i> , 2021, 103, .	1.1	20
4	Scalable and Predictive Spectra of Correlated Molecules with Moment Truncated Iterated Perturbation Theory. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7650-7658.	2.1	9
5	Reduced density matrix sampling: Self-consistent embedding and multiscale electronic structure on current generation quantum computers. <i>Physical Review Research</i> , 2021, 3, .	1.3	25
6	High harmonic generation in two-dimensional Mott insulators. <i>Npj Quantum Materials</i> , 2021, 6, .	1.8	18
7	Variational quantum eigensolver for dynamic correlation functions. <i>Physical Review A</i> , 2021, 104, .	1.0	19
8	Extending density matrix embedding: A static two-particle theory. <i>Physical Review B</i> , 2021, 104, .	1.1	8
9	Efficient compression of the environment of an open quantum system. <i>Physical Review B</i> , 2020, 102, .	1.1	5
10	Recent developments in the Pyscf SCF program package. <i>Journal of Chemical Physics</i> , 2020, 153, 024109.	1.2	388
11	Improved stochastic multireference perturbation theory for correlated systems with large active spaces. <i>Molecular Physics</i> , 2020, 118, e1802072.	0.8	7
12	Efficient Excitations and Spectra within a Perturbative Renormalization Approach. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6294-6304.	2.3	11
13	NECI: N -Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. <i>Journal of Chemical Physics</i> , 2020, 153, 034107.	1.2	55
14	Gaussian Process States: A Data-Driven Representation of Quantum Many-Body Physics. <i>Physical Review X</i> , 2020, 10, .	2.8	6
15	A Bayesian inference framework for compression and prediction of quantum states. <i>Journal of Chemical Physics</i> , 2020, 153, 124108.	1.2	8
16	Controlling arbitrary observables in correlated many-body systems. <i>Physical Review A</i> , 2020, 101, .	1.0	15
17	Driven Imposters: Controlling Expectations in Many-Body Systems. <i>Physical Review Letters</i> , 2020, 124, 183201.	2.9	20
18	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.	1.2	25

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19	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. <i>Physical Review X</i> , 2020, 10, .	2.8	68
20	Wave Function Perspective and Efficient Truncation of Renormalized Second-Order Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1090-1104.	2.3	12
21	Frequency-dependent and algebraic bath states for a dynamical mean-field theory with compact support. <i>Physical Review B</i> , 2020, 101, .	1.1	6
22	Equation of state of atomic solid hydrogen by stochastic many-body wave function methods. <i>Journal of Chemical Physics</i> , 2020, 153, 204107.	1.2	5
23	Four-component full configuration interaction quantum Monte Carlo for relativistic correlated electron problems. <i>Journal of Chemical Physics</i> , 2020, 153, 184103.	1.2	9
24	Energy-weighted density matrix embedding of open correlated chemical fragments. <i>Journal of Chemical Physics</i> , 2019, 151, 014115.	1.2	28
25	Pyscf: the Python-based simulations of chemistry framework. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1340.	6.2	894
26	Rigorous wave function embedding with dynamical fluctuations. <i>Physical Review B</i> , 2018, 98, .	1.1	36
27	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. <i>Physical Review B</i> , 2018, 98, .	1.1	16
28	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.	2.3	9
29	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.	1.2	35
30	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.	1.2	47
31	Projector Quantum Monte Carlo Method for Nonlinear Wave Functions. <i>Physical Review Letters</i> , 2017, 118, 176403.	2.9	25
32	From plane waves to local Gaussians for the simulation of correlated periodic systems. <i>Journal of Chemical Physics</i> , 2016, 145, 084111.	1.2	56
33	Assessment of multireference approaches to explicitly correlated full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2016, 145, 054117.	1.2	20
34	Spectral functions of strongly correlated extended systems via an exact quantum embedding. <i>Physical Review B</i> , 2015, 91, .	1.1	47
35	An excited-state approach within full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2015, 143, 134117.	1.2	77
36	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.	1.2	44

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37	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, .	1.1	14
38	Accurate <i>Ab Initio</i> 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.	2.9	42
39	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. <i>Journal of Chemical Physics</i> , 2015, 142, 184107.	1.2	83
40	Krylov-Projected Quantum Monte Carlo Method. <i>Physical Review Letters</i> , 2015, 115, 050603.	2.9	53
41	Stochastic Multiconfigurational Self-Consistent Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5316-5325.	2.3	86
42	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2015, 143, 054108.	1.2	24
43	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2014, 141, 244117.	1.2	90
44	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. <i>Molecular Physics</i> , 2014, 112, 1855-1869.	0.8	92
45	Intermediate and spin-liquid phase of the half-filled honeycomb Hubbard model. <i>Physical Review B</i> , 2014, 89, .	1.1	47
46	Spectroscopic accuracy directly from quantum chemistry: Application to ground and excited states of beryllium dimer. <i>Journal of Chemical Physics</i> , 2014, 140, 104112.	1.2	75
47	Symmetry Breaking and Broken Ergodicity in Full Configuration Interaction Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1915-1922.	2.3	15
48	Explicitly correlated plane waves: Accelerating convergence in periodic wavefunction expansions. <i>Journal of Chemical Physics</i> , 2013, 139, 084112.	1.2	62
49	Towards an exact description of electronic wavefunctions in real solids. <i>Nature</i> , 2013, 493, 365-370.	13.7	440
50	Full configuration interaction perspective on the homogeneous electron gas. <i>Physical Review B</i> , 2012, 85, .	1.1	99
51	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2012, 137, 164112.	1.2	49
52	Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models. <i>Journal of Chemical Physics</i> , 2012, 136, 244101.	1.2	86
53	Taming the First-Row Diatomics: A Full Configuration Interaction Quantum Monte Carlo Study. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4138-4152.	2.3	77
54	Full Configuration Interaction Excitations of Ethene and Butadiene: Resolution of an Ancient Question. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4441-4451.	2.3	57

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55	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.	1.2	47
56	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, .	1.1	101
57	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2780-2785.	2.3	117
58	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.	1.2	134
59	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.	1.2	89
60	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: A study of ionization potentials. <i>Journal of Chemical Physics</i> , 2010, 132, 174104.	1.2	110
61	Communications: Survival of the fittest: Accelerating convergence in full configuration-interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2010, 132, 041103.	1.2	308
62	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.	1.2	567