

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.

85
papers

4,437
citations

35
h-index

66
g-index

90
ext. papers

5,135
ext. citations

4.9
avg, IF

6.03
L-index

#	Paper	IF	Citations
85	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
84	Towards an exact description of electronic wavefunctions in real solids. <i>Nature</i> , 2013 , 493, 365-70	50.4	375
83	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 5925-5964	39.4	310
82	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
81	Ab initio molecular dynamics with excited electrons. <i>Physical Review Letters</i> , 1994 , 73, 2599-2602	7.4	213
80	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1595-1604	6.4	178
79	Combining the Complete Active Space Self-Consistent Field Method and the Full Configuration Interaction Quantum Monte Carlo within a Super-CI Framework, with Application to Challenging Metal-Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1245-58	6.4	134
78	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
77	Reconstruction of charged surfaces: General trends and a case study of Pt(110) and Au(110). <i>Physical Review B</i> , 2003 , 68,	3.3	113
76	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
75	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
74	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
73	Full configuration interaction perspective on the homogeneous electron gas. <i>Physical Review B</i> , 2012 , 85,	3.3	86
72	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. <i>Molecular Physics</i> , 2014 , 112, 1855-1869	1.7	82
71	Stochastic Multiconfigurational Self-Consistent Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5316-25	6.4	78
70	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
69	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

68	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
67	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. <i>Journal of Chemical Physics</i> , 2015 , 142, 184107	3.9	71
66	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
65	Where do the H atoms reside in PdH x systems?. <i>Molecular Physics</i> , 2003 , 101, 1781-1787	1.7	63
64	Multireference linearized coupled cluster theory for strongly correlated systems using matrix product states. <i>Journal of Chemical Physics</i> , 2015 , 143, 102815	3.9	60
63	An excited-state approach within full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2015 , 143, 134117	3.9	60
62	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
61	Explicitly correlated plane waves: accelerating convergence in periodic wavefunction expansions. <i>Journal of Chemical Physics</i> , 2013 , 139, 084112	3.9	55
60	Understanding the Mechanism Stabilizing Intermediate Spin States in Fe(II)-Porphyrin. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 4935-4947	2.8	53
59	The Ground State Electronic Energy of Benzene. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 8922-8929	7.4	52
58	Mechanism for the high reactivity of CO oxidation on a ruthenium oxide. <i>Journal of Chemical Physics</i> , 2001 , 114, 5956-5957	3.9	47
57	Combining Internally Contracted States and Matrix Product States To Perform Multireference Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 488-498	6.4	46
56	Krylov-Projected Quantum Monte Carlo Method. <i>Physical Review Letters</i> , 2015 , 115, 050603	7.4	44
55	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
54	Charge-transfer molecular dynamics. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1992 , 65, 489-500		43
53	Unbiasing the initiator approximation in full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2019 , 151, 224108	3.9	38
52	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
51	Two interacting electrons in a box: An exact diagonalization study. <i>Journal of Chemical Physics</i> , 2000 , 113, 7735-7745	3.9	35

50	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
49	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1492-1497	6.4	32
48	Two interacting electrons in a spherical box: An exact diagonalization study. <i>Physical Review B</i> , 2002 , 66,	3.3	32
47	Stochastic multi-reference perturbation theory with application to the linearized coupled cluster method. <i>Journal of Chemical Physics</i> , 2017 , 146, 044107	3.9	31
46	Efficient formulation of full configuration interaction quantum Monte Carlo in a spin eigenbasis via the graphical unitary group approach. <i>Journal of Chemical Physics</i> , 2019 , 151, 094104	3.9	30
45	Combining the Transcorrelated Method with Full Configuration Interaction Quantum Monte Carlo: Application to the Homogeneous Electron Gas. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1403-1411	6.4	30
44	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
43	Molecular-dynamics simulation of methane adsorbed on MgO: Evidence for a Kosterlitz-Thouless transition. <i>Molecular Physics</i> , 1990 , 71, 1173-1191	1.7	26
42	Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via nonunitary similarity transformations. <i>Physical Review B</i> , 2019 , 99,	3.3	25
41	The Intricate Case of Tetramethylethane: A Full Configuration Interaction Quantum Monte Carlo Benchmark and Multireference Coupled Cluster Studies. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2439-2445	6.4	24
40	Entropy of H ₂ O Wetting Layers \square <i>Journal of Physical Chemistry B</i> , 2004 , 108, 14362-14367	3.4	24
39	Similarity transformation of the electronic Schrödinger equation via Jastrow factorization. <i>Journal of Chemical Physics</i> , 2019 , 151, 061101	3.9	22
38	Projector Quantum Monte Carlo Method for Nonlinear Wave Functions. <i>Physical Review Letters</i> , 2017 , 118, 176403	7.4	19
37	Electronic correlations and magnetic interactions in infinite-layer NdNiO ₂ . <i>Physical Review B</i> , 2020 , 102,	3.3	19
36	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
35	Compression of Spin-Adapted Multiconfigurational Wave Functions in Exchange-Coupled Polynuclear Spin Systems. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2202-2215	6.4	16
34	Molecular-dynamics simulation of argon physisorbed on magnesium oxide. <i>Molecular Physics</i> , 1990 , 69, 703-713	1.7	16
33	The adaptive shift method in full configuration interaction quantum Monte Carlo: Development and applications. <i>Journal of Chemical Physics</i> , 2020 , 153, 224115	3.9	15

32	FCIQMC-Tailored Distinguishable Cluster Approach. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5621-5634	6.4	14
31	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
30	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
29	Correlation energies of the high-density spin-polarized electron gas to meV accuracy. <i>Physical Review B</i> , 2018 , 98,	3.3	13
28	Dynamics of quantum tunneling: Effects on the rate and transition path of OH on Cu(110). <i>Physical Review B</i> , 2010 , 81,	3.3	12
27	Chemical insights into the electronic structure of Fe(II) porphyrin using FCIQMC, DMRG, and generalized active spaces. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26454	2.1	11
26	Time Propagation and Spectroscopy of Fermionic Systems Using a Stochastic Technique. <i>Physical Review Letters</i> , 2018 , 121, 056401	7.4	10
25	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. <i>Journal of Chemical Physics</i> , 2015 , 143, 102601	3.9	10
24	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III)S] Cubanes. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 4727-4740	2.8	10
23	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	10
22	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. <i>Physical Review B</i> , 2018 , 98,	3.3	10
21	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron-Sulfur Clusters. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5684-5703	6.4	9
20	Accelerating the convergence of exact diagonalization with the transcorrelated method: Quantum gas in one dimension with contact interactions. <i>Physical Review A</i> , 2018 , 98,	2.6	8
19	Small polarons and the Janus nature of TiO ₂ (110). <i>Physical Review B</i> , 2020 , 101,	3.3	7
18	The color center singlet state of oxygen vacancies in TiO. <i>Journal of Chemical Physics</i> , 2020 , 153, 204704	3.9	7
17	Population control bias and importance sampling in full configuration interaction quantum Monte Carlo. <i>Physical Review B</i> , 2021 , 103,	3.3	6
16	Ammonium cyanate: a DFT study of crystal structure, rotational barriers and vibrational spectrum. <i>Molecular Physics</i> , 2004 , 102, 869-876	1.7	5
15	Synthesis and extensive characterisation of phosphorus doped graphite. <i>RSC Advances</i> , 2016 , 6, 62140-63145	3.7	4

14	Eliminating the wave-function singularity for ultracold atoms by a similarity transformation. <i>Physical Review Research</i> , 2020 , 2,	3.9	4
13	Binding curve of the beryllium dimer using similarity-transformed FCIQMC: Spectroscopic accuracy with triple-zeta basis sets. <i>Journal of Chemical Physics</i> , 2021 , 155, 011102	3.9	4
12	Dipole Amplification: A Principle for the Self-Assembly of Asymmetric Monomers on Metal Surfaces. <i>Angewandte Chemie</i> , 2008 , 120, 2456-2460	3.6	3
11	Transcorrelated coupled cluster methods. <i>Journal of Chemical Physics</i> , 2021 , 155, 191101	3.9	3
10	A full configuration interaction quantum Monte Carlo study of ScO, TiO, and VO molecules. <i>Journal of Chemical Physics</i> , 2021 , 154, 164302	3.9	3
9	Towards efficient and accurate ab initio solutions to periodic systems via transcorrelation and coupled cluster theory. <i>Physical Review Research</i> , 2021 , 3,	3.9	3
8	Are smooth pseudopotentials a good choice for representing short-range interactions?. <i>Physical Review A</i> , 2019 , 99,	2.6	2
7	Theory and Practice: Bulk Synthesis of C3B and its H ₂ - and Li-Storage Capacity. <i>Angewandte Chemie</i> , 2015 , 127, 6017-6021	3.6	2
6	Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo. <i>Physical Review B</i> , 2021 , 104,	3.3	2
5	Signatures of the BCS-BEC crossover in the yrast spectra of Fermi quantum rings. <i>Physical Review Research</i> , 2021 , 3,	3.9	2
4	The use of XANES and ELNES for the Characterisation of Stabilised Zirconia. <i>Materials Research Society Symposia Proceedings</i> , 2001 , 699, 821		1
3	Full configuration interaction quantum Monte Carlo treatment of fragments embedded in a periodic mean field.. <i>Journal of Chemical Physics</i> , 2022 , 156, 154107	3.9	1
2	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. <i>Nature Physics</i> , 2022 , 18, 190-195	16.2	1
1	General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides.. <i>Journal of Chemical Physics</i> , 2022 , 156, 124704	3.9	0