Cyrus Umrigar

List of Publications by Year
in descending order

49 papers	4,128 citations	159585 30 h-index	214800 47 g-index
50 all docs	50 docs citations	50 times ranked	2168 citing authors

#	Article	IF	Citations
1	A diffusion Monte Carlo algorithm with very small timeâ€step errors. Journal of Chemical Physics, 1993, 99, 2865-2890.	3.0	471
2	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	7.8	411
3	Heat-Bath Configuration Interaction: An Efficient Selected Configuration Interaction Algorithm Inspired by Heat-Bath Sampling. Journal of Chemical Theory and Computation, 2016, 12, 3674-3680.	5.3	294
4	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 1595-1604.	5.3	232
5	Optimization of quantum Monte Carlo wave functions by energy minimization. Journal of Chemical Physics, 2007, 126, 084102.	3.0	226
6	Multiconfiguration wave functions for quantum Monte Carlo calculations of firstâ€row diatomic molecules. Journal of Chemical Physics, 1996, 105, 213-226.	3.0	213
7	Full optimization of Jastrowâ€“Slater wave functions with application to the first-row atoms and homonuclear diatomic molecules. Journal of Chemical Physics, 2008, 128, 174101.	3.0	167
8	Comparison of exact and approximate density functionals for an exactly soluble model. Journal of Chemical Physics, 1994, 100, 1290-1296.	3.0	163
9	Energy and Variance Optimization of Many-Body Wave Functions. Physical Review Letters, 2005, 94, 150201.	7.8	155
10	Semistochastic Projector MonteÂCarlo Method. Physical Review Letters, 2012, 109, 230201.	7.8	151
11	Comparison of screened hybrid density functional theory to diffusion Monte Carlo in calculations of total energies of silicon phases and defects. Physical Review B, 2006, 74, .	3.2	131
12	Excited states using semistochastic heat-bath configuration interaction. Journal of Chemical Physics, 2017, 147, 164111.	3.0	108
13	Fast semistochastic heat-bath configuration interaction. Journal of Chemical Physics, 2018, 149, 214110.	3.0	99
14	Optimizing large parameter sets in variational quantum Monte Carlo. Physical Review B, 2012, 85, .	3.2	91
15	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
16	Approximating strongly correlated wave functions with correlator product states. Physical Review B, 2009, 80, .	3.2	88
17	Excited States of Methylene, Polyenes, and Ozone from Heat-Bath Configuration Interaction. Journal of Physical Chemistry A, 2018, 122, 2714-2722.	2.5	80
18	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

#	Article	IF	Citations
19	Correlation-induced inhomogeneity in circular quantum dots. Nature Physics, 2006, 2, 336-340.	16.7	72
20	Approaching chemical accuracy with quantum Monte Carlo. Journal of Chemical Physics, 2012, 136, 124116.	3.0	70
21	Efficient Heat-Bath Sampling in Fock Space. Journal of Chemical Theory and Computation, 2016, 12, 1561-1571.	5.3	66
22	Phase transformation in Si from semiconducting diamond to metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>-Sn</mml:mtext></mml:mrow></mml:math>phase in QMC and DFT under hydrostatic and anisotropic stress. Physical Review B, 2010, 82, .	3.2	65
23	The electronic complexity of the ground-state of the FeMo cofactor of nitrogenase as relevant to quantum simulations. Journal of Chemical Physics, 2019, 150, 024302.	3.0	59
24	Incipient Wigner localization in circular quantum dots. Physical Review B, 2007, 76, .	3.2	50
25	Spin contamination in quantum Monte Carlo wave functions. Journal of Chemical Physics, 1998, 108, 8838-8847.	3.0	44
26	Almost exact energies for the Gaussian-2 set with the semistochastic heat-bath configuration interaction method. Journal of Chemical Physics, 2020, 153, 124117.	3.0	41
27	Electron intracule densities with correct electron coalescence cusps from Hillerâ€“Becherâ€“Feinbergâ€type identities. Journal of Chemical Physics, 1995, 103, 6093-6103.	3.0	39
28	Quantum Monte Carlo study of composite fermions in quantum dots: The effect of Landau-level mixing. Physical Review B, 2005, 72, .	3.2	37
29	Localization in an inhomogeneous quantum wire. Physical Review B, 2009, 80, .	3.2	35
30	Energy landscape of silicon systems and its description by force fields, tight binding schemes, density functional methods, and quantum Monte Carlo methods. Physical Review B, 2010, 81, .	3.2	31
31	Accurate many-body electronic structure near the basis set limit: Application to the chromium dimer. Physical Review Research, 2020, 2, .	3.6	31
32	Zigzag Phase Transition in Quantum Wires. Physical Review Letters, 2013, 110, 246802.	7.8	29
33	Interaction-induced strong localization in quantum dots. Physical Review B, 2008, 77, .	3.2	27
34	Observations on variational and projector Monte Carlo methods. Journal of Chemical Physics, 2015, 143, 164105.	3.0	23
35	Orbital Optimization in Selected Configuration Interaction Methods. Journal of Chemical Theory and Computation, 2021, 17, 4183-4194.	5.3	23
36	Energy density functionals from the strong-coupling limit applied to the anions of the He isoelectronic series. Journal of Chemical Physics, 2014, 140, 18A532.	3.0	19

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37	Two aspects of quantum monte carlo: Determination of accurate wavefunctions and determination of potential energy surfaces of molecules. International Journal of Quantum Chemistry, 1989, 36, 217-230.	2.0	18
38	Externally Corrected CCSD with Renormalized Perturbative Triples (R-ecCCSD(T)) and the Density Matrix Renormalization Group and Selected Configuration Interaction External Sources. Journal of Chemical Theory and Computation, 2021, 17, 3414-3425.	5.3	18
39	Basis set construction for molecular electronic structure theory: Natural orbital and Gaussâ€“Slater basis for smooth pseudopotentials. Journal of Chemical Physics, 2011, 134, 064104.	3.0	15
40	Influence of the exchange-correlation potential in methods based on time-dependent density-functional theory. Physical Review A, 2013, 88, .	2.5	15
41	Path to Wigner localization in circular quantum dots. Physical Review B, 2009, 79, .	3.2	14
42	Composite-fermion antiparticle description of the hole excitation in a maximum-density droplet with a small number of electrons. Physical Review B, 2005, 72, .	3.2	9
43	Accurate energies of transition metal atoms, ions, and monoxides using selected configuration interaction and density-based basis-set corrections. Journal of Chemical Physics, 2021, 155, 204104.	3.0	9
44	Interaction effects in the mesoscopic regime: A quantum Monte Carlo study of irregular quantum dots. Physical Review B, 2005, 71, .	3.2	7
45	Nonlocal pseudopotentials and time-step errors in diffusion Monte Carlo. Journal of Chemical Physics, 2021, 154, 214110.	3.0	6
46	Monte Carlo Eigenvalue Methods in Quantum Mechanics and Statistical Mechanics. Advances in Chemical Physics, 0, , 65-115.	0.3	5
47	Monte Carlo Optimization of Trial Wave Functions in Quantum Mechanics and Statistical Mechanics. Recent Advances in Computational, 1997, , 201-227.	0.8	4
48	INTERATOMIC FORCES AND CORRELATED SAMPLING IN QUANTUM MONTE CARLO. Recent Advances in Computational, 2002, , 12-29.	0.8	2
49	POLARIZABILITY IN QUANTUM DOTS VIA CORRELATED QUANTUM MONTE CARLO. , 2008, , .		0