Cyrus Umrigar

List of Publications by Year
in descending order

49	4,128	159585	214800
papers	citations	30	47
		h-index	g-index

50	50	50	2168
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Orbital Optimization in Selected Configuration Interaction Methods. Journal of Chemical Theory and Computation, 2021, 17, 4183-4194.	5.3	23
3	Nonlocal pseudopotentials and time-step errors in diffusion Monte Carlo. Journal of Chemical Physics, 2021, 154, 214110.	3.0	6
4	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
5	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
6	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
7	Accurate many-body electronic structure near the basis set limit: Application to the chromium dimer. Physical Review Research, 2020, 2, .	3.6	31
8	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
9	Excited States of Methylene, Polyenes, and Ozone from Heat-Bath Configuration Interaction. Journal of Physical Chemistry A, 2018, 122, 2714-2722.	2.5	80
10	Fast semistochastic heat-bath configuration interaction. Journal of Chemical Physics, 2018, 149, 214110.	3.0	99
11	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
12	Excited states using semistochastic heat-bath configuration interaction. Journal of Chemical Physics, 2017, 147, 164111.	3.0	108
13	Efficient Heat-Bath Sampling in Fock Space. Journal of Chemical Theory and Computation, 2016, 12, 1561-1571.	5.3	66
14	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
15	Observations on variational and projector Monte Carlo methods. Journal of Chemical Physics, 2015, 143, 164105.	3.0	23
16	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
17	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
18	Influence of the exchange-correlation potential in methods based on time-dependent density-functional theory. Physical Review A, 2013, 88, .	2.5	15

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19	Zigzag Phase Transition in Quantum Wires. Physical Review Letters, 2013, 110, 246802.	7.8	29
20	Approaching chemical accuracy with quantum Monte Carlo. Journal of Chemical Physics, 2012, 136, 124116.	3.0	70
21	Optimizing large parameter sets in variational quantum Monte Carlo. Physical Review B, 2012, 85, .	3.2	91
22	Semistochastic Projector Monte Carlo Method. Physical Review Letters, 2012, 109, 230201.	7.8	151
23	Basis set construction for molecular electronic structure theory: Natural orbital and Gauss–Slater basis for smooth pseudopotentials. Journal of Chemical Physics, 2011, 134, 064104.	3.0	15
24	Phase transformation in Si from semiconducting diamond to metallic β-Sn phase in QMC and DFT under hydrostatic and anisotropic stress. Physical Review B, 2010, 82, .	3.2	65
25	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
26	Path to Wigner localization in circular quantum dots. Physical Review B, 2009, 79, .	3.2	14
27	Localization in an inhomogeneous quantum wire. Physical Review B, 2009, 80, .	3.2	35
28	Approximating strongly correlated wave functions with correlator product states. Physical Review B, 2009, 80, .	3.2	88
29	Full optimization of Jastrow–Slater wave functions with application to the first-row atoms and homonuclear diatomic molecules. Journal of Chemical Physics, 2008, 128, 174101.	3.0	167
30	Interaction-induced strong localization in quantum dots. Physical Review B, 2008, 77, .	3.2	27
31	POLARIZABILITY IN QUANTUM DOTS VIA CORRELATED QUANTUM MONTE CARLO. , 2008, , .		0
32	Incipient Wigner localization in circular quantum dots. Physical Review B, 2007, 76, .	3.2	50
33	Optimization of quantum Monte Carlo wave functions by energy minimization. Journal of Chemical Physics, 2007, 126, 084102.	3.0	226
34	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	7.8	411
35	Correlation-induced inhomogeneity in circular quantum dots. Nature Physics, 2006, 2, 336-340.	16.7	72
36	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

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37	Interaction effects in the mesoscopic regime: A quantum Monte Carlo study of irregular quantum dots. Physical Review B, 2005, 71, .	3.2	7
38	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
39	Energy and Variance Optimization of Many-Body Wave Functions. Physical Review Letters, 2005, 94, 150201.	7.8	155
40	Quantum Monte Carlo study of composite fermions in quantum dots: The effect of Landau-level mixing. Physical Review B, 2005, 72, .	3.2	37
41	INTERATOMIC FORCES AND CORRELATED SAMPLING IN QUANTUM MONTE CARLO. Recent Advances in Computational, 2002, , 12-29.	0.8	2
42	Spin contamination in quantum Monte Carlo wave functions. Journal of Chemical Physics, 1998, 108, 8838-8847.	3.0	44
43	Monte Carlo Optimization of Trial Wave Functions in Quantum Mechanics and Statistical Mechanics. Recent Advances in Computational, 1997, , 201-227.	0.8	4
44	Multiconfiguration wave functions for quantum Monte Carlo calculations of firstâ€row diatomic molecules. Journal of Chemical Physics, 1996, 105, 213-226.	3.0	213
45	Electron intracule densities with correct electron coalescence cusps from Hillerâ€"Sucherâ€"Feinbergâ€type identities. Journal of Chemical Physics, 1995, 103, 6093-6103.	3.0	39
46	Comparison of exact and approximate density functionals for an exactly soluble model. Journal of Chemical Physics, 1994, 100, 1290-1296.	3.0	163
47	A diffusion Monte Carlo algorithm with very small timeâ€step errors. Journal of Chemical Physics, 1993, 99, 2865-2890.	3.0	471
48	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
49	Monte Carlo Eigenvalue Methods in Quantum Mechanics and Statistical Mechanics. Advances in Chemical Physics, 0, , 65-115.	0.3	5