C J Umrigar

List of Publications by Year
in descending order

70 papers	6,584 citations	76196 40 h-index	98622 67 g-index
71 all docs	71 docs citations	71 times ranked	3116 citing authors

#	Article	IF	Citations
1	Optimized trial wave functions for quantum Monte Carlo calculations. Physical Review Letters, 1988, 60, 1719-1722.	2.9	584
2	A diffusion Monte Carlo algorithm with very small timeâ€step errors. Journal of Chemical Physics, 1993, 99, 2865-2890.	1.2	471
3	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	2.9	411
4	Accurate exchange-correlation potentials and total-energy components for the helium isoelectronic series. Physical Review A, 1994, 50, 3827-3837.	1.0	344
5	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.	2.3	294
6	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 1595-1604.	2.3	232
7	Optimization of quantum Monte Carlo wave functions by energy minimization. Journal of Chemical Physics, 2007, 126, 084102.	1.2	226
8	Natural Orbital Functional for the Many-Electron Problem. Physical Review Letters, 1998, 81, 866-869.	2.9	224
9	Multiconfiguration wave functions for quantum Monte Carlo calculations of firstâ€row diatomic molecules. Journal of Chemical Physics, 1996, 105, 213-226.	1.2	213
10	All-electron study of gradient corrections to the local-density functional in metallic systems. Physical Review B, 1995, 51, 4105-4109.	1.1	202
11	All-electron local-density and generalized-gradient calculations of the structural properties of semiconductors. Physical Review B, 1994, 50, 14947-14951.	1.1	172
12	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.	1.2	167
13	Comparison of exact and approximate density functionals for an exactly soluble model. Journal of Chemical Physics, 1994, 100, 1290-1296.	1.2	163
14	Critical assessment of the self-interaction-correctedâ€“local-density-functional method and its algorithmic implementation. Physical Review A, 1997, 55, 1765-1771.	1.0	155
15	Energy and Variance Optimization of Many-Body Wave Functions. Physical Review Letters, 2005, 94, 150201.	2.9	155
16	Semistochastic Projector MonteÂCarlo Method. Physical Review Letters, 2012, 109, 230201.	2.9	151
17	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, .	1.1	131
18	Excited states using semistochastic heat-bath configuration interaction. Journal of Chemical Physics, 2017, 147, 164111.	1.2	108

#	Article	IF	Citations
19	Diffusion Monte Carlo study of circular quantum dots. Physical Review B, 2000, 62, 8120-8125.	1.1	101
20	Fast semistochastic heat-bath configuration interaction. Journal of Chemical Physics, 2018, 149, 214110.	1.2	99
21	Optimizing large parameter sets in variational quantum Monte Carlo. Physical Review B, 2012, 85, .	1.1	91
22	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	2.1	90
23	Correlated sampling in quantum Monte Carlo: A route to forces. Physical Review B, 2000, 61, R16291-R16294.	1.1	89
24	Excitation energies from density functional perturbation theory. Journal of Chemical Physics, 1997, 107, 9994-10002.	1.2	84
25	Excited States of Methylene, Polyenes, and Ozone from Heat-Bath Configuration Interaction. Journal of Physical Chemistry A, 2018, 122, 2714-2722.	1.1	80
26	Spectroscopic accuracy directly from quantum chemistry: Application to ground and excited states of beryllium dimer. Journal of Chemical Physics, 2014, 140, 104112.	1.2	75
27	Accelerated Metropolis method. Physical Review Letters, 1993, 71, 408-411.	2.9	73
28	Correlation-induced inhomogeneity in circular quantum dots. Nature Physics, 2006, 2, 336-340.	6.5	72
29	Excited states of methylene from quantum Monte Carlo. Journal of Chemical Physics, 2009, 131, 124103.	1.2	70
30	Approaching chemical accuracy with quantum Monte Carlo. Journal of Chemical Physics, 2012, 136, 124116.	1.2	70
31	Efficient Heat-Bath Sampling in Fock Space. Journal of Chemical Theory and Computation, 2016, 12, 1561-1571.	2.3	66
32	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, .	1.1	65
33	Local correlation energies of two-electron atoms and model systems. Physical Review A, 1997, 56, 290-296.	1.0	64
34	Questioning the existence of a unique ground-state structure for Si clusters. Physical Review B, 2007, 75, .	1.1	62
35	Accuracy of electronic wave functions in quantum Monte Carlo: The effect of high-order correlations. Journal of Chemical Physics, 1997, 107, 3007-3013.	1.2	59
36	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.	1.2	59

#	Article	IF	Citations
37	Separation of the exchange-correlation potential into exchange plus correlation: An optimized effective potential approach. Physical Review A, 1996, 54, 4810-4814.	1.0	54
38	Incipient Wigner localization in circular quantum dots. Physical Review B, 2007, 76, .	1.1	50
39	Spin contamination in quantum Monte Carlo wave functions. Journal of Chemical Physics, 1998, 108, 8838-8847.	1.2	44
40	Quantum Monte Carlo with Jastrow-valence-bond wave functions. Journal of Chemical Physics, 2011, 134, 084108.	1.2	43
41	Almost exact energies for the Gaussian-2 set with the semistochastic heat-bath configuration interaction method. Journal of Chemical Physics, 2020, 153, 124117.	1.2	41
42	Electron intracule densities with correct electron coalescence cusps from Hillerâ€“Sucherâ€“Feinbergâ€¢type identities. Journal of Chemical Physics, 1995, 103, 6093-6103.	1.2	39
43	Quantum Monte Carlo study of composite fermions in quantum dots: The effect of Landau-level mixing. Physical Review B, 2005, 72, .	1.1	37
44	Localization in an inhomogeneous quantum wire. Physical Review B, 2009, 80, .	1.1	35
45	Evidence of physical reality in the Kohn-Sham potential: The case of atomic Ne. Physical Review A, 1998, 57, 2466-2469.	1.0	33
46	Zero-variance zero-bias quantum Monte Carlo estimators of the spherically and system-averaged pair density. Journal of Chemical Physics, 2007, 126, 244112.	1.2	32
47	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, .	1.1	31
48	Accurate many-body electronic structure near the basis set limit: Application to the chromium dimer. Physical Review Research, 2020, 2, .	1.3	31
49	Natural Orbital Functional Theory. Mathematical and Computational Chemistry, 2000, , 165-181.	0.3	30
50	Zigzag Phase Transition in Quantum Wires. Physical Review Letters, 2013, 110, 246802.	2.9	29
51	Interaction-induced strong localization in quantum dots. Physical Review B, 2008, 77, .	1.1	27
52	Observations on variational and projector Monte Carlo methods. Journal of Chemical Physics, 2015, 143, 164105.	1.2	23
53	Orbital Optimization in Selected Configuration Interaction Methods. Journal of Chemical Theory and Computation, 2021, 17, 4183-4194.	2.3	23
54	Maximum-density droplet to lower-density droplet transition in quantum dots. Physical Review B, 2005, 72, .	1.1	21

#	Article	IF	Citations
55	Energy density functionals from the strong-coupling limit applied to the anions of the He isoelectronic series. Journal of Chemical Physics, 2014, 140, 18A532.	1.2	19
56	Variational Monte Carlo Basics and Applications to Atoms and Molecules. , 1999, , 129-160.		19
57	Energies, densities, and pair correlation functions of jellium spheres by the variational Monte Carlo method. Physical Review B, 1992, 45, 6293-6296.	1.1	18
58	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.	1.0	18
59	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.	2.3	18
60	Basis set construction for molecular electronic structure theory: Natural orbital and Gaussâ€“Slater basis for smooth pseudopotentials. Journal of Chemical Physics, 2011, 134, 064104.	1.2	15
61	Influence of the exchange-correlation potential in methods based on time-dependent density-functional theory. Physical Review A, 2013, 88, .	1.0	15
62	Fixed-node diffusion Monte Carlo study of the structures of m-benzyne. Journal of Chemical Physics, 2008, 128, 154324.	1.2	13
63	Composite-fermion antiparticle description of the hole excitation in a maximum-density droplet with a small number of electrons. Physical Review B, 2005, 72, .	1.1	9
64	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.	1.2	9
65	Compact and flexible basis functions for quantum Monte Carlo calculations. Journal of Chemical Physics, 2010, 132, 094109.	1.2	8
66	Interaction effects in the mesoscopic regime: A quantum Monte Carlo study of irregular quantum dots. Physical Review B, 2005, 71, .	1.1	7
67	Nonlocal pseudopotentials and time-step errors in diffusion Monte Carlo. Journal of Chemical Physics, 2021, 154, 214110.	1.2	6
68	Monte Carlo Eigenvalue Methods in Quantum Mechanics and Statistical Mechanics. Advances in Chemical Physics, 0, , 65-115.	0.3	5
69	Are Unoccupied Kohn-Sham Eigenvalues Related to Excitation Energies?. , 1998, , 167-176.		5
70	Quantum Monte Carlo Calculations of Electronic Excitation Energies: The Case of the Singlet nâ†'Ï€âˆ— (CO) Transition in Acrolein. Progress in Theoretical Chemistry and Physics, 2012, , 343-351.	0.2	5