C J Umrigar

List of Publications by Citations

70 papers	5,714 citations	38 h-index	71 g-index
71 ext. papers	6,137 ext. citations	4.2 avg, IF	5.89 L-index

#	Paper	IF	Citations
70	Optimized trial wave functions for quantum Monte Carlo calculations. *Physical Review Letters*, **1988**, 60, 1719-1722	7.4	534
69	A diffusion Monte Carlo algorithm with very small time-step errors. *Journal of Chemical Physics*, **1993**, 99, 2865-2890	3.9	421
68	Alleviation of the Fermion-sign problem by optimization of many-body wave functions. *Physical Review Letters*, **2007**, 98, 110201	7.4	355
67	Accurate exchange-correlation potentials and total-energy components for the helium isoelectronic series. *Physical Review A*, **1994**, 50, 3827-3837	2.6	330
66	Heat-Bath Configuration Interaction: An Efficient Selected Configuration Interaction Algorithm Inspired by Heat-Bath Sampling. *Journal of Chemical Theory and Computation*, **2016**, 12, 3674-80	6.4	215
65	Natural Orbital Functional for the Many-Electron Problem. *Physical Review Letters*, **1998**, 81, 866-869	7.4	203
64	Optimization of quantum Monte Carlo wave functions by energy minimization. *Journal of Chemical Physics*, **2007**, 126, 084102	3.9	200
63	All-electron study of gradient corrections to the local-density functional in metallic systems. *Physical Review B*, **1995**, 51, 4105-4109	3.3	193
62	Multiconfiguration wave functions for quantum Monte Carlo calculations of first-row diatomic molecules. *Journal of Chemical Physics*, **1996**, 105, 213-226	3.9	193
61	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 1595-1604	6.4	178
60	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	3.9	160
59	Comparison of exact and approximate density functionals for an exactly soluble model. *Journal of Chemical Physics*, **1994**, 100, 1290-1296	3.9	152
58	Critical assessment of the self-interaction-corrected-local-density-functional method and its algorithmic implementation. *Physical Review A*, **1997**, 55, 1765-1771	2.6	146
57	All-electron local-density and generalized-gradient calculations of the structural properties of semiconductors. *Physical Review B*, **1994**, 50, 14947-14951	3.3	146
56	Energy and variance optimization of many-body wave functions. *Physical Review Letters*, **2005**, 94, 150201	7.4	134
55	Semistochastic projector Monte Carlo method. *Physical Review Letters*, **2012**, 109, 230201	7.4	130
54	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,	3.3	119

53	Diffusion Monte Carlo study of circular quantum dots. *Physical Review B*, **2000**, 62, 8120-8125	3.3	93
52	Excited states using semistochastic heat-bath configuration interaction. *Journal of Chemical Physics*, **2017**, 147, 164111	3.9	82
51	Excitation energies from density functional perturbation theory. *Journal of Chemical Physics*, **1997**, 107, 9994-10002	3.9	81
50	Correlated sampling in quantum Monte Carlo: A route to forces. *Physical Review B*, **2000**, 61, R16291-R16294	3.3	77
49	Optimizing large parameter sets in variational quantum Monte Carlo. *Physical Review B*, **2012**, 85,	3.3	73
48	Fast semistochastic heat-bath configuration interaction. *Journal of Chemical Physics*, **2018**, 149, 214110	3.9	71
47	Accelerated Metropolis method. *Physical Review Letters*, **1993**, 71, 408-411	7.4	68
46	Spectroscopic accuracy directly from quantum chemistry: application to ground and excited states of beryllium dimer. *Journal of Chemical Physics*, **2014**, 140, 104112	3.9	65
45	Approaching chemical accuracy with quantum Monte Carlo. *Journal of Chemical Physics*, **2012**, 136, 124116	3.9	64
44	Excited States of Methylene, Polyenes, and Ozone from Heat-Bath Configuration Interaction. *Journal of Physical Chemistry A*, **2018**, 122, 2714-2722	2.8	63
43	Excited states of methylene from quantum Monte Carlo. *Journal of Chemical Physics*, **2009**, 131, 124103	3.9	63
42	Questioning the existence of a unique ground-state structure for Si clusters. *Physical Review B*, **2007**, 75,	3.3	62
41	Correlation-induced inhomogeneity in circular quantum dots. *Nature Physics*, **2006**, 2, 336-340	16.2	62
40	Local correlation energies of two-electron atoms and model systems. *Physical Review A*, **1997**, 56, 290-296	2.6	59
39	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,	3.3	58
38	Accuracy of electronic wave functions in quantum Monte Carlo: The effect of high-order correlations. *Journal of Chemical Physics*, **1997**, 107, 3007-3013	3.9	56
37	Efficient Heat-Bath Sampling in Fock Space. *Journal of Chemical Theory and Computation*, **2016**, 12, 1561-71	6.4	56
36	Separation of the exchange-correlation potential into exchange plus correlation: An optimized effective potential approach. *Physical Review A*, **1996**, 54, 4810-4814	2.6	54

35	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
34	Incipient Wigner localization in circular quantum dots. *Physical Review B*, **2007**, 76,	3.3	44
33	Quantum Monte Carlo with Jastrow-valence-bond wave functions. *Journal of Chemical Physics*, **2011**, 134, 084108	3.9	38
32	Electron intracule densities with correct electron coalescence cusps from HillerSucherFeinberg-type identities. *Journal of Chemical Physics*, **1995**, 103, 6093-6103	3.9	36
31	Localization in an inhomogeneous quantum wire. *Physical Review B*, **2009**, 80,	3.3	32
30	Evidence of physical reality in the Kohn-Sham potential: The case of atomic Ne. *Physical Review A*, **1998**, 57, 2466-2469	2.6	32
29	Spin contamination in quantum Monte Carlo wave functions. *Journal of Chemical Physics*, **1998**, 108, 8838-8847	3.9	31
28	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	3.9	31
27	Zero-variance zero-bias quantum Monte Carlo estimators of the spherically and system-averaged pair density. *Journal of Chemical Physics*, **2007**, 126, 244112	3.9	30
26	Natural Orbital Functional Theory. *Mathematical and Computational Chemistry*, **2000**, 165-181		29
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,	3.3	27
24	Quantum Monte Carlo study of composite fermions in quantum dots: The effect of Landau-level mixing. *Physical Review B*, **2005**, 72,	3.3	27
23	Interaction-induced strong localization in quantum dots. *Physical Review B*, **2008**, 77,	3.3	26
22	Zigzag phase transition in quantum wires. *Physical Review Letters*, **2013**, 110, 246802	7.4	22
21	Accurate many-body electronic structure near the basis set limit: Application to the chromium dimer. *Physical Review Research*, **2020**, 2,	3.9	21
20	Observations on variational and projector Monte Carlo methods. *Journal of Chemical Physics*, **2015**, 143, 164105	3.9	19
19	Variational Monte Carlo Basics and Applications to Atoms and Molecules **1999**, 129-160		19
18	Almost exact energies for the Gaussian-2 set with the semistochastic heat-bath configuration interaction method. *Journal of Chemical Physics*, **2020**, 153, 124117	3.9	18

17	Energies, densities, and pair correlation functions of jellium spheres by the variational Monte Carlo method. *Physical Review B*, **1992**, 45, 6293-6296	3.3	18
16	Maximum-density droplet to lower-density droplet transition in quantum dots. *Physical Review B*, **2005**, 72,	3.3	17
15	Influence of the exchange-correlation potential in methods based on time-dependent density-functional theory. *Physical Review A*, **2013**, 88,	2.6	15
14	Energy density functionals from the strong-coupling limit applied to the anions of the He isoelectronic series. *Journal of Chemical Physics*, **2014**, 140, 18A532	3.9	15
13	Basis set construction for molecular electronic structure theory: natural orbital and Gauss-Slater basis for smooth pseudopotentials. *Journal of Chemical Physics*, **2011**, 134, 064104	3.9	15
12	Two aspects of quantum monte carlo: Determination of accurate wavefunctions and determination of potential energy surfaces of molecules. *International Journal of Quantum Chemistry*, **2009**, 36, 217-230	2.1	13
11	Fixed-node diffusion Monte Carlo study of the structures of m-benzyne. *Journal of Chemical Physics* , **2008**, 128, 154324	3.9	13
10	Orbital Optimization in Selected Configuration Interaction Methods. *Journal of Chemical Theory and Computation*, **2021**, 17, 4183-4194	6.4	10
9	Compact and flexible basis functions for quantum Monte Carlo calculations. *Journal of Chemical Physics*, **2010**, 132, 094109	3.9	8
8	Composite-fermion antiparticle description of the hole excitation in a maximum-density droplet with a small number of electrons. *Physical Review B*, **2005**, 72,	3.3	8
7	Interaction effects in the mesoscopic regime: A quantum Monte Carlo study of irregular quantum dots. *Physical Review B*, **2005**, 71,	3.3	7
6	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	6.4	7
5	Are Unoccupied Kohn-Sham Eigenvalues Related to Excitation Energies? **1998**, 167-176		5
4	Quantum Monte Carlo Calculations of Electronic Excitation Energies: The Case of the Singlet n-π (CO) Transition in Acrolein. *Progress in Theoretical Chemistry and Physics*, **2012**, 343-351	0.6	4
3	Monte Carlo Eigenvalue Methods in Quantum Mechanics and Statistical Mechanics. *Advances in Chemical Physics*,65-115		4
2	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	3.9	3
1	Nonlocal pseudopotentials and time-step errors in diffusion Monte Carlo. *Journal of Chemical Physics*, **2021**, 154, 214110	3.9	2