Michel Caffarel

List of Publications by Year
in descending order

81 papers	3,554 citations	136950 32 h-index	133252 59 g-index
81 all docs	81 docs citations	81 times ranked	2193 citing authors

#	Article	IF	Citations
1	Exact diagonalization approach to correlated fermions in infinite dimensions: Mott transition and superconductivity. Physical Review Letters, 1994, 72, 1545-1548.	7.8	549
2	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. Journal of Chemical Theory and Computation, 2018, 14, 4360-4379.	5.3	211
3	Gutzwiller wave function for a model of strongly interacting bosons. Physical Review B, 1992, 45, 3137-3140.	3.2	192
4	Reference Energies for Double Excitations. Journal of Chemical Theory and Computation, 2019, 15, 1939-1956.	5.3	116
5	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. Journal of Chemical Theory and Computation, 2019, 15, 3591-3609.	5.3	108
6	Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory. Journal of Chemical Physics, 2017, 147, 034101.	3.0	106
7	Using perturbatively selected configuration interaction in quantum Monte Carlo calculations. Canadian Journal of Chemistry, 2013, 91, 879-885.	1.1	105
8	Zero-variance zero-bias principle for observables in quantum Monte Carlo: Application to forces. Journal of Chemical Physics, 2003, 119, 10536-10552.	3.0	102
9	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
10	Zero-Variance Principle for Monte Carlo Algorithms. Physical Review Letters, 1999, 83, 4682-4685.	7.8	98
11	Selected configuration interaction dressed by perturbation. Journal of Chemical Physics, 2018, 149, 064103.	3.0	92
12	Development of a pure diffusion quantum Monte Carlo method using a full generalized Feynmanâ€“Kac formula. I. Formalism. Journal of Chemical Physics, 1988, 88, 1088-1099.	3.0	90
13	<scp>QUESTDB</scp>: A database of highly accurate excitation energies for the electronic structure community. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1517.	14.6	84
14	Computing forces with quantum Monte Carlo. Journal of Chemical Physics, 2000, 113, 4028-4034.	3.0	77
15	Metal-insulator transition in the one-dimensionalSU(N)Hubbard model. Physical Review B, 1999, 60, 2299-2318.	3.2	76
16	Diffusion Monte Carlo methods with a fixed number of walkers. Physical Review E, 2000, 61, 4566-4575.	2.1	75
17	Fixed-node diffusion Monte Carlo potential energy curve of the fluorine molecule F2 using selected configuration interaction trial wavefunctions. Journal of Chemical Physics, 2015, 142, 044115.	3.0	70
18	Development of a pure diffusion quantum Monte Carlo method using a full generalized Feynmanâ€“Kac formula. II. Applications to simple systems. Journal of Chemical Physics, 1988, 88, 1100-1109.	3.0	52

#	Article	IF	Citations
19	Maximum probability domains from Quantum Monte Carlo calculations. Journal of Computational Chemistry, 2007, 28, 442-454.	3.3	52
20	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. Journal of Chemical Physics, 2018, 149, 034108.	3.0	50
21	Electron pair localization function: A practical tool to visualize electron localization in molecules from quantum Monte Carlo data. Journal of Chemical Physics, 2004, 121, 1725-1735.	3.0	48
22	Communication: Toward an improved control of the fixed-node error in quantum Monte Carlo: The case of the water molecule. Journal of Chemical Physics, 2016, 144, 151103.	3.0	48
23	Deterministic Construction of Nodal Surfaces within Quantum Monte Carlo: The Case of FeS. Journal of Chemical Theory and Computation, 2018, 14, 1395-1402.	5.3	48
24	A Bayesian analysis of Greenâ€™s function Monte Carlo correlation functions. Journal of Chemical Physics, 1992, 97, 8415-8423.	3.0	43
25	Quantum Monte Carlo with Jastrow-valence-bond wave functions. Journal of Chemical Physics, 2011, 134, 084108.	3.0	43
26	Spin Density Distribution in Open-Shell Transition Metal Systems: A Comparative Post-Hartreeâ€“Fock, Density Functional Theory, and Quantum Monte Carlo Study of the CuCl₂ Molecule. Journal of Chemical Theory and Computation, 2014, 10, 5286-5296.	5.3	39
27	Evaluating dynamic multipole polarizabilities and van der Waals dispersion coefficients of two-electron systems with a quantum Monte Carlo calculation: A comparison with someab initiocalculations. Physical Review A, 1993, 47, 3704-3717.	2.5	37
28	Accurate nonrelativistic ground-state energies of 3d transition metal atoms. Journal of Chemical Physics, 2014, 141, 244110.	3.0	37
29	Secondâ€order exchange effects in intermolecular interactions. The water dimer. Journal of Chemical Physics, 1990, 92, 6049-6060.	3.0	35
30	Dynamical Symmetry Enlargement versus Spin-Charge Decoupling in the One-Dimensional SU(4) Hubbard Model. Physical Review Letters, 2004, 93, .	7.8	34
31	A perturbational study of some hydrogenâ€bonded dimers. Journal of Chemical Physics, 1995, 103, 8043-8057.	3.0	33
32	Towards accurate all-electron quantum Monte Carlo calculations of transition-metal systems: Spectroscopy of the copper atom. Journal of Chemical Physics, 2005, 123, 094102.	3.0	32
33	Quantum Monte Carlo with very large multideterminant wavefunctions. Journal of Computational Chemistry, 2016, 37, 1866-1875.	3.3	30
34	Using CIPSI Nodes in Diffusion Monte Carlo. ACS Symposium Series, 2016, , 15-46.	0.5	30
35	Excited States from State-Specific Orbital-Optimized Pair Coupled Cluster. Journal of Chemical Theory and Computation, 2021, 17, 4756-4768.	5.3	29
36	Quantum Monte Carlo for large chemical systems: Implementing efficient strategies for petascale platforms and beyond. Journal of Computational Chemistry, 2013, 34, 938-951.	3.3	28

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37	A Quantum Monte Carlo Study of the Reactions of CH with Acrolein. Journal of Physical Chemistry A, 2015, 119, 4214-4223.	2.5	28
38	Improved Monte Carlo estimators for the one-body density. Physical Review E, 2007, 75, 035701.	2.1	27
39	Quantum Monte Carlo method for some model and realistic coupled anharmonic oscillators. Journal of Chemical Physics, 1989, 90, 990-1002.	3.0	26
40	Spin stiffness and topological defects in two-dimensional frustrated spin systems. Physical Review B, 2001, 64, .	3.2	26
41	An efficient sampling algorithm for variational Monte Carlo. Journal of Chemical Physics, 2006, 125, 114105.	3.0	26
42	Multireference Quantum Monte Carlo Study of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>Molecule. Physical Review Letters, 2007, 99, 153001.	7.8	26
43	LanczÃ³s-Type Algorithm for Quantum Monte Carlo Data. Europhysics Letters, 1991, 16, 249-254.	2.0	23
44	Dynamic polarizabilities and van der Waals coefficients of the 21Sand 23Smetastable states of helium. Physical Review A, 1993, 48, 161-165.	2.5	23
45	A study of the fixed-node error in quantum Monte Carlo calculations of electronic transitions: The case of the singlet nâ†'Ï€âˆ— (CO) transition of the acrolein. Journal of Chemical Physics, 2009, 130, 114107.	3.0	20
46	Multi-Jastrow trial wavefunctions for electronic structure calculations with quantum Monte Carlo. Journal of Chemical Physics, 2010, 133, 044111.	3.0	18
47	Influence of pseudopotentials on excitation energies from selected configuration interaction and diffusion Monte Carlo. Results in Chemistry, 2019, 1, 100002.	2.0	18
48	Electron Pair Localization Function (EPLF) for Density Functional Theory andab InitioWave Function-Based Methods: A New Tool for Chemical Interpretation. Journal of Chemical Theory and Computation, 2011, 7, 618-624.	5.3	17
49	One-dimensional pair hopping and attractive Hubbard models: A comparative study. Physical Review B, 1996, 54, 17414-17421.	3.2	16
50	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solidsâ€"A case study in diamond. Journal of Chemical Physics, 2020, 153, 184111.	3.0	16
51	Treatment of the SchrÃ¶dinger equation through a Monte Carlo method based upon the generalized Feynman-Kac formula. Journal of Statistical Physics, 1986, 43, 797-801.	1.2	15
52	Quantum Monte Carlo perturbation calculations of interaction energies. Physical Review A, 1991, 43, 2139-2151.	2.5	15
53	The fermion Monte Carlo revisited. Journal of Physics A: Mathematical and Theoretical, 2007, 40, 1181-1214.	2.1	15
54	Structural and optical properties of a neutral Nickel bisdithiolene complex: density functional versus ab initio methods. Theoretical Chemistry Accounts, 2010, 126, 243-255.	1.4	15

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55	Spinâ€driven activation of dioxygen in various metalloenzymes and their inspired models. Journal of Computational Chemistry, 2011, 32, 1178-1182.	3.3	14
56	Accurate full configuration interaction correlation energy estimates for five- and six-membered rings. Journal of Chemical Physics, 2021, 155, 134104.	3.0	14
57	A quantum Monte Carlo perturbational study of the Heâ€“He interaction. Journal of Chemical Physics, 1996, 104, 4621-4631.	3.0	13
58	Quantum Monte Carlo Calculations with Multi-Reference Trial Wave Functions. Recent Advances in Computational, 1997, , 73-98.	0.8	13
59	Systematic comparison and cross-validation of fixed-node diffusion Monte Carlo and phaseless auxiliary-field quantum Monte Carlo in solids. Physical Review B, 2020, 102, .	3.2	13
60	Chaotic versus Nonchaotic Stochastic Dynamics in MonteÂCarlo Simulations: A Route for Accurate Energy Differences in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>-Body Systems. Physical Review Letters, 2011, 106, 150601.	7.8	12
61	Comment on â€˜â€˜Feynman-Kac path-integral calculation of the ground-state energies of atomsâ€™â€™. Physical Review Letters, 1993, 71, 2159-2159.	7.8	10
62	Bond Breaking and Bond Making in Tetraoxygen: Analysis of the O₂(X³Î£_g^{â^’}) + O₂(X³Î£_g^{â^’}) â‡† O₄Reaction Using the Electron Pair Localization Function. Journal of Physical Chemistry A, 2009, 113, 9014-9021.	2.5	10
63	The lithiumâ€“thiophene interaction: a critical study using highly correlated electronic structure approaches of quantum chemistry. Theoretical Chemistry Accounts, 2010, 126, 275-287.	1.4	10
64	Evaluating two-electron-repulsion integrals over arbitrary orbitals using zero variance Monte Carlo: Application to full configuration interaction calculations with Slater-type orbitals. Journal of Chemical Physics, 2019, 151, .	3.0	10
65	Monte Carlo Calculation of the Spin Stiffness of the Two-Dimensional Heisenberg Model. Europhysics Letters, 1994, 26, 493-498.	2.0	9
66	Hubbard model ondâ^’dimensional hypercubes: Exact solution for the two-electron case. Physical Review B, 1998, 57, R12651-R12654.	3.2	9
67	QMC=Chem: A Quantum Monte Carlo Program for Large-Scale Simulations in Chemistry at the Petascale Level and beyond. Lecture Notes in Computer Science, 2013, , 118-127.	1.3	8
68	A pedagogical introduction to Quantum Monte-Carlo. Lecture Notes in Quantum Chemistry II, 2000, , 45-73.	0.3	7
69	On the stability of Be3: A benchmark complete active space self-consistent field + averaged quadratic coupled cluster study. Journal of Chemical Physics, 2011, 135, 104311.	3.0	6
70	Large-Scale Quantum Monte Carlo Electronic Structure Calculations on the EGEE Grid. , 2012, , 195-207.		5
71	Quantum Monte Carlo Calculations of Electronic Excitation Energies: The Case of the Singlet nâ†’Ï€â^— (CO) Transition in Acrolein. Progress in Theoretical Chemistry and Physics, 2012, , 343-351.	0.2	5
72	Stochastic Methods in Quantum Mechanics. , 1989, , 85-105.		5

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73	On the Nonconservation of the Number of Nodal Cells of Eigenfunctions. Europhysics Letters, 1992, 20, 581-588.	2.0	4
74	Block-diagonalization of pairing Hamiltonians using spin transpositions. Journal of Physics A, 2004, 37, 623-636.	1.6	4
75	FIXED-NODE QUANTUM MONTE CARLO FOR CHEMISTRY. , 2008, , .		2
76	A quantum Monte Carlo study of systems with effective core potentials and node nonlinearities. Chemical Physics, 2022, 554, 111402.	1.9	2
77	Computing Response Properties with Quantum Monte Carlo. AIP Conference Proceedings, 1991, , .	0.4	1
78	Hubbard model on hypercubes. Physica B: Condensed Matter, 1999, 259-261, 787-789.	2.7	0
79	Self-consistent electronâ€“nucleus cusp correction for molecular orbitals. Advances in Quantum Chemistry, 2019, 79, 113-132.	0.8	0
80	Talking Across Fields: A Physicistâ€™s Presentation of some Mathematical Aspects of Quantum Monte Carlo Methods. Annales De La FacultÃ© Des Sciences De Toulouse, 2015, 24, 949-972.	0.3	0
81	Quantum Monte Carlo Methods in Chemistry. , 2015, , 1191-1197.		0