W Matthew C Foulkes

List of Publications by Year
in descending order

74 papers	6,497 citations	109321 35 h-index	85541 71 g-index
74 all docs	74 docs citations	74 times ranked	4387 citing authors

#	Article	IF	Citations
1	Quantum Monte Carlo simulations of solids. Reviews of Modern Physics, 2001, 73, 33-83.	45.6	1,813
2	Tight-binding models and density-functional theory. Physical Review B, 1989, 39, 12520-12536.	3.2	591
3	Electronic states inLa2â^'xSrxCuO4+Î´probed by soft-x-ray absorption. Physical Review Letters, 1991, 66, 104-107.	7.8	463
4	Finite-size effects and Coulomb interactions in quantum Monte Carlo calculations for homogeneous systems with periodic boundary conditions. Physical Review B, 1996, 53, 1814-1832.	3.2	265
5	Ab initio solution of the many-electron SchrÃ¶dinger equation with deep neural networks. Physical Review Research, 2020, 2, .	3.6	227
6	Supercell size scaling of density functional theory formation energies of charged defects. Physical Review B, 2009, 79, .	3.2	180
7	Finite-size errors in continuum quantum Monte Carlo calculations. Physical Review B, 2008, 78, .	3.2	173
8	On the growth of Al2O3 scales. Acta Materialia, 2013, 61, 6670-6683.	7.9	140
9	AbÂinitio Exchange-Correlation Free Energy of the Uniform Electron Gas at Warm Dense Matter Conditions. Physical Review Letters, 2017, 119, 135001.	7.8	139
10	AbÂInitioQuantum Monte Carlo Simulation of the Warm Dense Electron Gas in the Thermodynamic Limit. Physical Review Letters, 2016, 117, 156403.	7.8	136
11	Model for low-energy electronic states probed by x-ray absorption in high-Tccuprates. Physical Review B, 1992, 45, 10032-10050.	3.2	121
12	The treatment of electronic excitations in atomistic models of radiation damage in metals. Reports on Progress in Physics, 2010, 73, 116501.	20.1	109
13	Dissociation of High-Pressure Solid Molecular Hydrogen: A Quantum MonteÂCarlo and Anharmonic Vibrational Study. Physical Review Letters, 2014, 112, 165501.	7.8	102
14	Pseudopotentials with position-dependent electron masses. Physical Review B, 1990, 42, 11505-11529.	3.2	101
15	Elimination of Coulomb finite-size effects in quantum many-body simulations. Physical Review B, 1997, 55, R4851-R4854.	3.2	99
16	Finite-size errors in quantum many-body simulations of extended systems. Physical Review B, 1999, 59, 1917-1929.	3.2	98
17	The sign problem and population dynamics in the full configuration interaction quantum Monte Carlo method. Journal of Chemical Physics, 2012, 136, 054110.	3.0	88
18	Accurate Exchange-Correlation Energies for the Warm Dense Electron Gas. Physical Review Letters, 2016, 117, 115701.	7.8	88

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19	Accurate and efficient method for the treatment of exchange in a plane-wave basis. Journal of Chemical Physics, 2006, 124, 064105.	3.0	87
20	Density-matrix quantum Monte Carlo method. Physical Review B, 2014, 89, .	3.2	84
21	Variational and diffusion quantum Monte Carlo calculations at nonzero wave vectors: Theory and application to diamond-structure germanium. Physical Review B, 1995, 51, 10591-10600.	3.2	79
22	Quantum Monte Carlo Calculations for Solids Using SpecialkPoints Methods. Physical Review Letters, 1994, 73, 1959-1962.	7.8	72
23	Symmetry constraints and variational principles in diffusion quantum Monte Carlo calculations of excited-state energies. Physical Review B, 1999, 60, 4558-4570.	3.2	71
24	Interaction picture density matrix quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 044116.	3.0	69
25	Electron Elevator: Excitations across the Band Gap via a Dynamical Gap State. Physical Review Letters, 2016, 116, 043201.	7.8	68
26	Quantum Monte Carlo Investigation of Exchange and Correlation in Silicon. Physical Review Letters, 1997, 78, 3350-3353.	7.8	65
27	Fate of density functional theory in the study of high-pressure solid hydrogen. Physical Review B, 2013, 88, .	3.2	62
28	Ab initio quantum Monte Carlo simulation of the warm dense electron gas. Physics of Plasmas, 2017, 24, .	1.9	59
29	Optimized wave functions for quantum Monte Carlo studies of atoms and solids. Physical Review B, 1996, 53, 9640-9648.	3.2	57
30	Ab initiocalculations of the cohesive energy and the bulk modulus of aluminium. Journal of Physics Condensed Matter, 2002, 14, 8787-8793.	1.8	53
31	The Band Structure of Polycrystalline Al₂O₃ and Its Influence on Transport Phenomena. Journal of the American Ceramic Society, 2016, 99, 733-747.	3.8	51
32	Electronic damping of atomic dynamics in irradiation damage of metals. Journal of Physics Condensed Matter, 2007, 19, 436209.	1.8	50
33	Quantum Monte Carlo study of high pressure solid molecular hydrogen. New Journal of Physics, 2013, 15, 113005.	2.9	45
34	Quantum Monte Carlo Analysis of Exchange and Correlation in the Strongly Inhomogeneous Electron Gas. Physical Review Letters, 2001, 87, 036401.	7.8	38
35	How good is damped molecular dynamics as a method to simulate radiation damage in metals?. New Journal of Physics, 2009, 11, 013004.	2.9	37
36	Quantum Monte Carlo calculations of the surface energy of an electron gas. Physical Review B, 2007, 76, .	3.2	35

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37	Nature of the metallization transition in solid hydrogen. Physical Review B, 2017, 95, .	3.2	34
38	Modelling non-adiabatic processes using correlated electron-ion dynamics. European Physical Journal B, 2010, 77, 305-329.	1.5	33
39	The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. Journal of Chemical Theory and Computation, 2019, 15, 1728-1742.	5.3	33
40	Systematic study of finite-size effects in quantum Monte Carlo calculations of real metallic systems. Journal of Chemical Physics, 2015, 143, 102807.	3.0	26
41	Hubbard-like Hamiltonians for interacting electrons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>s</mml:mi><mml:mo>,</mml:mo><mml:mi>p</mml:mi></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>orbitals. Physical Review B, 2016, 93, .	3.2	26
42	The effect of quantization on the full configuration interaction quantum Monte Carlo sign problem. Journal of Chemical Physics, 2013, 138, 024110.	3.0	25
43	The Ehrenfest approximation for electrons coupled to a phonon system. Journal of Physics Condensed Matter, 2008, 20, 125212.	1.8	24
44	Structural and electronic properties of Î£7 grain boundaries in Î±-Al2O3. Acta Materialia, 2015, 99, 16-28.	7.9	24
45	Accuracy of the chemical-pseudopotential method for tetrahedral semiconductors. Physical Review B, 1993, 48, 14216-14225.	3.2	23
46	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. Journal of Open Research Software, 2015, 3, 9.	5.9	21
47	Quantum Monte Carlo investigations of density functional theory of the strongly inhomogeneous electron gas. Physical Review B, 2003, 68, .	3.2	20
48	Inhomogeneous random-phase approximation and many-electron trial wave functions. Physical Review B, 2001, 63, .	3.2	17
49	Quantum Monte Carlo Calculations of the Energy of the Relativistic Homogeneous Electron Gas. Physical Review Letters, 1996, 77, 1099-1102.	7.8	16
50	Efficient method for grand-canonical twist averaging in quantum Monte Carlo calculations. Physical Review B, 2019, 100, .	3.2	16
51	An accelerated Metropolis method. Journal of Chemical Physics, 1998, 109, 2630-2634.	3.0	15
52	Resonant charging and stopping power of slow channelling atoms in a crystalline metal. New Journal of Physics, 2012, 14, 073009.	2.9	15
53	Coulomb finite-size effects in quasi-two-dimensional systems. Journal of Physics Condensed Matter, 2004, 16, 891-902.	1.8	13
54	Quantumâ€“classical simulations of the electronic stopping force and charge on slow heavy channelling ions in metals. Journal of Physics Condensed Matter, 2013, 25, 125501.	1.8	13

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55	Quasiparticle Effective Mass of the Three-Dimensional Fermi Liquid by Quantum MonteÂCarlo. Physical Review Letters, 2021, 127, 086401.	7.8	12
56	Localization lengths over metal to band insulator transitions. Journal of Physics Condensed Matter, 2007, 19, 506212.	1.8	11
57	Adiabatic perturbation theory of electronic stopping in insulators. Physical Review B, 2016, 93, .	3.2	11
58	A Quantum Monte Carlo Approach to the Adiabatic Connection Method. Advances in Quantum Chemistry, 1998, 33, 189-207.	0.8	10
59	Comment on â€˜â€˜Feynman-Kac path-integral calculation of the ground-state energies of atomsâ€™â€™. Physical Review Letters, 1993, 71, 2158-2158.	7.8	6
60	A recursive solution of Heisenberg's equation and its interpretation. Journal of Physics Condensed Matter, 1994, 6, 6455-6475.	1.8	6
61	Neural Systems Under Change of Scale. Frontiers in Computational Neuroscience, 2021, 15, 643148.	2.1	6
62	Improved many-electron wavefunctions from plasmon normal modes. Journal of Physics Condensed Matter, 2006, 18, 2305-2326.	1.8	4
63	The microscopic Einstein-de Haas effect. Journal of Chemical Physics, 2019, 150, 224109.	3.0	4
64	Conservation laws by virtue of scale symmetries in neural systems. PLoS Computational Biology, 2020, 16, e1007865.	3.2	4
65	A simple model for large-scale simulations of fcc metals with explicit treatment of electrons. Philosophical Magazine Letters, 2010, 90, 51-60.	1.2	3
66	Free-energy coarse-grained potential for C60. Journal of Chemical Physics, 2015, 143, 164509.	3.0	3
67	Quantum Monte Carlo studies of density functional theory. Mathematics and Computers in Simulation, 2003, 62, 463-470.	4.4	2
68	Aiding the Design of Radiation Resistant Materials with Multiphysics Simulations of Damage Processes. Materials Research Society Symposia Proceedings, 2009, 1229, 30601.	0.1	2
69	Rendering neuronal state equations compatible with the principle of stationary action. Journal of Mathematical Neuroscience, 2021, 11, 10.	2.4	2
70	Perfect localized basis functions for solids: chemical pseudopotentials and the Kronig-Penney model. Journal of Physics Condensed Matter, 1993, 5, 7987-8004.	1.8	1
71	Diffusion of oxygen in Mg-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^’</mml:mtext><mml:msub mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> : The corundum conundrum explained. Physical Review Materials, 2022, 6, .	2.4	1
72	A two-phase Hessian approach improves the DFT relaxation of slabs. Journal of Physics Condensed Matter, 2018, 30, 315901.	1.8	0

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73	Comment on â€œSelf-diffusion in high-purity Î±-Al2O3: Comparison of Ti-doped, Mg-doped and undoped single crystalsâ€•P. Fielitz, S. Ganschow, K. Klemens, and G. Borchardt, J. Eur. Ceram. Soc., 41, (2021), 663â€“668â€. Journal of the European Ceramic Society, 2022, 42, 1829-1831.	5.7	0
74	Estimating anisotropy directly via neural timeseries. Journal of Computational Neuroscience, 2022, 50, 241-249.	1.0	0