W Matthew C Foulkes

List of Publications by Year
in descending order

74 papers	6,497 citations	109264 35 h-index	85498 71 g-index
74 all docs	74 docs citations	74 times ranked	4387 citing authors

#	Article	IF	Citations
1	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.	2.8	0
2	Estimating anisotropy directly via neural timeseries. Journal of Computational Neuroscience, 2022, 50, 241-249.	0.6	0
3	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, .	0.9	1
4	Neural Systems Under Change of Scale. Frontiers in Computational Neuroscience, 2021, 15, 643148.	1.2	6
5	Rendering neuronal state equations compatible with the principle of stationary action. Journal of Mathematical Neuroscience, 2021, 11, 10.	2.4	2
6	Quasiparticle Effective Mass of the Three-Dimensional Fermi Liquid by Quantum MonteÂCarlo. Physical Review Letters, 2021, 127, 086401.	2.9	12
7	Conservation laws by virtue of scale symmetries in neural systems. PLoS Computational Biology, 2020, 16, e1007865.	1.5	4
8	Ab initio solution of the many-electron SchrÃ¶dinger equation with deep neural networks. Physical Review Research, 2020, 2, .	1.3	227
9	The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. Journal of Chemical Theory and Computation, 2019, 15, 1728-1742.	2.3	33
10	The microscopic Einstein-de Haas effect. Journal of Chemical Physics, 2019, 150, 224109.	1.2	4
11	Efficient method for grand-canonical twist averaging in quantum Monte Carlo calculations. Physical Review B, 2019, 100, .	1.1	16
12	A two-phase Hessian approach improves the DFT relaxation of slabs. Journal of Physics Condensed Matter, 2018, 30, 315901.	0.7	0
13	Ab initio quantum Monte Carlo simulation of the warm dense electron gas. Physics of Plasmas, 2017, 24, .	0.7	59
14	AbÂinitio Exchange-Correlation Free Energy of the Uniform Electron Gas at Warm Dense Matter Conditions. Physical Review Letters, 2017, 119, 135001.	2.9	139
15	Nature of the metallization transition in solid hydrogen. Physical Review B, 2017, 95, .	1.1	34
16	Accurate Exchange-Correlation Energies for the Warm Dense Electron Gas. Physical Review Letters, 2016, 117, 115701.	2.9	88
17	AbÂInitioQuantum Monte Carlo Simulation of the Warm Dense Electron Gas in the Thermodynamic Limit. Physical Review Letters, 2016, 117, 156403.	2.9	136
18	Adiabatic perturbation theory of electronic stopping in insulators. Physical Review B, 2016, 93, .	1.1	11

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19	Electron Elevator: Excitations across the Band Gap via a Dynamical Gap State. Physical Review Letters, 2016, 116, 043201.	2.9	68
20	The Band Structure of Polycrystalline Al₂O₃ and Its Influence on Transport Phenomena. Journal of the American Ceramic Society, 2016, 99, 733-747.	1.9	51
21	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, .	1.1	26
22	Interaction picture density matrix quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 044116.	1.2	69
23	Free-energy coarse-grained potential for C60. Journal of Chemical Physics, 2015, 143, 164509.	1.2	3
24	Structural and electronic properties of Î£7 grain boundaries in Î±-Al2O3. Acta Materialia, 2015, 99, 16-28.	3.8	24
25	Systematic study of finite-size effects in quantum Monte Carlo calculations of real metallic systems. Journal of Chemical Physics, 2015, 143, 102807.	1.2	26
26	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. Journal of Open Research Software, 2015, 3, 9.	2.7	21
27	Density-matrix quantum Monte Carlo method. Physical Review B, 2014, 89, .	1.1	84
28	Dissociation of High-Pressure Solid Molecular Hydrogen: A Quantum MonteÂCarlo and Anharmonic Vibrational Study. Physical Review Letters, 2014, 112, 165501.	2.9	102
29	Fate of density functional theory in the study of high-pressure solid hydrogen. Physical Review B, 2013, 88, .	1.1	62
30	On the growth of Al2O3 scales. Acta Materialia, 2013, 61, 6670-6683.	3.8	140
31	The effect of quantization on the full configuration interaction quantum Monte Carlo sign problem. Journal of Chemical Physics, 2013, 138, 024110.	1.2	25
32	Quantum Monte Carlo study of high pressure solid molecular hydrogen. New Journal of Physics, 2013, 15, 113005.	1.2	45
33	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.	0.7	13
34	Resonant charging and stopping power of slow channelling atoms in a crystalline metal. New Journal of Physics, 2012, 14, 073009.	1.2	15
35	The sign problem and population dynamics in the full configuration interaction quantum Monte Carlo method. Journal of Chemical Physics, 2012, 136, 054110.	1.2	88
36	Modelling non-adiabatic processes using correlated electron-ion dynamics. European Physical Journal B, 2010, 77, 305-329.	0.6	33

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37	A simple model for large-scale simulations of fcc metals with explicit treatment of electrons. Philosophical Magazine Letters, 2010, 90, 51-60.	0.5	3
38	The treatment of electronic excitations in atomistic models of radiation damage in metals. Reports on Progress in Physics, 2010, 73, 116501.	8.1	109
39	Aiding the Design of Radiation Resistant Materials with Multiphysics Simulations of Damage Processes. Materials Research Society Symposia Proceedings, 2009, 1229, 30601.	0.1	2
40	How good is damped molecular dynamics as a method to simulate radiation damage in metals?. New Journal of Physics, 2009, 11, 013004.	1.2	37
41	Supercell size scaling of density functional theory formation energies of charged defects. Physical Review B, 2009, 79, .	1.1	180
42	The Ehrenfest approximation for electrons coupled to a phonon system. Journal of Physics Condensed Matter, 2008, 20, 125212.	0.7	24
43	Finite-size errors in continuum quantum Monte Carlo calculations. Physical Review B, 2008, 78, .	1.1	173
44	Localization lengths over metal to band insulator transitions. Journal of Physics Condensed Matter, 2007, 19, 506212.	0.7	11
45	Electronic damping of atomic dynamics in irradiation damage of metals. Journal of Physics Condensed Matter, 2007, 19, 436209.	0.7	50
46	Quantum Monte Carlo calculations of the surface energy of an electron gas. Physical Review B, 2007, 76, .	1.1	35
47	Improved many-electron wavefunctions from plasmon normal modes. Journal of Physics Condensed Matter, 2006, 18, 2305-2326.	0.7	4
48	Accurate and efficient method for the treatment of exchange in a plane-wave basis. Journal of Chemical Physics, 2006, 124, 064105.	1.2	87
49	Coulomb finite-size effects in quasi-two-dimensional systems. Journal of Physics Condensed Matter, 2004, 16, 891-902.	0.7	13
50	Quantum Monte Carlo studies of density functional theory. Mathematics and Computers in Simulation, 2003, 62, 463-470.	2.4	2
51	Quantum Monte Carlo investigations of density functional theory of the strongly inhomogeneous electron gas. Physical Review B, 2003, 68, .	1.1	20
52	Ab initiocalculations of the cohesive energy and the bulk modulus of aluminium. Journal of Physics Condensed Matter, 2002, 14, 8787-8793.	0.7	53
53	Quantum Monte Carlo simulations of solids. Reviews of Modern Physics, 2001, 73, 33-83.	16.4	1,813
54	Quantum Monte Carlo Analysis of Exchange and Correlation in the Strongly Inhomogeneous Electron Gas. Physical Review Letters, 2001, 87, 036401.	2.9	38

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55	Inhomogeneous random-phase approximation and many-electron trial wave functions. Physical Review B, 2001, 63, .	1.1	17
56	Finite-size errors in quantum many-body simulations of extended systems. Physical Review B, 1999, 59, 1917-1929.	1.1	98
57	Symmetry constraints and variational principles in diffusion quantum Monte Carlo calculations of excited-state energies. Physical Review B, 1999, 60, 4558-4570.	1.1	71
58	An accelerated Metropolis method. Journal of Chemical Physics, 1998, 109, 2630-2634.	1.2	15
59	A Quantum Monte Carlo Approach to the Adiabatic Connection Method. Advances in Quantum Chemistry, 1998, 33, 189-207.	0.4	10
60	Elimination of Coulomb finite-size effects in quantum many-body simulations. Physical Review B, 1997, 55, R4851-R4854.	1.1	99
61	Quantum Monte Carlo Investigation of Exchange and Correlation in Silicon. Physical Review Letters, 1997, 78, 3350-3353.	2.9	65
62	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.	1.1	265
63	Quantum Monte Carlo Calculations of the Energy of the Relativistic Homogeneous Electron Gas. Physical Review Letters, 1996, 77, 1099-1102.	2.9	16
64	Optimized wave functions for quantum Monte Carlo studies of atoms and solids. Physical Review B, 1996, 53, 9640-9648.	1.1	57
65	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.	1.1	79
66	A recursive solution of Heisenberg's equation and its interpretation. Journal of Physics Condensed Matter, 1994, 6, 6455-6475.	0.7	6
67	Quantum Monte Carlo Calculations for Solids Using SpecialkPoints Methods. Physical Review Letters, 1994, 73, 1959-1962.	2.9	72
68	Perfect localized basis functions for solids: chemical pseudopotentials and the Kronig-Penney model. Journal of Physics Condensed Matter, 1993, 5, 7987-8004.	0.7	1
69	Accuracy of the chemical-pseudopotential method for tetrahedral semiconductors. Physical Review B, 1993, 48, 14216-14225.	1.1	23
70	Comment on â€˜â€˜Feynman-Kac path-integral calculation of the ground-state energies of atomsâ€™â€™. Physical Review Letters, 1993, 71, 2158-2158.	2.9	6
71	Model for low-energy electronic states probed by x-ray absorption in high-Tccuprates. Physical Review B, 1992, 45, 10032-10050.	1.1	121
72	Electronic states inLa2â^'xSrxCuO4+Î´probed by soft-x-ray absorption. Physical Review Letters, 1991, 66, 104-107.	2.9	463

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73	Pseudopotentials with position-dependent electron masses. Physical Review B, 1990, 42, 11505-11529.	1.1	101
74	Tight-binding models and density-functional theory. Physical Review B, 1989, 39, 12520-12536.	1.1	591