Fionn D Malone

List of Publications by Year
in descending order

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21	1,049	516710	713466
papers	citations	16 h-index	21 g-index

21	21	21	614
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<tt>QMCPACK</tt>: an open sourceab initioquantum Monte Carlo package for the electronic structure of atoms, molecules and solids. Journal of Physics Condensed Matter, 2018, 30, 195901.	1.8	187
2	AbÂinitio Exchange-Correlation Free Energy of the Uniform Electron Gas at Warm Dense Matter Conditions. Physical Review Letters, 2017, 119, 135001.	7.8	139
3	AbÂInitioQuantum Monte Carlo Simulation of the Warm Dense Electron Gas in the Thermodynamic Limit. Physical Review Letters, 2016, 117, 156403.	7.8	136
4	Accurate Exchange-Correlation Energies for the Warm Dense Electron Gas. Physical Review Letters, 2016, 117, 115701.	7.8	88
5	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 174105.	3.0	80
6	Interaction picture density matrix quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 044116.	3.0	69
7	Ab initio quantum Monte Carlo simulation of the warm dense electron gas. Physics of Plasmas, 2017, 24, .	1.9	59
8	Overcoming the Memory Bottleneck in Auxiliary Field Quantum Monte Carlo Simulations with Interpolative Separable Density Fitting. Journal of Chemical Theory and Computation, 2019, 15, 256-264.	5.3	38
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.	5.3	33
10	A phaseless auxiliary-field quantum Monte Carlo perspective on the uniform electron gas at finite temperatures: Issues, observations, and benchmark study. Journal of Chemical Physics, 2021, 154, 064109.	3.0	31
11	Utilizing Essential Symmetry Breaking in Auxiliary-Field Quantum Monte Carlo: Application to the Spin Gaps of the C₃₆ Fullerene and an Iron Porphyrin Model Complex. Journal of Chemical Theory and Computation, 2020, 16, 3019-3027.	5.3	30
12	Auxiliary-field quantum Monte Carlo calculations of the structural properties of nickel oxide. Journal of Chemical Physics, 2018, 149, 164102.	3.0	24
13	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. Journal of Open Research Software, 2015, 3, 9.	5.9	21
14	Accelerating Auxiliary-Field Quantum Monte Carlo Simulations of Solids with Graphical Processing Units. Journal of Chemical Theory and Computation, 2020, 16, 4286-4297.	5.3	18
15	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. Journal of Chemical Physics, 2020, 153, 126101.	3.0	17
16	Towards the simulation of large scale proteinâ€“ligand interactions on NISQ-era quantum computers. Chemical Science, 2022, 13, 3094-3108.	7.4	16
17	An auxiliary-Field quantum Monte Carlo perspective on the ground state of the dense uniform electron gas: An investigation with Hartree-Fock trial wavefunctions. Journal of Chemical Physics, 2019, 151, 064122.	3.0	15
18	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

#	Article	IF	Citations
19	Using Density Matrix Quantum Monte Carlo for Calculating Exact-on-Average Energies for ab Initio Hamiltonians in a Finite Basis Set. Journal of Chemical Theory and Computation, 2020, 16, 1029-1038.	5.3	13
20	Accelerating the convergence of auxiliary-field quantum Monte Carlo in solids with optimized Gaussian basis sets. Journal of Chemical Physics, 2020, 153, 194111.	3.0	12
21	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended Koopmansâ€™ Theorem Approach. Journal of Chemical Theory and Computation, 2021, 17, 3372-3387.	5.3	10