

Fionn D Malone

List of Publications by Year in descending order

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Version: 2024-02-01

21
papers

1,049
citations

516710

16
h-index

713466

21
g-index

21
all docs

21
docs citations

21
times ranked

614
citing authors

#	ARTICLE	IF	CITATIONS
1	Towards the simulation of large scale protein–ligand interactions on NISQ-era quantum computers. <i>Chemical Science</i> , 2022, 13, 3094-3108.	7.4	16
2	A phaseless auxiliary-field quantum Monte Carlo perspective on the uniform electron gas at finite temperatures: Issues, observations, and benchmark study. <i>Journal of Chemical Physics</i> , 2021, 154, 064109.	3.0	31
3	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended Koopmans’s™ Theorem Approach. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3372-3387.	5.3	10
4	Systematic comparison and cross-validation of fixed-node diffusion Monte Carlo and phaseless auxiliary-field quantum Monte Carlo in solids. <i>Physical Review B</i> , 2020, 102, .	3.2	13
5	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. <i>Journal of Chemical Physics</i> , 2020, 153, 126101.	3.0	17
6	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2020, 152, 174105.	3.0	80
7	Accelerating Auxiliary-Field Quantum Monte Carlo Simulations of Solids with Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4286-4297.	5.3	18
8	Using Density Matrix Quantum Monte Carlo for Calculating Exact-on-Average Energies for <i>ab initio</i> Hamiltonians in a Finite Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1029-1038.	5.3	13
9	Utilizing Essential Symmetry Breaking in Auxiliary-Field Quantum Monte Carlo: Application to the Spin Gaps of the C ₃₆ Fullerene and an Iron Porphyrin Model Complex. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3019-3027.	5.3	30
10	Accelerating the convergence of auxiliary-field quantum Monte Carlo in solids with optimized Gaussian basis sets. <i>Journal of Chemical Physics</i> , 2020, 153, 194111.	3.0	12
11	An auxiliary-Field quantum Monte Carlo perspective on the ground state of the dense uniform electron gas: An investigation with Hartree-Fock trial wavefunctions. <i>Journal of Chemical Physics</i> , 2019, 151, 064122.	3.0	15
12	The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1728-1742.	5.3	33
13	Overcoming the Memory Bottleneck in Auxiliary Field Quantum Monte Carlo Simulations with Interpolative Separable Density Fitting. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 256-264.	5.3	38
14	Auxiliary-field quantum Monte Carlo calculations of the structural properties of nickel oxide. <i>Journal of Chemical Physics</i> , 2018, 149, 164102.	3.0	24
15	QMCPACK: an open source <i>ab initio</i> quantum Monte Carlo package for the electronic structure of atoms, molecules and solids. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 195901.	1.8	187
16	<i>Ab initio</i> quantum Monte Carlo simulation of the warm dense electron gas. <i>Physics of Plasmas</i> , 2017, 24, .	1.9	59
17	<i>Ab initio</i> Exchange-Correlation Free Energy of the Uniform Electron Gas at Warm Dense Matter Conditions. <i>Physical Review Letters</i> , 2017, 119, 135001.	7.8	139
18	Accurate Exchange-Correlation Energies for the Warm Dense Electron Gas. <i>Physical Review Letters</i> , 2016, 117, 115701.	7.8	88

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19	<i>Ab Initio</i> Quantum Monte Carlo Simulation of the Warm Dense Electron Gas in the Thermodynamic Limit. <i>Physical Review Letters</i> , 2016, 117, 156403.	7.8	136
20	Interaction picture density matrix quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2015, 143, 044116.	3.0	69
21	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. <i>Journal of Open Research Software</i> , 2015, 3, 9.	5.9	21