Mario Motta

List of Publications by Year
in descending order

21 papers	1,943 citations	471509 17 h-index	677142 22 g-index
23 all docs	23 docs citations	23 times ranked	1106 citing authors

#	Article	IF	Citations
1	Digital Quantum Simulation of Open Quantum Systems Using Quantum Imaginaryâ€“Time Evolution. PRX Quantum, 2022, 3, .	9.2	48
2	Quantum Circuits for the Preparation of Spin Eigenfunctions on Quantum Computers. Symmetry, 2022, 14, 624.	2.2	4
3	Emerging quantum computing algorithms for quantum chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	41
4	Ab initio electronic density in solids by many-body plane-wave auxiliary-field quantum Monte Carlo calculations. Physical Review B, 2021, 103, .	3.2	8
5	Quantum Computation of Finite-Temperature Static and Dynamical Properties of Spin Systems Using Quantum Imaginary Time Evolution. PRX Quantum, 2021, 2, .	9.2	68
6	Quantum computation of dominant products in lithiumâ€“sulfur batteries. Journal of Chemical Physics, 2021, 154, 134115.	3.0	42
7	Low rank representations for quantum simulation of electronic structure. Npj Quantum Information, 2021, 7, .	6.7	54
8	Quantum Filter Diagonalization with Compressed Double-Factorized Hamiltonians. PRX Quantum, 2021, 2, .	9.2	22
9	Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution. Nature Physics, 2020, 16, 205-210.	16.7	317
10	Quantum Algorithms for Quantum Chemistry and Quantum Materials Science. Chemical Reviews, 2020, 120, 12685-12717.	47.7	311
11	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
12	Quantum simulation of electronic structure with a transcorrelated Hamiltonian: improved accuracy with a smaller footprint on the quantum computer. Physical Chemistry Chemical Physics, 2020, 22, 24270-24281.	2.8	43
13	Ground-State Properties of the Hydrogen Chain: Dimerization, Insulator-to-Metal Transition, and Magnetic Phases. Physical Review X, 2020, 10, .	8.9	42
14	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. Physical Review X, 2020, 10, .	8.9	68
15	Hamiltonian symmetries in auxiliary-field quantum Monte Carlo calculations for electronic structure. Physical Review B, 2019, 100, .	3.2	19
16	Efficient Ab Initio Auxiliary-Field Quantum Monte Carlo Calculations in Gaussian Bases via Low-Rank Tensor Decomposition. Journal of Chemical Theory and Computation, 2019, 15, 3510-3521.	5.3	39
17	Communication: Calculation of interatomic forces and optimization of molecular geometry with auxiliary-field quantum Monte Carlo. Journal of Chemical Physics, 2018, 148, 181101.	3.0	24
18	Ab initio computations of molecular systems by the auxiliaryâ€field quantum Monte Carlo method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1364.	14.6	96

#	Article	IF	Citations
19	Towards the Solution of the Many-Electron Problem in Real Materials: Equation of State of the Hydrogen Chain with State-of-the-Art Many-Body Methods. Physical Review X, 2017, 7, .	8.9	171
20	Computation of Ground-State Properties in Molecular Systems: Back-Propagation with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2017, 13, 5367-5378.	5.3	41
21	Qubitization of Arbitrary Basis Quantum Chemistry Leveraging Sparsity and Low Rank Factorization. Quantum - the Open Journal for Quantum Science, 0, 3, 208.	0.0	89