James Daniel Whitfield

List of Publications by Year
in descending order

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31	2,471	394421 19	414414 32
papers	citations	h-index	g-index

33	33	33	1860
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Towards quantum chemistry on a quantum computer. Nature Chemistry, 2010, 2, 106-111.	13.6	568
2	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
3	Simulation of electronic structure Hamiltonians using quantum computers. Molecular Physics, 2011, 109, 735-750.	1.7	310
4	Simulating Chemistry Using Quantum Computers. Annual Review of Physical Chemistry, 2011, 62, 185-207.	10.8	224
5	Quantum Simulation of Helium Hydride Cation in a Solid-State Spin Register. ACS Nano, 2015, 9, 7769-7774.	14.6	113
6	Faster quantum chemistry simulation on fault-tolerant quantum computers. New Journal of Physics, 2012, 14, 115023.	2.9	91
7	Quantum stochastic walks: A generalization of classical random walks and quantum walks. Physical Review A, 2010, 81, .	2.5	83
8	Bravyi-Kitaev Superfast simulation of electronic structure on a quantum computer. Journal of Chemical Physics, 2018, 148, 164104.	3.0	73
9	Reducing Qubit Requirements for Quantum Simulations Using Molecular Point Group Symmetries. Journal of Chemical Theory and Computation, 2020, 16, 6091-6097.	5.3	68
10	Operator locality in the quantum simulation of fermionic models. Physical Review A, 2017, 95, .	2.5	65
11	Adiabatic quantum simulators. AIP Advances, 2011, 1, .	1.3	57
12	Superfast encodings for fermionic quantum simulation. Physical Review Research, 2019, 1, .	3.6	55
13	Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance. Scientific Reports, 2011, 1, 88.	3.3	51
14	Ground-state spin logic. Europhysics Letters, 2012, 99, 57004.	2.0	51
15	Quantum Transport Enhancement by Time-Reversal Symmetry Breaking. Scientific Reports, 2013, 3, 2361.	3.3	49
16	Local spin operators for fermion simulations. Physical Review A, 2016, 94, .	2.5	44
17	Computational complexity in electronic structure. Physical Chemistry Chemical Physics, 2013, 15, 397-411.	2.8	42
18	Simulation of classical thermal states on a quantum computer: A transfer-matrix approach. Physical Review A, 2010, 82, .	2.5	24

#	Article	IF	Citations
19	Generalized Pauli constraints in small atoms. Physical Review A, 2018, 97, .	2.5	22
20	Communication: Spin-free quantum computational simulations and symmetry adapted states. Journal of Chemical Physics, 2013, 139, 021105.	3.0	18
21	Hardware-efficient fermionic simulation with a cavityâ€“QED system. Npj Quantum Information, 2018, 4, .	6.7	18
22	Intractability of Electronic Structure in a Fixed Basis. PRX Quantum, 2022, 3, .	9.2	9
23	Solver for the Electronic V-Representation Problem of Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 6014-6026.	5.3	8
24	On the NP-completeness of the Hartree-Fock method for translationally invariant systems. Journal of Chemical Physics, 2014, 141, 234103.	3.0	4
25	Analysis of superfast encoding performance for electronic structure simulations. Physical Review A, 2019, 100, .	2.5	3
26	Limitations of Hartreeâ€“Fock with quantum resources. Journal of Chemical Physics, 2021, 154, 044112.	3.0	3
27	The Computational Complexity of Density Functional Theory. Letters in Mathematical Physics, 2014, , 245-260.	0.6	3
28	Floquet graphene antidot lattices. Physical Review B, 2021, 104, .	3.2	3
29	Basis set convergence of Wilson basis functions for electronic structure. Journal of Chemical Physics, 2019, 151, 064118.	3.0	1
30	A Comparison of Three Ways to Measure Time-Dependent Densities With Quantum Simulators. Frontiers in Physics, 2021, 9, .	2.1	1
31	Linear-Optical Generation of Eigenstates of the Two-SiteXYModel. Physical Review X, 2015, 5, .	8.9	0