

# James Daniel Whitfield

## List of Publications by Year in descending order

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31  
papers

2,471  
citations

394421

19  
h-index

414414

32  
g-index

33  
all docs

33  
docs citations

33  
times ranked

1860  
citing authors

#	ARTICLE	IF	CITATIONS
1	Intractability of Electronic Structure in a Fixed Basis. PRX Quantum, 2022, 3, .	9.2	9
2	Limitations of Hartree-Fock with quantum resources. Journal of Chemical Physics, 2021, 154, 044112.	3.0	3
3	A Comparison of Three Ways to Measure Time-Dependent Densities With Quantum Simulators. Frontiers in Physics, 2021, 9, .	2.1	1
4	Floquet graphene antidot lattices. Physical Review B, 2021, 104, .	3.2	3
5	Recent developments in the PySCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
6	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
7	Reducing Qubit Requirements for Quantum Simulations Using Molecular Point Group Symmetries. Journal of Chemical Theory and Computation, 2020, 16, 6091-6097.	5.3	68
8	Analysis of superfast encoding performance for electronic structure simulations. Physical Review A, 2019, 100, .	2.5	3
9	Basis set convergence of Wilson basis functions for electronic structure. Journal of Chemical Physics, 2019, 151, 064118.	3.0	1
10	Superfast encodings for fermionic quantum simulation. Physical Review Research, 2019, 1, .	3.6	55
11	Hardware-efficient fermionic simulation with a cavity-QED system. Npj Quantum Information, 2018, 4, .	6.7	18
12	Bravyi-Kitaev Superfast simulation of electronic structure on a quantum computer. Journal of Chemical Physics, 2018, 148, 164104.	3.0	73
13	Generalized Pauli constraints in small atoms. Physical Review A, 2018, 97, .	2.5	22
14	Operator locality in the quantum simulation of fermionic models. Physical Review A, 2017, 95, .	2.5	65
15	Local spin operators for fermion simulations. Physical Review A, 2016, 94, .	2.5	44
16	Linear-Optical Generation of Eigenstates of the Two-Site XY Model. Physical Review X, 2015, 5, .	8.9	0
17	Quantum Simulation of Helium Hydride Cation in a Solid-State Spin Register. ACS Nano, 2015, 9, 7769-7774.	14.6	113
18	On the NP-completeness of the Hartree-Fock method for translationally invariant systems. Journal of Chemical Physics, 2014, 141, 234103.	3.0	4

#	ARTICLE	IF	CITATIONS
19	The Computational Complexity of Density Functional Theory. <i>Letters in Mathematical Physics</i> , 2014, , 245-260.	0.6	3
20	Computational complexity in electronic structure. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 397-411.	2.8	42
21	Quantum Transport Enhancement by Time-Reversal Symmetry Breaking. <i>Scientific Reports</i> , 2013, 3, 2361.	3.3	49
22	Communication: Spin-free quantum computational simulations and symmetry adapted states. <i>Journal of Chemical Physics</i> , 2013, 139, 021105.	3.0	18
23	Faster quantum chemistry simulation on fault-tolerant quantum computers. <i>New Journal of Physics</i> , 2012, 14, 115023.	2.9	91
24	Ground-state spin logic. <i>Europhysics Letters</i> , 2012, 99, 57004.	2.0	51
25	Simulation of electronic structure Hamiltonians using quantum computers. <i>Molecular Physics</i> , 2011, 109, 735-750.	1.7	310
26	Simulating Chemistry Using Quantum Computers. <i>Annual Review of Physical Chemistry</i> , 2011, 62, 185-207.	10.8	224
27	Adiabatic quantum simulators. <i>AIP Advances</i> , 2011, 1, .	1.3	57
28	Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance. <i>Scientific Reports</i> , 2011, 1, 88.	3.3	51
29	Towards quantum chemistry on a quantum computer. <i>Nature Chemistry</i> , 2010, 2, 106-111.	13.6	568
30	Simulation of classical thermal states on a quantum computer: A transfer-matrix approach. <i>Physical Review A</i> , 2010, 82, .	2.5	24
31	Quantum stochastic walks: A generalization of classical random walks and quantum walks. <i>Physical Review A</i> , 2010, 81, .	2.5	83