B Scott Fales

List of Publications by Year
in descending order

21 papers	**750** citations	516710 **16** h-index	713466 **21** g-index
21 all docs	**21** docs citations	**21** times ranked	**901** citing authors

#	Article	IF	Citations
1	Rank-reduced coupled-cluster. III. Tensor hypercontraction of the doubles amplitudes. Journal of Chemical Physics, 2022, 156, 054102.	3.0	15
2	<scp>TeraChem</scp>: A graphical processing unit<scp>â€accelerated</scp> electronic structure package for <scp>largeâ€scale</scp> ab initio molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1494.	14.6	143
3	Cover Image, Volume 11, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1523.	14.6	5
4	Efficient Treatment of Large Active Spaces through Multi-GPU Parallel Implementation of Direct Configuration Interaction. Journal of Chemical Theory and Computation, 2020, 16, 1586-1596.	5.3	20
5	PySpawn: Software for Nonadiabatic Quantum Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 5485-5498.	5.3	10
6	Fast transformations between configuration state function and Slater determinant bases for direct configuration interaction. Journal of Chemical Physics, 2020, 152, 164111.	3.0	11
7	TeraChem: Accelerating electronic structure and <i>ab initio</i> molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110.	3.0	87
8	Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures. Journal of Chemical Theory and Computation, 2020, 16, 4021-4028.	5.3	22
9	Electronic and Structural Comparisons between Iron(II/III) and Ruthenium(II/III) Imide Analogs. Inorganic Chemistry, 2019, 58, 11699-11715.	4.0	8
10	Conical Intersections at the Nanoscale: Molecular Ideas for Materials. Annual Review of Physical Chemistry, 2019, 70, 21-43.	10.8	31
11	Dynamics of recombination via conical intersection in a semiconductor nanocrystal. Chemical Science, 2018, 9, 681-687.	7.4	22
12	Simulating Electron Dynamics of Complex Molecules with Time-Dependent Complete Active Space Configuration Interaction. Journal of Chemical Theory and Computation, 2018, 14, 4129-4138.	5.3	29
13	Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. Journal of Chemical Theory and Computation, 2018, 14, 4139-4150.	5.3	23
14	A direct-compatible formulation of the coupled perturbed complete active space self-consistent field equations on graphical processing units. Journal of Chemical Physics, 2017, 146, 174113.	3.0	50
15	Robust and Efficient Spin Purification for Determinantal Configuration Interaction. Journal of Chemical Theory and Computation, 2017, 13, 4162-4172.	5.3	17
16	Understanding Nonradiative Recombination through Defect-Induced Conical Intersections. Journal of Physical Chemistry Letters, 2017, 8, 4091-4099.	4.6	27
17	Complete active space configuration interaction from state-averaged configuration interaction singles natural orbitals: Analytic first derivatives and derivative coupling vectors. Journal of Chemical Physics, 2017, 147, 094104.	3.0	25
18	Mechanisms and time-resolved dynamics for trihydrogen cation (H3 +) formation from organic molecules in strong laser fields. Scientific Reports, 2017, 7, 4703.	3.3	62

#	Article	IF	Citations
19	Defect-Induced Conical Intersections Promote Nonradiative Recombination. Nano Letters, 2015, 15, 6247-6253.	9.1	47
20	Nanoscale Multireference Quantum Chemistry: Full Configuration Interaction on Graphical Processing Units. Journal of Chemical Theory and Computation, 2015, 11, 4708-4716.	5.3	72
21	Infrared Multiple Photon Dissociation Action Spectroscopy and Theoretical Studies of Diethyl Phosphate Complexes: Effects of Protonation and Sodium Cationization on Structure. Journal of the American Society for Mass Spectrometry, 2011, 22, 81-92.	2.8	24