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	<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
2	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110.	3.0	87
3	Nanoscale Multireference Quantum Chemistry: Full Configuration Interaction on Graphical Processing Units. Journal of Chemical Theory and Computation, 2015, 11, 4708-4716.	5.3	72
4	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
5	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
6	Defect-Induced Conical Intersections Promote Nonradiative Recombination. Nano Letters, 2015, 15, 6247-6253.	9.1	47
7	Conical Intersections at the Nanoscale: Molecular Ideas for Materials. Annual Review of Physical Chemistry, 2019, 70, 21-43.	10.8	31
8	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
9	Understanding Nonradiative Recombination through Defect-Induced Conical Intersections. Journal of Physical Chemistry Letters, 2017, 8, 4091-4099.	4.6	27
10	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
11	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
12	Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. Journal of Chemical Theory and Computation, 2018, 14, 4139-4150.	5.3	23
13	Dynamics of recombination via conical intersection in a semiconductor nanocrystal. Chemical Science, 2018, 9, 681-687.	7.4	22
14	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
15	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
16	Robust and Efficient Spin Purification for Determinantal Configuration Interaction. Journal of Chemical Theory and Computation, 2017, 13, 4162-4172.	5.3	17
17	Rank-reduced coupled-cluster. III. Tensor hypercontraction of the doubles amplitudes. Journal of Chemical Physics, 2022, 156, 054102.	3.0	15
18	Fast transformations between configuration state function and Slater determinant bases for direct configuration interaction. Journal of Chemical Physics, 2020, 152, 164111.	3.0	11

#	Article	IF	Citations
19	PySpawn: Software for Nonadiabatic Quantum Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 5485-5498.	5.3	10
20	Electronic and Structural Comparisons between Iron(II/III) and Ruthenium(II/III) Imide Analogs. Inorganic Chemistry, 2019, 58, 11699-11715.	4.0	8
21	Cover Image, Volume 11, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1523.	14.6	5