Lee M Thompson

List of Publications by Year
in descending order

22 papers	232 citations	933447 10 h-index	996975 15 g-index
32 all docs	32 docs citations	32 times ranked	238 citing authors

#	Article	IF	Citations
1	Analytical Harmonic Vibrational Frequencies for the Green Fluorescent Protein Computed with ONIOM: Chromophore Mode Character and Its Response to Environment. Journal of Chemical Theory and Computation, 2014, 10, 751-766.	5.3	24
2	Natural ionization orbitals for interpreting electron detachment processes. Journal of Chemical Physics, 2016, 144, 204117.	3.0	19
3	Spin projection with double hybrid density functional theory. Journal of Chemical Physics, 2014, 141, 034108.	3.0	18
4	Modeling the Photoelectron Spectra of MoNbO₂^{â€“} Accounting for Spin Contamination in Density Functional Theory. Journal of Physical Chemistry A, 2015, 119, 8744-8751.	2.5	18
5	Nonâ€Covalent Substrate Directed Enantioselective Heck Desymmetrization of cis â€Cyclohexâ€4â€eneâ€1,2â€diol: Synthesis of all cis Chiral 5â€Arylâ€cyclohexâ€3â€eneâ€1,2â€diols and Mechanistic Investigation. Advanced Synthesis and Catalysis, 2018, 360, 3760-3767.	4.3	17
6	Second derivatives for approximate spin projection methods. Journal of Chemical Physics, 2015, 142, 054106.	3.0	16
7	The role of substituents in retro Dielsâ€“Alder extrusion of CO2 from 2(H)-pyrone cycloadducts. Tetrahedron, 2016, 72, 6021-6024.	1.9	14
8	Explaining the MoVO4â^' photoelectron spectrum: Rationalization of geometric and electronic structure. Journal of Chemical Physics, 2017, 146, 104301.	3.0	14
9	On approximate projection models. Molecular Physics, 2019, 117, 1421-1429.	1.7	13
10	Effect of Oriented External Electric Fields on the Photo and Thermal Isomerization of Azobenzene. Journal of Physical Chemistry A, 2020, 124, 3520-3529.	2.5	12
11	Ultrafast vibrational dynamics of parallel excited state proton transfer reactions in the Green Fluorescent Protein. Vibrational Spectroscopy, 2012, 62, 1-6.	2.2	10
12	Deconstructing the ONIOM Hessian: Investigating Method Combinations for Transition Structures. Journal of Chemical Theory and Computation, 2012, 8, 4907-4914.	5.3	10
13	Global elucidation of broken symmetry solutions to the independent particle model through a Lie algebraic approach. Journal of Chemical Physics, 2018, 149, 194106.	3.0	9
14	Orbital optimization in nonorthogonal multiconfigurational self-consistent field applied to the study of conical intersections and avoided crossings. Journal of Chemical Physics, 2021, 154, 244101.	3.0	9
15	Global Elucidation of Self-Consistent Field Solution Space Using Basin Hopping. Journal of Chemical Theory and Computation, 2020, 16, 5635-5644.	5.3	8
16	Assessing the Calculation of Exchange Coupling Constants and Spin Crossover Gaps Using the Approximate Projection Model To Improve Density Functional Calculations. Journal of Chemical Theory and Computation, 2020, 16, 154-163.	5.3	6
17	Kinetics of phosphotungstic acid-catalyzed condensation of levulinic acid with phenol to diphenolic acid: Temperature-controlled regioselectivity. Molecular Catalysis, 2021, 514, 111848.	2.0	4
18	The Influence of Î²â€Ammonium Substitution on the Reaction Kinetics of Aminooxy Condensations with Aldehydes and Ketones. ChemPhysChem, 2019, 20, 815-822.	2.1	3

#	Article	IF	Citations
19	Difference projection-after-variation double-hybrid density functional theory applied to the calculation of vertical excitation energies. Journal of Chemical Physics, 2020, 153, 074103.	3.0	3
20	Excited State Electronic Structure of Single-Site Vanadium Oxide Photocatalysts Supported on Mesoporous Silica. ACS Symposium Series, 2019, , 327-341.	0.5	2
21	Oriented External Electric Field Tuning of Unsubstituted Azoheteroarene Thermal Isomerization Half-Lives. Journal of Physical Chemistry A, 2021, 125, 8238-8248.	2.5	2
22	On the linear geometry of lanthanide hydroxide (Ln-OH, Ln = Laâ€“Lu). Physical Chemistry Chemical Physics, 2019, 21, 21890-21897.	2.8	1