Lee M Thompson

List of Publications by Year
in descending order

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

933447

996975

#	Article	IF	Citations
1	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
2	Oriented External Electric Field Tuning of Unsubstituted Azoheteroarene Thermal Isomerization Half-Lives. Journal of Physical Chemistry A, 2021, 125, 8238-8248.	2.5	2
3	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
4	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
5	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
6	Global Elucidation of Self-Consistent Field Solution Space Using Basin Hopping. Journal of Chemical Theory and Computation, 2020, 16, 5635-5644.	5.3	8
7	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
8	The Influence of β-Ammonium Substitution on the Reaction Kinetics of Aminooxy Condensations with Aldehydes and Ketones. ChemPhysChem, 2019, 20, 815-822.	2.1	3
9	Excited State Electronic Structure of Single-Site Vanadium Oxide Photocatalysts Supported on Mesoporous Silica. ACS Symposium Series, 2019, , 327-341.	0.5	2
10	On the linear geometry of lanthanide hydroxide (Ln-OH, Ln = La–Lu). Physical Chemistry Chemical Physics, 2019, 21, 21890-21897.	2.8	1
11	On approximate projection models. Molecular Physics, 2019, 117, 1421-1429.	1.7	13
12	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
13	Non-Covalent Substrate Directed Enantioselective Heck Desymmetrization of cis -Cyclohex-4-ene-1,2-diol: Synthesis of all cis Chiral 5-Aryl-cyclohex-3-ene-1,2-diols and Mechanistic Investigation. Advanced Synthesis and Catalysis, 2018, 360, 3760-3767.	4.3	17
14	Explaining the MoVO4⁻ photoelectron spectrum: Rationalization of geometric and electronic structure. Journal of Chemical Physics, 2017, 146, 104301.	3.0	14
15	Natural ionization orbitals for interpreting electron detachment processes. Journal of Chemical Physics, 2016, 144, 204117.	3.0	19
16	The role of substituents in retro Diels–Alder extrusion of CO_2 from 2(H)-pyrone cycloadducts. Tetrahedron, 2016, 72, 6021-6024.	1.9	14
17	Second derivatives for approximate spin projection methods. Journal of Chemical Physics, 2015, 142, 054106.	3.0	16
18	Modeling the Photoelectron Spectra of $MoNbO_2^-$ Accounting for Spin Contamination in Density Functional Theory. Journal of Physical Chemistry A, 2015, 119, 8744-8751.	2.5	18

#	Article	IF	Citations
19	Spin projection with double hybrid density functional theory. Journal of Chemical Physics, 2014, 141, 034108.	3.0	18
20	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
21	Ultrafast vibrational dynamics of parallel excited state proton transfer reactions in the Green Fluorescent Protein. Vibrational Spectroscopy, 2012, 62, 1-6.	2.2	10
22	Deconstructing the ONIOM Hessian: Investigating Method Combinations for Transition Structures. Journal of Chemical Theory and Computation, 2012, 8, 4907-4914.	5.3	10