Christopher J Stein

List of Publications by Year
in descending order

33 papers	2,736 citations	430874 18 h-index	434195 31 g-index
38 all docs	38 docs citations	38 times ranked	2529 citing authors

#	Article	IF	Citations
1	Origin of the different reactivity of the highâ€valent coinageâ€metal complexes [RCu^{<scp>iii</scp>}Me₃]^{â¯} and [RAg^{<scp>iii</scp>}Me₃]^{â¯} (R=allyl)**. Chemistry - A European Journal, 2022, 28, .	3.3	2
2	NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces. , 2022, 1, 333-343.		42
3	A benchmark dataset for Hydrogen Combustion. Scientific Data, 2022, 9, 215.	5.3	6
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
5	Stripping away ion hydration shells in electrical double-layer formation: Water networks matter. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	20
6	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
7	Semiclassical Dispersion Corrections Efficiently Improve Multiconfigurational Theory with Short-Range Density-Functional Dynamic Correlation. Journal of Physical Chemistry A, 2020, 124, 2834-2841.	2.5	4
8	Orbital Entanglement Analysis of Exchange-Coupled Systems. Journal of Physical Chemistry Letters, 2019, 10, 6762-6770.	4.6	14
9	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
10	<scp>autoCAS</scp>: A Program for Fully Automated Multiconfigurational Calculations. Journal of Computational Chemistry, 2019, 40, 2216-2226.	3.3	60
11	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 094113.	3.0	29
12	The Poissonâ€“Boltzmann model for implicit solvation of electrolyte solutions: Quantum chemical implementation and assessment via Sechenov coefficients. Journal of Chemical Physics, 2019, 151, 224111.	3.0	24
13	Structure and dynamics of the radical cation of ethane arising from the Jahnâ€“Teller and pseudo-Jahnâ€“Teller effects. Physical Chemistry Chemical Physics, 2018, 20, 1072-1081.	2.8	11
14	Engineering Molecular Iodine Catalysis for Alkylâ€“Nitrogen Bond Formation. ACS Catalysis, 2018, 8, 3918-3925.	11.2	83
15	Measuring multi-configurational character by orbital entanglement. Molecular Physics, 2017, 115, 2110-2119.	1.7	49
16	Kooperative Lichtâ€aktivierte Iodâ€und Photoredoxâ€Katalyse zur Aminierung von Câ€Hâ€Bindungen. Angewandte Chemie, 2017, 129, 8117-8121.	2.0	63
17	Cooperative Lightâ€Activated Iodine and Photoredox Catalysis for the Amination of Câ¯H Bonds. Angewandte Chemie - International Edition, 2017, 56, 8004-8008.	13.8	181
18	Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. Photochemistry and Photobiology, 2017, 93, 815-833.	2.5	9

#	Article	IF	Citations
19	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. Journal of the American Chemical Society, 2017, 139, 9672-9683.	13.7	45
20	Vibrational Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 3764-3777.	5.3	46
21	Automated Identification of Relevant Frontier Orbitals for Chemical Compounds and Processes. Chimia, 2017, 71, 170.	0.6	63
22	New Approaches for ab initio Calculations of Molecules with Strong Electron Correlation. Chimia, 2016, 70, 244.	0.6	94
23	Highly Accurate Spectroscopic Parameters from Ab Initio Calculations. , 2016, , .		0
24	The Delicate Balance of Static and Dynamic Electron Correlation. Journal of Chemical Theory and Computation, 2016, 12, 3764-3773.	5.3	78
25	Automated Selection of Active Orbital Spaces. Journal of Chemical Theory and Computation, 2016, 12, 1760-1771.	5.3	237
26	Theoretical rovibrational spectroscopy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si63.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mi mathvariant="normal">NO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:mrow><mml:mo>+</mml:m Journal of Molecular Spectroscopy, 2015, 311, 12-18.	1.2	5
27	High-level theoretical spectroscopic parameters for three ions of astrochemical interest. Molecular Physics, 2015, 113, 2169-2178.	1.7	10
28	Challenging High-Level ab initio Rovibrational Spectroscopy: The Nitrous Oxide Molecule. Zeitschrift Fur Physikalische Chemie, 2015, 229, 1663-1690.	2.8	17
29	Accurate Calculation of the Dissociation Energy of the Highly Anharmonic System ClHCl^{â€“}. Journal of Physical Chemistry A, 2015, 119, 5158-5164.	2.5	4
30	STRONG THEORETICAL SUPPORT FOR THE ASSIGNMENT OF B11244 TOl-C₃H⁺. Astrophysical Journal, 2014, 787, 72.	4.5	30
31	Accurate bond dissociation energies (D0) for FHFâ¯isotopologues. Molecular Physics, 2013, 111, 2647-2652.	1.7	17
32	Rovibrational States of N₃^{â€“} and CO₂ Up to High J: A Theoretical Study Beyond fc-CCSD(T). Journal of Physical Chemistry A, 2013, 117, 13806-13814.	2.5	13
33	FHF^{â€“} Isotopologues: Highly Anharmonic Hydrogen-Bonded Systems with Strong Coriolis Interaction. Journal of Physical Chemistry A, 2013, 117, 9695-9703.	2.5	16