

Christopher J Stein

List of Publications by Year in descending order

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33
papers

2,736
citations

430874

18
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434195

31
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38
all docs

38
docs citations

38
times ranked

2529
citing authors

#	ARTICLE	IF	CITATIONS
1	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	5.3	661
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
3	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020, 152, 214117.	3.0	281
4	Automated Selection of Active Orbital Spaces. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1760-1771.	5.3	237
5	Cooperative Light-Activated Iodine and Photoredox Catalysis for the Amination of C-H Bonds. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8004-8008.	13.8	181
6	New Approaches for ab initio Calculations of Molecules with Strong Electron Correlation. <i>Chimia</i> , 2016, 70, 244.	0.6	94
7	Engineering Molecular Iodine Catalysis for Alkyl-Nitrogen Bond Formation. <i>ACS Catalysis</i> , 2018, 8, 3918-3925.	11.2	83
8	The Delicate Balance of Static and Dynamic Electron Correlation. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3764-3773.	5.3	78
9	Kooperative Licht-aktivierte Iod- und Photoredox-Katalyse zur Aminierung von C-H-Bindungen. <i>Angewandte Chemie</i> , 2017, 129, 8117-8121.	2.0	63
10	Automated Identification of Relevant Frontier Orbitals for Chemical Compounds and Processes. <i>Chimia</i> , 2017, 71, 170.	0.6	63
11	<sc>autoCAS</sc>: A Program for Fully Automated Multiconfigurational Calculations. <i>Journal of Computational Chemistry</i> , 2019, 40, 2216-2226.	3.3	60
12	Measuring multi-configurational character by orbital entanglement. <i>Molecular Physics</i> , 2017, 115, 2110-2119.	1.7	49
13	Vibrational Density Matrix Renormalization Group. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3764-3777.	5.3	46
14	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. <i>Journal of the American Chemical Society</i> , 2017, 139, 9672-9683.	13.7	45
15	NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces. , 2022, 1, 333-343.		42
16	STRONG THEORETICAL SUPPORT FOR THE ASSIGNMENT OF B11244 TO C^3H^+ . <i>Astrophysical Journal</i> , 2014, 787, 72.	4.5	30
17	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. <i>Journal of Chemical Physics</i> , 2019, 150, 094113.	3.0	29
18	The Poisson-Boltzmann model for implicit solvation of electrolyte solutions: Quantum chemical implementation and assessment via Sechenov coefficients. <i>Journal of Chemical Physics</i> , 2019, 151, 224111.	3.0	24

#	ARTICLE	IF	CITATIONS
19	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
20	Accurate bond dissociation energies (D0) for FHF ⁺ isotopologues. Molecular Physics, 2013, 111, 2647-2652.	1.7	17
21	Challenging High-Level <i>ab initio</i> Rovibrational Spectroscopy: The Nitrous Oxide Molecule. Zeitschrift Fur Physikalische Chemie, 2015, 229, 1663-1690.	2.8	17
22	FHF ⁺ Isotopologues: Highly Anharmonic Hydrogen-Bonded Systems with Strong Coriolis Interaction. Journal of Physical Chemistry A, 2013, 117, 9695-9703.	2.5	16
23	Orbital Entanglement Analysis of Exchange-Coupled Systems. Journal of Physical Chemistry Letters, 2019, 10, 6762-6770.	4.6	14
24	Rovibrational States of N ₃ ⁺ and CO ₂ Up to High <i>J</i> : A Theoretical Study Beyond <i>fc</i> -CCSD(T). Journal of Physical Chemistry A, 2013, 117, 13806-13814.	2.5	13
25	Structure and dynamics of the radical cation of ethane arising from the Jahn-Teller and pseudo-Jahn-Teller effects. Physical Chemistry Chemical Physics, 2018, 20, 1072-1081.	2.8	11
26	High-level theoretical spectroscopic parameters for three ions of astrochemical interest. Molecular Physics, 2015, 113, 2169-2178.	1.7	10
27	Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. Photochemistry and Photobiology, 2017, 93, 815-833.	2.5	9
28	A benchmark dataset for Hydrogen Combustion. Scientific Data, 2022, 9, 215.	5.3	6
29	Theoretical rovibrational spectroscopy of NO_2^+ . Journal of Molecular Spectroscopy, 2015, 311, 12-18.	1.2	5
30	Accurate Calculation of the Dissociation Energy of the Highly Anharmonic System ClHCl ⁺ . Journal of Physical Chemistry A, 2015, 119, 5158-5164.	2.5	4
31	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
32	Origin of the different reactivity of the high-valent coinage-metal complexes [RCu ^{III} Me ₃] ⁺ and [RAg ^{III} Me ₃] ⁺ (R=allyl)**. Chemistry - A European Journal, 2022, 28, .	3.3	2
33	Highly Accurate Spectroscopic Parameters from Ab Initio Calculations. , 2016, , .		0