

Joseph Ivanic

List of Publications by Year in descending order

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25
papers

2,301
citations

430874

18
h-index

580821

25
g-index

25
all docs

25
docs citations

25
times ranked

2322
citing authors

#	ARTICLE	IF	CITATIONS
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
2	Direct configuration interaction and multiconfigurational self-consistent-field method for multiple active spaces with variable occupations. I. Method. Journal of Chemical Physics, 2003, 119, 9364-9376.	3.0	247
3	Identification of deadwood in configuration spaces through general direct configuration interaction. Theoretical Chemistry Accounts, 2001, 106, 339-351.	1.4	157
4	Rapid and stable determination of rotation matrices between spherical harmonics by direct recursion. Journal of Chemical Physics, 1999, 111, 8825-8831.	3.0	146
5	<i>In Vivo</i> Activation of Duocarmycin Antibody Conjugates by Near-Infrared Light. ACS Central Science, 2017, 3, 329-337.	11.3	125
6	Reactive species involved in the regioselective photooxidation of heptamethine cyanines. Chemical Science, 2015, 6, 6556-6563.	7.4	112
7	Rotation Matrices for Real Spherical Harmonics. Direct Determination by Recursion. The Journal of Physical Chemistry, 1996, 100, 6342-6347.	2.9	104
8	Direct configuration interaction and multiconfigurational self-consistent-field method for multiple active spaces with variable occupations. II. Application to oxoMn(salen) and N2O4. Journal of Chemical Physics, 2003, 119, 9377-9385.	3.0	87
9	Covalent bonds are created by the drive of electron waves to lower their kinetic energy through expansion. Journal of Chemical Physics, 2014, 140, 204104.	3.0	77
10	Split-localized orbitals can yield stronger configuration interaction convergence than natural orbitals. Journal of Chemical Physics, 2003, 119, 8217-8224.	3.0	66
11	Targeted multicolor in vivo imaging over 1,000 nm enabled by nonamethine cyanines. Nature Methods, 2022, 19, 353-358.	19.0	65
12	Impact of Cyanine Conformational Restraint in the Near-Infrared Range. Journal of Organic Chemistry, 2020, 85, 5907-5915.	3.2	60
13	Solvent-Induced Shifts in Electronic Spectra of Uracil. Journal of Physical Chemistry A, 2011, 115, 4574-4582.	2.5	54
14	Violation of the weak noncrossing rule between totally symmetric closed-shell states in the valence-isoelectronic series O3, S3, SO2, and S2O. Journal of Chemical Physics, 1997, 107, 4307-4317.	3.0	51
15	Intrinsic local constituents of molecular electronic wave functions. I. Exact representation of the density matrix in terms of chemically deformed and oriented atomic minimal basis set orbitals. Theoretical Chemistry Accounts, 2008, 120, 281-294.	1.4	44
16	Core remodeling leads to long wavelength fluoro-coumarins. Chemical Science, 2020, 11, 7302-7307.	7.4	38
17	Deadwood in configuration spaces. II. Singles + doubles and singles + doubles + triples + quadruples spaces. Theoretical Chemistry Accounts, 2002, 107, 220-228.	1.4	33
18	Intrinsic local constituents of molecular electronic wave functions. II. Electronic structure analyses in terms of intrinsic oriented quasi-atomic molecular orbitals for the molecules FOOH, H2BH2BH2, H2CO and the isomerization HNO \leftrightarrow NOH. Theoretical Chemistry Accounts, 2008, 120, 295-305.	1.4	23

#	ARTICLE	IF	CITATIONS
19	Ketone Incorporation Extends the Emission Properties of the Xanthene Scaffold Beyond 1000 nm. <i>Photochemistry and Photobiology</i> , 2022, 98, 325-333.	2.5	18
20	A systematic multireference perturbation-theory study of the low-lying states of SiC ₃ . <i>Journal of Chemical Physics</i> , 2006, 124, 034303.	3.0	17
21	High-level theoretical study of the NO dimer and tetramer: Has the tetramer been observed?. <i>Journal of Chemical Physics</i> , 2012, 137, 214316.	3.0	15
22	The transition from the open minimum to the ring minimum on the ground state and on the lowest excited state of like symmetry in ozone: A configuration interaction study. <i>Journal of Chemical Physics</i> , 2016, 144, 104304.	3.0	13
23	Protonation-Dependent Sequencing of 5-Formylcytidine in RNA. <i>Biochemistry</i> , 2022, 61, 535-544.	2.5	10
24	Hybrid Correlation Energy (HyCE): An Approach Based on Separate Evaluations of Internal and External Components. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5223-5237.	2.5	3
25	Repurposing the Pummerer Rearrangement: Determination of Methionine Sulfoxides in Peptides. <i>ChemBioChem</i> , 2020, 21, 508-516.	2.6	2