

Alberto Baiardi

List of Publications by Year in Descending Order

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Version: 2024-04-28

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

45
papers

1,341
citations

18
h-index

36
g-index

47
ext. papers

1,661
ext. citations

5.1
avg. IF

5.28
L-index

#	Paper	IF	Citations
45	Quantum Proton Effects from Density Matrix Renormalization Group Calculations.. <i>Journal of Chemical Theory and Computation</i> , 2022 ,	6.4	2
44	Expansive Quantum Mechanical Exploration of Chemical Reaction Paths.. <i>Accounts of Chemical Research</i> , 2021 ,	24.3	5
43	Excited-State DMRG Made Simple with FEAST.. <i>Journal of Chemical Theory and Computation</i> , 2021 ,	6.4	2
42	Simplified State Interaction for Matrix Product State Wave Functions. <i>Journal of Chemical Theory and Computation</i> , 2021 ,	6.4	1
41	Electron Dynamics with the Time-Dependent Density Matrix Renormalization Group. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3320-3334	6.4	6
40	Nuclear-electronic all-particle density matrix renormalization group. <i>Journal of Chemical Physics</i> , 2020 , 152, 204103	3.9	8
39	Hardware efficient quantum algorithms for vibrational structure calculations. <i>Chemical Science</i> , 2020 , 11, 6842-6855	9.4	19
38	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020 , 152, 214117	3.9	106
37	The density matrix renormalization group in chemistry and molecular physics: Recent developments and new challenges. <i>Journal of Chemical Physics</i> , 2020 , 152, 040903	3.9	71
36	Interplay of Stereoelectronic and Vibrational Modulation Effects in Tuning the UPS Spectra of Unsaturated Hydrocarbon Cage Compounds. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5218-5226 ¹	6.4	1
35	Transcorrelated density matrix renormalization group. <i>Journal of Chemical Physics</i> , 2020 , 153, 164115	3.9	9
34	Theory meets experiment for unravelling the C1s X-ray photoelectron spectra of pyridine, 2-fluoropyridine, and 2,6-difluoropyridine. <i>Journal of Chemical Physics</i> , 2019 , 151, 124105	3.9	3
33	Large-Scale Quantum Dynamics with Matrix Product States. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3481-3498	6.4	39
32	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. <i>Journal of Chemical Physics</i> , 2019 , 150, 094113	3.9	20
31	Approximate Analytical Gradients and Nonadiabatic Couplings for the State-Average Density Matrix Renormalization Group Self-Consistent-Field Method. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6724-6737	6.4	10
30	Computational simulation of vibrationally resolved spectra for spin-forbidden transitions. <i>Chirality</i> , 2018 , 30, 850-865	2.1	11
29	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6370-6390	6.4	20

28	A combined theoretical and experimental study of the ionic states of iodopentafluorobenzene. <i>Journal of Chemical Physics</i> , 2017 , 146, 084302	3.9	3
27	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2804-2822	6.4	28
26	A combined theoretical and experimental study of the valence and Rydberg states of iodopentafluorobenzene. <i>Journal of Chemical Physics</i> , 2017 , 146, 174301	3.9	5
25	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2789-2803	6.4	18
24	Assessment of Electron Propagator Methods for the Simulation of Vibrationally Resolved Valence and Core Photoionization Spectra. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3120-3135	6.4	8
23	Theoretical and experimental investigation of UV-vis absorption spectrum in a Eu(3+) based complex for luminescent downshifting applications. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	1
22	The ionic states of difluoromethane: A reappraisal of the low energy photoelectron spectrum including ab initio configuration interaction computations. <i>Journal of Chemical Physics</i> , 2017 , 147, 074305	3.9	3
21	Spectroscopic Characterization of Key Aromatic Molecules: A Route toward The Origin of Life. <i>Astronomical Journal</i> , 2017 , 154,	4.9	9
20	Understanding the interplay between the solvent and nuclear rearrangements in the negative solvatochromism of a push-pull flexible quinolinium cation. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 32544-32555	3.6	7
19	Vibrational Density Matrix Renormalization Group. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3764-3777	6.4	31
18	Aiming at an accurate prediction of vibrational and electronic spectra for medium-to-large molecules: An overview. <i>International Journal of Quantum Chemistry</i> , 2016 , 116, 1543-1574	2.1	132
17	Temperature Dependence of Radiative and Nonradiative Rates from Time-Dependent Correlation Function Methods. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 774-86	6.4	26
16	Combined theoretical and experimental study of the valence, Rydberg, and ionic states of chlorobenzene. <i>Journal of Chemical Physics</i> , 2016 , 144, 124302	3.9	7
15	Combined theoretical and experimental study of the valence, Rydberg and ionic states of fluorobenzene. <i>Journal of Chemical Physics</i> , 2016 , 144, 204305	3.9	12
14	General formulation of vibronic spectroscopy in internal coordinates. <i>Journal of Chemical Physics</i> , 2016 , 144, 084114	3.9	47
13	Vibronic Effects on Rates of Excitation Energy Transfer and Their Temperature Dependence. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2357-65	6.4	9
12	Accurate Simulation of Resonance-Raman Spectra of Flexible Molecules: An Internal Coordinates Approach. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3267-80	6.4	43
11	The ionic states of iodobenzene studied by photoionization and ab initio configuration interaction and DFT computations. <i>Journal of Chemical Physics</i> , 2015 , 142, 134301	3.9	16

10	Virtual Eyes Designed for Quantitative Spectroscopy of Inorganic Complexes: Vibronic Signatures in the Phosphorescence Spectra of Terpyridine Derivatives. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 7253-7	3.4	15
9	Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMS-Draw tool. <i>Journal of Computational Chemistry</i> , 2015 , 36, 321-34	3.5	73
8	Vibrationally resolved NEXAFS at C and N K-edges of pyridine, 2-fluoropyridine and 2,6-difluoropyridine: A combined experimental and theoretical assessment. <i>Journal of Chemical Physics</i> , 2015 , 143, 204102	3.9	14
7	Interpretation of the photoelectron, ultraviolet, and vacuum ultraviolet photoabsorption spectra of bromobenzene by ab initio configuration interaction and DFT computations. <i>Journal of Chemical Physics</i> , 2015 , 143, 164303	3.9	15
6	Interpretation of the vacuum ultraviolet photoabsorption spectrum of iodobenzene by ab initio computations. <i>Journal of Chemical Physics</i> , 2015 , 142, 134302	3.9	37
5	New developments of a multifrequency virtual spectrometer: stereo-electronic, dynamical, and environmental effects on chiroptical spectra. <i>Chirality</i> , 2014 , 26, 588-600	2.1	30
4	Accurate yet feasible computations of resonance Raman spectra for metal complexes in solution: [Ru(bpy) ₃](2+) as a case study. <i>Dalton Transactions</i> , 2014 , 43, 17610-4	4.3	15
3	A general time-dependent route to resonance-Raman spectroscopy including Franck-Condon, Herzberg-Teller and Duschinsky effects. <i>Journal of Chemical Physics</i> , 2014 , 141, 114108	3.9	45
2	General Time Dependent Approach to Vibronic Spectroscopy Including Franck-Condon, Herzberg-Teller, and Duschinsky Effects. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4097-115 ^{6.4}		235
1	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12404-22	3.6	122