Alberto Baiardi

List of Publications by Year
in descending order

46 papers	1,996 citations	361388 20 h-index	243610 44 g-index
47 all docs	47 docs citations	47 times ranked	1897 citing authors

#	Article	IF	Citations
1	General Time Dependent Approach to Vibronic Spectroscopy Including Franckâ€“Condon, Herzbergâ€“Teller, and Duschinsky Effects. Journal of Chemical Theory and Computation, 2013, 9, 4097-4115.	5.3	314
2	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
3	Aiming at an accurate prediction of vibrational and electronic spectra for mediumâ€toâ€large molecules: An overview. International Journal of Quantum Chemistry, 2016, 116, 1543-1574.	2.0	161
4	The density matrix renormalization group in chemistry and molecular physics: Recent developments and new challenges. Journal of Chemical Physics, 2020, 152, 040903.	3.0	152
5	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. Physical Chemistry Chemical Physics, 2012, 14, 12404.	2.8	128
6	Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMSâ€Draw tool. Journal of Computational Chemistry, 2015, 36, 321-334.	3.3	84
7	Large-Scale Quantum Dynamics with Matrix Product States. Journal of Chemical Theory and Computation, 2019, 15, 3481-3498.	5.3	66
8	General formulation of vibronic spectroscopy in internal coordinates. Journal of Chemical Physics, 2016, 144, 084114.	3.0	62
9	A general time-dependent route to Resonance-Raman spectroscopy including Franck-Condon, Herzberg-Teller and Duschinsky effects. Journal of Chemical Physics, 2014, 141, 114108.	3.0	52
10	Interpretation of the vacuum ultraviolet photoabsorption spectrum of iodobenzene by ab initio computations. Journal of Chemical Physics, 2015, 142, 134302.	3.0	51
11	Accurate Simulation of Resonance-Raman Spectra of Flexible Molecules: An Internal Coordinates Approach. Journal of Chemical Theory and Computation, 2015, 11, 3267-3280.	5.3	50
12	Hardware efficient quantum algorithms for vibrational structure calculations. Chemical Science, 2020, 11, 6842-6855.	7.4	50
13	Vibrational Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 3764-3777.	5.3	46
14	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. Journal of Chemical Theory and Computation, 2017, 13, 2804-2822.	5.3	40
15	Temperature Dependence of Radiative and Nonradiative Rates from Time-Dependent Correlation Function Methods. Journal of Chemical Theory and Computation, 2016, 12, 774-786.	5.3	37
16	New Developments of a Multifrequency Virtual Spectrometer: Stereoâ€Electronic, Dynamical, and Environmental Effects on Chiroptical Spectra. Chirality, 2014, 26, 588-600.	2.6	35
17	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 094113.	3.0	29
18	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 6370-6390.	5.3	26

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19	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. Journal of Chemical Theory and Computation, 2017, 13, 2789-2803.	5.3	23
20	Transcorrelated density matrix renormalization group. Journal of Chemical Physics, 2020, 153, 164115.	3.0	23
21	Interpretation of the photoelectron, ultraviolet, and vacuum ultraviolet photoabsorption spectra of bromobenzene by ab initio configuration interaction and DFT computations. Journal of Chemical Physics, 2015, 143, 164303.	3.0	19
22	Accurate yet feasible computations of resonance Raman spectra for metal complexes in solution: [Ru(bpy)₃]²⁺ as a case study. Dalton Transactions, 2014, 43, 17610-17614.	3.3	18
23	The ionic states of iodobenzene studied by photoionization and ab initio configuration interaction and DFT computations. Journal of Chemical Physics, 2015, 142, 134301.	3.0	18
24	Vibrationally resolved NEXAFS at C and N K-edges of pyridine, 2-fluoropyridine and 2,6-difluoropyridine: A combined experimental and theoretical assessment. Journal of Chemical Physics, 2015, 143, 204102.	3.0	17
25	Virtual Eyes Designed for Quantitative Spectroscopy of Inorganic Complexes: Vibronic Signatures in the Phosphorescence Spectra of Terpyridine Derivatives. Journal of Physical Chemistry B, 2015, 119, 7253-7257.	2.6	17
26	Approximate Analytical Gradients and Nonadiabatic Couplings for the State-Average Density Matrix Renormalization Group Self-Consistent-Field Method. Journal of Chemical Theory and Computation, 2019, 15, 6724-6737.	5.3	17
27	Nuclear-electronic all-particle density matrix renormalization group. Journal of Chemical Physics, 2020, 152, 204103.	3.0	16
28	Combined theoretical and experimental study of the valence, Rydberg and ionic states of fluorobenzene. Journal of Chemical Physics, 2016, 144, 204305.	3.0	15
29	Computational simulation of vibrationally resolved spectra for spinâ€forbidden transitions. Chirality, 2018, 30, 850-865.	2.6	15
30	Electron Dynamics with the Time-Dependent Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2021, 17, 3320-3334.	5.3	14
31	Expansive Quantum Mechanical Exploration of Chemical Reaction Paths. Accounts of Chemical Research, 2022, 55, 35-43.	15.6	14
32	Excited-State DMRG Made Simple with FEAST. Journal of Chemical Theory and Computation, 2022, 18, 415-430.	5.3	13
33	Spectroscopic Characterization of Key Aromatic and Heterocyclic Molecules: A Route toward the Origin of Life. Astronomical Journal, 2017, 154, 82.	4.7	12
34	Combined theoretical and experimental study of the valence, Rydberg, and ionic states of chlorobenzene. Journal of Chemical Physics, 2016, 144, 124302.	3.0	11
35	Assessment of Electron Propagator Methods for the Simulation of Vibrationally Resolved Valence and Core Photoionization Spectra. Journal of Chemical Theory and Computation, 2017, 13, 3120-3135.	5.3	10
36	Quantum Proton Effects from Density Matrix Renormalization Group Calculations. Journal of Chemical Theory and Computation, 2022, 18, 234-250.	5.3	10

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37	Vibronic Effects on Rates of Excitation Energy Transfer and Their Temperature Dependence. Journal of Chemical Theory and Computation, 2016, 12, 2357-2365.	5.3	9
38	Explicitly Correlated Electronic Structure Calculations with Transcorrelated Matrix Product Operators. Journal of Chemical Theory and Computation, 2022, 18, 4203-4217.	5.3	9
39	Understanding the interplay between the solvent and nuclear rearrangements in the negative solvatochromism of a pushâ€“pull flexible quinolinium cation. Physical Chemistry Chemical Physics, 2017, 19, 32544-32555.	2.8	7
40	A combined theoretical and experimental study of the valence and Rydberg states of iodopentafluorobenzene. Journal of Chemical Physics, 2017, 146, 174301.	3.0	6
41	Theory meets experiment for unravelling the C1s X-ray photoelectron spectra of pyridine, 2-fluoropyridine, and 2,6-difluoropyridine. Journal of Chemical Physics, 2019, 151, 124105.	3.0	6
42	Simplified State Interaction for Matrix Product State Wave Functions. Journal of Chemical Theory and Computation, 2021, 17, 7477-7485.	5.3	4
43	A combined theoretical and experimental study of the ionic states of iodopentafluorobenzene. Journal of Chemical Physics, 2017, 146, 084302.	3.0	3
44	The ionic states of difluoromethane: A reappraisal of the low energy photoelectron spectrum including ab initio configuration interaction computations. Journal of Chemical Physics, 2017, 147, 074305.	3.0	3
45	Theoretical and experimental investigation of UVâ€“Vis absorption spectrum in a Eu(3+) based complex for luminescent downshifting applications. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	1
46	Interplay of Stereoelectronic and Vibrational Modulation Effects in Tuning the UPS Spectra of Unsaturated Hydrocarbon Cage Compounds. Journal of Chemical Theory and Computation, 2020, 16, 5218-5226.	5.3	1