Alberto Baiardi

List of Publications by Citations

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	General Time Dependent Approach to Vibronic Spectroscopy Including Franck-Condon, Herzberg-Teller, and Duschinsky Effects. *Journal of Chemical Theory and Computation*, **2013**, 9, 4097-115	6.4	235
44	Aiming at an accurate prediction of vibrational and electronic spectra for medium-to-large molecules: An overview. *International Journal of Quantum Chemistry*, **2016**, 116, 1543-1574	2.1	132
43	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. *Physical Chemistry Chemical Physics*, **2012**, 14, 12404-22	3.6	122
42	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
41	Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMS-Draw tool. *Journal of Computational Chemistry*, **2015**, 36, 321-34	3.5	73
40	The density matrix renormalization group in chemistry and molecular physics: Recent developments and new challenges. *Journal of Chemical Physics*, **2020**, 152, 040903	3.9	71
39	General formulation of vibronic spectroscopy in internal coordinates. *Journal of Chemical Physics*, **2016**, 144, 084114	3.9	47
38	A general time-dependent route to resonance-Raman spectroscopy including Franck-Condon, Herzberg-Teller and Duschinsky effects. *Journal of Chemical Physics*, **2014**, 141, 114108	3.9	45
37	Accurate Simulation of Resonance-Raman Spectra of Flexible Molecules: An Internal Coordinates Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 3267-80	6.4	43
36	Large-Scale Quantum Dynamics with Matrix Product States. *Journal of Chemical Theory and Computation*, **2019**, 15, 3481-3498	6.4	39
35	Interpretation of the vacuum ultraviolet photoabsorption spectrum of iodobenzene by ab initio computations. *Journal of Chemical Physics*, **2015**, 142, 134302	3.9	37
34	Vibrational Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 3764-3777	6.4	31
33	New developments of a multifrequency virtual spectrometer: stereo-electronic, dynamical, and environmental effects on chiroptical spectra. *Chirality*, **2014**, 26, 588-600	2.1	30
32	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 2804-2822	6.4	28
31	Temperature Dependence of Radiative and Nonradiative Rates from Time-Dependent Correlation Function Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 774-86	6.4	26
30	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 094113	3.9	20
29	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. *Journal of Chemical Theory and Computation*, **2018**, 14, 6370-6390	6.4	20

28	Hardware efficient quantum algorithms for vibrational structure calculations. *Chemical Science*, **2020**, 11, 6842-6855	9.4	19
27	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. *Journal of Chemical Theory and Computation*, **2017**, 13, 2789-2803	6.4	18
26	The ionic states of iodobenzene studied by photoionization and ab initio configuration interaction and DFT computations. *Journal of Chemical Physics*, **2015**, 142, 134301	3.9	16
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, 7253-7	3.4	15
24	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, 17610-4	4.3	15
23	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	3.9	15
22	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	3.9	14
21	Combined theoretical and experimental study of the valence, Rydberg and ionic states of fluorobenzene. *Journal of Chemical Physics*, **2016**, 144, 204305	3.9	12
20	Computational simulation of vibrationally resolved spectra for spin-forbidden transitions. *Chirality*, **2018**, 30, 850-865	2.1	11
19	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	6.4	10
18	Spectroscopic Characterization of Key Aromatic Molecules: A Route toward The Origin of Life. *Astronomical Journal*, **2017**, 154,	4.9	9
17	Transcorrelated density matrix renormalization group. *Journal of Chemical Physics*, **2020**, 153, 164115	3.9	9
16	Vibronic Effects on Rates of Excitation Energy Transfer and Their Temperature Dependence. *Journal of Chemical Theory and Computation*, **2016**, 12, 2357-65	6.4	9
15	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	6.4	8
14	Nuclear-electronic all-particle density matrix renormalization group. *Journal of Chemical Physics*, **2020**, 152, 204103	3.9	8
13	Understanding the interplay between the solvent and nuclear rearrangements in the negative solvatochromism of a push-pull flexible quinolinium cation. *Physical Chemistry Chemical Physics*, **2017**, 19, 32544-32555	3.6	7
12	Combined theoretical and experimental study of the valence, Rydberg, and ionic states of chlorobenzene. *Journal of Chemical Physics*, **2016**, 144, 124302	3.9	7
11	Electron Dynamics with the Time-Dependent Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2021**, 17, 3320-3334	6.4	6

10	A combined theoretical and experimental study of the valence and Rydberg states of iodopentafluorobenzene. *Journal of Chemical Physics*, **2017**, 146, 174301	3.9	5
9	Expansive Quantum Mechanical Exploration of Chemical Reaction Paths.. *Accounts of Chemical Research*, **2021**,	24.3	5
8	A combined theoretical and experimental study of the ionic states of iodopentafluorobenzene. *Journal of Chemical Physics*, **2017**, 146, 084302	3.9	3
7	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	3.9	3
6	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	3.9	3
5	Excited-State DMRG Made Simple with FEAST.. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
4	Quantum Proton Effects from Density Matrix Renormalization Group Calculations.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
3	Theoretical and experimental investigation of UV□Vis absorption spectrum in a Eu(3+) based complex for luminescent downshifting applications. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	1
2	Simplified State Interaction for Matrix Product State Wave Functions. *Journal of Chemical Theory and Computation*, **2021**,	6.4	1
1	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	6.4	1