Julien Bloino

List of Publications by Year
in descending order

97 papers	6,815 citations	76031 42 h-index	68831 81 g-index
102 all docs	102 docs citations	102 times ranked	4543 citing authors

#	Article	IF	Citations
1	Accurate Quantum Chemical Spectroscopic Characterization of Glycolic Acid: A Route Toward its Astrophysical Detection. Journal of Physical Chemistry A, 2022, 126, 2373-2387.	1.1	16
2	Modulation of Ï€ character upon complexation captured by molecular rotation spectra. Physical Chemistry Chemical Physics, 2022, , .	1.3	0
3	Accounting for molecular flexibility in photoionization: case of tert-butyl hydroperoxide. Physical Chemistry Chemical Physics, 2022, 24, 10826-10837.	1.3	3
4	Unusual binary aggregates of perylene bisimide revealed by their electronic transitions in helium nanodroplets and DFT calculations. Physical Chemistry Chemical Physics, 2021, 23, 13862-13872.	1.3	1
5	Unraveling the internal conversion process within the Q-bands of a chlorophyll-like-system through surface-hopping molecular dynamics simulations. Journal of Chemical Physics, 2021, 154, 094110.	1.2	8
6	Accuracy and Reliability in the Simulation of Vibrational Spectra: A Comprehensive Benchmark of Energies and Intensities Issuing From Generalized Vibrational Perturbation Theory to Second Order (GVPT2). Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	32
7	Interplay of stereo-electronic, vibronic and environmental effects in tuning the chiroptical properties of an Ir(III) cyclometalated N-heterocyclic carbene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 254, 119631.	2.0	4
8	General Perturb-Then-Diagonalize Model for the Vibrational Frequencies and Intensities of Molecules Belonging to Abelian and Non-Abelian Symmetry Groups. Journal of Chemical Theory and Computation, 2021, 17, 4332-4358.	2.3	15
9	Theoretical Investigation of the Circularly Polarized Luminescence of a Chiral Boron Dipyrromethene (BODIPY) Dye. Frontiers in Chemistry, 2020, 8, 801.	1.8	10
10	The Italian National Project of Astrobiologyâ€"Life in Spaceâ€"Origin, Presence, Persistence of Life in Space, from Molecules to Extremophiles. Astrobiology, 2020, 20, 580-582.	1.5	10
11	Toward Fully Unsupervised Anharmonic Computations Complementing Experiment for Robust and Reliable Assignment and Interpretation of IR and VCD Spectra from Mid-IR to NIR: The Case of 2,3-Butanediol and trans-1,2-Cyclohexanediol. Journal of Physical Chemistry A, 2020, 124, 1011-1024.	1.1	26
12	Role of specific soluteâ€"solvent interactions on the photophysical properties of distyryl substituted BODIPY derivatives. Physical Chemistry Chemical Physics, 2020, 22, 10981-10994.	1.3	13
13	State-of-the-art computation of the rotational and IR spectra of the methyl-cyclopropyl cation: hints on its detection in space. Physical Chemistry Chemical Physics, 2019, 21, 3431-3439.	1.3	17
14	On the simulation of vibrationally resolved electronic spectra of medium-size molecules: the case of styryl substituted BODIPYs. Physical Chemistry Chemical Physics, 2019, 21, 3512-3526.	1.3	28
15	Vibrational circular dichroism under the quantum magnifying glass: from the electronic flow to the spectroscopic observable. Physical Chemistry Chemical Physics, 2019, 21, 4224-4239.	1.3	13
16	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. Chemical Reviews, 2019, 119, 8131-8191.	23.0	167
17	The vibrational CD spectra of propylene oxide in liquid xenon: a proof-of-principle CryoVCD study that challenges theory. Physical Chemistry Chemical Physics, 2019, 21, 6582-6587.	1.3	18
18	Ferrocenes with simple chiral substituents: an in-depth theoretical and experimental VCD and ECD study. Physical Chemistry Chemical Physics, 2019, 21, 9419-9432.	1.3	19

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19	Computational simulation of vibrationally resolved spectra for spinâ€forbidden transitions. Chirality, 2018, 30, 850-865.	1.3	15
20	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. Astrophysical Journal, 2018, 855, 123.	1.6	35
21	Computational challenges in Astrochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1349.	6.2	43
22	Cover Image, Volume 8, Issue 3. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1368.	6.2	1
23	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 6370-6390.	2.3	26
24	Accurate rest frequencies for propargylamine in the ground and low-lying vibrational states. Astronomy and Astrophysics, 2018, 615, A176.	2.1	10
25	Accurate Vibrationalâ€“Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study. Journal of Physical Chemistry A, 2017, 121, 3305-3317.	1.1	18
26	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. Journal of Chemical Theory and Computation, 2017, 13, 2804-2822.	2.3	40
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.	2.3	23
28	Spectroscopic Characterization of Key Aromatic and Heterocyclic Molecules: A Route toward the Origin of Life. Astronomical Journal, 2017, 154, 82.	1.9	12
29	General formulation of vibronic spectroscopy in internal coordinates. Journal of Chemical Physics, 2016, 144, 084114.	1.2	62
30	Vibronic Effects on Rates of Excitation Energy Transfer and Their Temperature Dependence. Journal of Chemical Theory and Computation, 2016, 12, 2357-2365.	2.3	9
31	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.	1.0	161
32	Temperature Dependence of Radiative and Nonradiative Rates from Time-Dependent Correlation Function Methods. Journal of Chemical Theory and Computation, 2016, 12, 774-786.	2.3	37
33	Reliable vibrational wavenumbers for Cî€O and Nâ€“H stretchings of isolated and hydrogen-bonded nucleic acid bases. Physical Chemistry Chemical Physics, 2016, 18, 8479-8490.	1.3	47
34	Vibronic Coupling Investigation to Compute Phosphorescence Spectra of Pt(II) Complexes. Inorganic Chemistry, 2015, 54, 5588-5595.	1.9	34
35	Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism, and Raman Optical Activity. Journal of Physical Chemistry A, 2015, 119, 11862-11874.	1.1	101
36	Accurate Simulation of Resonance-Raman Spectra of Flexible Molecules: An Internal Coordinates Approach. Journal of Chemical Theory and Computation, 2015, 11, 3267-3280.	2.3	50

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37	Generalized vibrational perturbation theory for rotovibrational energies of linear, symmetric and asymmetric tops: Theory, approximations, and automated approaches to deal with mediumâ€toâ€large molecular systems. International Journal of Quantum Chemistry, 2015, 115, 948-982.	1.0	95
38	Benchmarking TD-DFT against Vibrationally Resolved Absorption Spectra at Room Temperature: 7-Aminocoumarins as Test Cases. Journal of Chemical Theory and Computation, 2015, 11, 5371-5384.	2.3	68
39	CC/DFT Route toward Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as a Case Study. Journal of Chemical Theory and Computation, 2015, 11, 4342-4363.	2.3	75
40	Toward the design of alkynylimidazole fluorophores: computational and experimental characterization of spectroscopic features in solution and in poly(methyl methacrylate). Physical Chemistry Chemical Physics, 2015, 17, 26710-26723.	1.3	13
41	A VPT2 Route to Near-Infrared Spectroscopy: The Role of Mechanical and Electrical Anharmonicity. Journal of Physical Chemistry A, 2015, 119, 5269-5287.	1.1	90
42	A general time-dependent route to Resonance-Raman spectroscopy including Franck-Condon, Herzberg-Teller and Duschinsky effects. Journal of Chemical Physics, 2014, 141, 114108.	1.2	52
43	Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane. Journal of Chemical Physics, 2014, 141, 034107.	1.2	57
44	A Multifrequency Virtual Spectrometer for Complex Bioâ€Organic Systems: Vibronic and Environmental Effects on the UV/Vis Spectrum of Chlorophyll a. ChemPhysChem, 2014, 15, 3355-3364.	1.0	31
45	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF OXIRANE: A VALUABLE ROUTE TO ITS IDENTIFICATION IN TITAN'S ATMOSPHERE AND THE ASSIGNMENT OF UNIDENTIFIED INFRARED BANDS. Astrophysical Journal, 2014, 785, 107.	1.6	47
46	Synthesis and Optical Properties of Imidazoleâ€Based Fluorophores having High Quantum Yields. ChemPlusChem, 2014, 79, 366-370.	1.3	13
47	Stereoelectronic, Vibrational, and Environmental Contributions to Polarizabilities of Large Molecular Systems: A Feasible Anharmonic Protocol. Journal of Chemical Theory and Computation, 2014, 10, 2456-2464.	2.3	35
48	Environmental and complexation effects on the structures and spectroscopic signatures of organic pigments relevant to cultural heritage: the case of alizarin and alizarinâ€“Mg(ii)/Al(iii) complexes. Physical Chemistry Chemical Physics, 2014, 16, 2897.	1.3	32
49	A Robust and Effective Time-Independent Route to the Calculation of Resonance Raman Spectra of Large Molecules in Condensed Phases with the Inclusion of Duschinsky, Herzbergâ€“Teller, Anharmonic, and Environmental Effects. Journal of Chemical Theory and Computation, 2014, 10, 346-363.	2.3	71
50	Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation. Physical Chemistry Chemical Physics, 2014, 16, 1759-1787.	1.3	363
51	New Developments of a Multifrequency Virtual Spectrometer: Stereoâ€Electronic, Dynamical, and Environmental Effects on Chiroptical Spectra. Chirality, 2014, 26, 588-600.	1.3	35
52	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.	1.6	18
53	Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test cases. Computational and Theoretical Chemistry, 2014, 1037, 35-48.	1.1	21
54	Reprint of â€œEnvironmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test casesâ€• Computational and Theoretical Chemistry, 2014, 1040-1041, 144-157.	1.1	1

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55	ANHARMONIC VIBRATIONAL SPECTROSCOPY ON METAL TRANSITION COMPLEXES. , 2014, , .		0
56	ACCURATE ANHARMONIC IR SPECTRA FROM INTEGRATED CC/DFT APPROACH. , 2014, , .		0
57	SIMULATION OF ACCURATE VIBRATIONALLY RESOLVED ELECTRONIC SPECTRA: THE INTEGRATED TIME-DEPENDENT AND TIME-INDEPENDENT FRAMEWORK. , 2014, , .		0
58	ANHARMONIC IR SPECTRA OF BIOMOLECULES: NUCLEOBASES AND THEIR OLIGOMERS. , 2014, , .		0
59	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.	2.3	314
60	Development of a Virtual Spectrometer for Chiroptical Spectroscopies: The Case of Nicotine. Chirality, 2013, 25, 701-708.	1.3	22
61	Anharmonicity Effects in the Vibrational CD Spectra of Propylene Oxide. Journal of Physical Chemistry Letters, 2013, 4, 3424-3428.	2.1	46
62	Glycine conformers: a never-ending story?. Physical Chemistry Chemical Physics, 2013, 15, 1358-1363.	1.3	81
63	Characterization of the Elusive Conformers of Glycine from State-of-the-Art Structural, Thermodynamic, and Spectroscopic Computations: Theory Complements Experiment. Journal of Chemical Theory and Computation, 2013, 9, 1533-1547.	2.3	72
64	Tuning of NMR and EPR parameters by vibrational averaging and environmental effects: an integrated computational approach. Molecular Physics, 2013, 111, 1345-1354.	0.8	12
65	Accurate structure, thermodynamic and spectroscopic parameters from CC and CC/DFT schemes: the challenge of the conformational equilibrium in glycine. Physical Chemistry Chemical Physics, 2013, 15, 10094.	1.3	117
66	Circular Dichroism and Optical Rotation of Lactamide and 2-Aminopropanol in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 5136-5147.	1.2	16
67	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. Journal of Chemical Physics, 2013, 139, 164302.	1.2	36
68	Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical. Journal of Chemical Physics, 2013, 138, 234303.	1.2	28
69	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Highlights in Theoretical Chemistry, 2013, , 319-337.	0.0	0
70	Toward Ab Initio Anharmonic Vibrational Circular Dichroism Spectra in the Condensed Phase. Journal of Physical Chemistry Letters, 2012, 3, 1766-1773.	2.1	50
71	Toward an Accurate Modeling of Optical Rotation for Solvated Systems: Anharmonic Vibrational Contributions Coupled to the Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2012, 8, 585-597.	2.3	46
72	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. Physical Chemistry Chemical Physics, 2012, 14, 12404.	1.3	128

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73	A second-order perturbation theory route to vibrational averages and transition properties of molecules: General formulation and application to infrared and vibrational circular dichroism spectroscopies. Journal of Chemical Physics, 2012, 136, 124108.	1.2	311
74	Role of Hostâ€“Guest Interactions in Tuning the Optical Properties of Coumarin Derivatives Incorporated in MCM-41: A TD-DFT Investigation. Journal of Physical Chemistry C, 2012, 116, 17807-17818.	1.5	47
75	General Perturbative Approach for Spectroscopy, Thermodynamics, and Kinetics: Methodological Background and Benchmark Studies. Journal of Chemical Theory and Computation, 2012, 8, 1015-1036.	2.3	256
76	Toward anharmonic computations of vibrational spectra for large molecular systems. International Journal of Quantum Chemistry, 2012, 112, 2185-2200.	1.0	101
77	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	64
78	Fully ab initio IR spectra for complex molecular systems from perturbative vibrational approaches: Glycine as a test case. Journal of Molecular Structure, 2012, 1009, 74-82.	1.8	48
79	Reliable structural, thermodynamic, and spectroscopic properties of organic molecules adsorbed on silicon surfaces from computational modeling: the case of glycine@Si(100). Physical Chemistry Chemical Physics, 2011, 13, 16713.	1.3	37
80	Noncovalent Interactions in the Gas Phase: The Anisoleâ€“Phenol Complex. Journal of Physical Chemistry A, 2011, 115, 9603-9611.	1.1	38
81	Multipolar symmetric squaraines with large two-photon absorption cross-sections in the NIR region. Physical Chemistry Chemical Physics, 2011, 13, 12087.	1.3	26
82	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. Physical Chemistry Chemical Physics, 2011, 13, 2160-2166.	1.3	57
83	Towards an accurate description of anharmonic infrared spectra in solution within the polarizable continuum model: Reaction field, cavity field and nonequilibrium effects. Journal of Chemical Physics, 2011, 135, 104505.	1.2	48
84	A fully automated implementation of VPT2 Infrared intensities. Chemical Physics Letters, 2010, 496, 157-161.	1.2	140
85	Absorption and emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study. Physical Chemistry Chemical Physics, 2010, 12, 1000-1006.	1.3	67
86	General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra. Journal of Chemical Theory and Computation, 2010, 6, 1256-1274.	2.3	253
87	Harmonic and Anharmonic Vibrational Frequency Calculations with the Double-Hybrid B2PLYP Method: Analytic Second Derivatives and Benchmark Studies. Journal of Chemical Theory and Computation, 2010, 6, 2115-2125.	2.3	274
88	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. Physical Chemistry Chemical Physics, 2010, 12, 10550.	1.3	43
89	Validation of the DFT/N07D computational model on the magnetic, vibrational and electronic properties of vinyl radical. Physical Chemistry Chemical Physics, 2010, 12, 1092-1101.	1.3	69
90	Integrated experimental and computational spectroscopy study on Ï€-stacking interaction: the anisole dimer. Physical Chemistry Chemical Physics, 2010, 12, 13547.	1.3	24

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91	The Gas Phase Anisole Dimer: A Combined High-Resolution Spectroscopy and Computational Study of a Stacked Molecular System. Journal of Physical Chemistry A, 2009, 113, 14343-14351.	1.1	52
92	First principle simulation of vibrationally resolved <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si127.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi>A</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m accent="true"><mml:mrow><mml:mtext>X</mml:mtext></mml:mrow><mml:mrow><mml:mo>Ëœ</mml:mo></mm. Chemical Physics Letters, 2009, 471, 143-147.	1.2	27
93	Fully Integrated Approach to Compute Vibrationally Resolved Optical Spectra: From Small Molecules to Macrosystems. Journal of Chemical Theory and Computation, 2009, 5, 540-554.	2.3	406
94	Integrated computational approach to vibrationally resolved electronic spectra: Anisole as a test case. Journal of Chemical Physics, 2008, 128, 244105.	1.2	117
95	Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzbergâ€“Teller effect: The Qx band of porphyrin as a case study. Journal of Chemical Physics, 2008, 128, 224311.	1.2	523
96	Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. Journal of Chemical Physics, 2007, 126, 084509.	1.2	445
97	Ultraviolet resonance Raman spectroscopy of anthracene: Experiment and theory. Journal of Raman Spectroscopy, 0, , .	1.2	5