Julien Bloino

List of Publications by Year
in descending order

97 papers	6,815 citations	66336 42 h-index	60616 81 g-index
102 all docs	102 docs citations	102 times ranked	4090 citing authors

#	Article	IF	Citations
1	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.	3.0	523
2	Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. Journal of Chemical Physics, 2007, 126, 084509.	3.0	445
3	Fully Integrated Approach to Compute Vibrationally Resolved Optical Spectra: From Small Molecules to Macrosystems. Journal of Chemical Theory and Computation, 2009, 5, 540-554.	5.3	406
4	Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation. Physical Chemistry Chemical Physics, 2014, 16, 1759-1787.	2.8	363
5	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
6	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.	3.0	311
7	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.	5.3	274
8	General Perturbative Approach for Spectroscopy, Thermodynamics, and Kinetics: Methodological Background and Benchmark Studies. Journal of Chemical Theory and Computation, 2012, 8, 1015-1036.	5.3	256
9	General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra. Journal of Chemical Theory and Computation, 2010, 6, 1256-1274.	5.3	253
10	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. Chemical Reviews, 2019, 119, 8131-8191.	47.7	167
11	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
12	A fully automated implementation of VPT2 Infrared intensities. Chemical Physics Letters, 2010, 496, 157-161.	2.6	140
13	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
14	Integrated computational approach to vibrationally resolved electronic spectra: Anisole as a test case. Journal of Chemical Physics, 2008, 128, 244105.	3.0	117
15	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.	2.8	117
16	Toward anharmonic computations of vibrational spectra for large molecular systems. International Journal of Quantum Chemistry, 2012, 112, 2185-2200.	2.0	101
17	Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism, and Raman Optical Activity. Journal of Physical Chemistry A, 2015, 119, 11862-11874.	2.5	101
18	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.	2.0	95

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19	A VPT2 Route to Near-Infrared Spectroscopy: The Role of Mechanical and Electrical Anharmonicity. Journal of Physical Chemistry A, 2015, 119, 5269-5287.	2.5	90
20	Glycine conformers: a never-ending story?. Physical Chemistry Chemical Physics, 2013, 15, 1358-1363.	2.8	81
21	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.	5.3	75
22	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.	5.3	72
23	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.	5.3	71
24	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.	2.8	69
25	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.	5.3	68
26	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.	2.8	67
27	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.	1.4	64
28	General formulation of vibronic spectroscopy in internal coordinates. Journal of Chemical Physics, 2016, 144, 084114.	3.0	62
29	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. Physical Chemistry Chemical Physics, 2011, 13, 2160-2166.	2.8	57
30	Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane. Journal of Chemical Physics, 2014, 141, 034107.	3.0	57
31	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.	2.5	52
32	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
33	Toward Ab Initio Anharmonic Vibrational Circular Dichroism Spectra in the Condensed Phase. Journal of Physical Chemistry Letters, 2012, 3, 1766-1773.	4.6	50
34	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
35	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.	3.0	48
36	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.	3.6	48

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37	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.	3.1	47
38	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.	4.5	47
39	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.	2.8	47
40	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.	5.3	46
41	Anharmonicity Effects in the Vibrational CD Spectra of Propylene Oxide. Journal of Physical Chemistry Letters, 2013, 4, 3424-3428.	4.6	46
42	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. Physical Chemistry Chemical Physics, 2010, 12, 10550.	2.8	43
43	Computational challenges in Astrochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1349.	14.6	43
44	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. Journal of Chemical Theory and Computation, 2017, 13, 2804-2822.	5.3	40
45	Noncovalent Interactions in the Gas Phase: The Anisoleâ€“Phenol Complex. Journal of Physical Chemistry A, 2011, 115, 9603-9611.	2.5	38
46	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.	2.8	37
47	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
48	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. Journal of Chemical Physics, 2013, 139, 164302.	3.0	36
49	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.	5.3	35
50	New Developments of a Multifrequency Virtual Spectrometer: Stereoâ€Electronic, Dynamical, and Environmental Effects on Chiroptical Spectra. Chirality, 2014, 26, 588-600.	2.6	35
51	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. Astrophysical Journal, 2018, 855, 123.	4.5	35
52	Vibronic Coupling Investigation to Compute Phosphorescence Spectra of Pt(II) Complexes. Inorganic Chemistry, 2015, 54, 5588-5595.	4.0	34
53	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.	2.8	32
54	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, .	2.8	32

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55	A Multifrequency Virtual Spectrometer for Complex Bioâ€Organic Systems: Vibronic and Environmental Effects on the UV/Vis Spectrum of Chlorophyll <i>a</i>. ChemPhysChem, 2014, 15, 3355-3364.	2.1	31
56	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.	3.0	28
57	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.	2.8	28
58	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.	2.6	27
59	Multipolar symmetric squaraines with large two-photon absorption cross-sections in the NIR region. Physical Chemistry Chemical Physics, 2011, 13, 12087.	2.8	26
60	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 6370-6390.	5.3	26
61	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 <i>trans</i>-1,2-Cyclohexanediol. Journal of Physical Chemistry A, 2020, 124, 1011-1024.	2.5	26
62	Integrated experimental and computational spectroscopy study on Ï€-stacking interaction: the anisole dimer. Physical Chemistry Chemical Physics, 2010, 12, 13547.	2.8	24
63	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
64	Development of a Virtual Spectrometer for Chiroptical Spectroscopies: The Case of Nicotine. Chirality, 2013, 25, 701-708.	2.6	22
65	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.	2.5	21
66	Ferrocenes with simple chiral substituents: an in-depth theoretical and experimental VCD and ECD study. Physical Chemistry Chemical Physics, 2019, 21, 9419-9432.	2.8	19
67	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
68	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.	2.5	18
69	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.	2.8	18
70	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.	2.8	17
71	Circular Dichroism and Optical Rotation of Lactamide and 2-Aminopropanol in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 5136-5147.	2.6	16
72	Accurate Quantum Chemical Spectroscopic Characterization of Glycolic Acid: A Route Toward its Astrophysical Detection. Journal of Physical Chemistry A, 2022, 126, 2373-2387.	2.5	16

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73	Computational simulation of vibrationally resolved spectra for spinâ€forbidden transitions. Chirality, 2018, 30, 850-865.	2.6	15
74	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.	5.3	15
75	Synthesis and Optical Properties of Imidazoleâ€Based Fluorophores having High Quantum Yields. ChemPlusChem, 2014, 79, 366-370.	2.8	13
76	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.	2.8	13
77	Vibrational circular dichroism under the quantum magnifying glass: from the electronic flow to the spectroscopic observable. Physical Chemistry Chemical Physics, 2019, 21, 4224-4239.	2.8	13
78	Role of specific soluteâ€“solvent interactions on the photophysical properties of distyryl substituted BODIPY derivatives. Physical Chemistry Chemical Physics, 2020, 22, 10981-10994.	2.8	13
79	Tuning of NMR and EPR parameters by vibrational averaging and environmental effects: an integrated computational approach. Molecular Physics, 2013, 111, 1345-1354.	1.7	12
80	Spectroscopic Characterization of Key Aromatic and Heterocyclic Molecules: A Route toward the Origin of Life. Astronomical Journal, 2017, 154, 82.	4.7	12
81	Accurate rest frequencies for propargylamine in the ground and low-lying vibrational states. Astronomy and Astrophysics, 2018, 615, A176.	5.1	10
82	Theoretical Investigation of the Circularly Polarized Luminescence of a Chiral Boron Dipyrromethene (BODIPY) Dye. Frontiers in Chemistry, 2020, 8, 801.	3.6	10
83	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.	3.0	10
84	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
85	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.	3.0	8
86	Ultraviolet resonance Raman spectroscopy of anthracene: Experiment and theory. Journal of Raman Spectroscopy, 0, , .	2.5	5
87	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.	3.9	4
88	Accounting for molecular flexibility in photoionization: case of tert-butyl hydroperoxide. Physical Chemistry Chemical Physics, 2022, 24, 10826-10837.	2.8	3
89	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.	2.5	1
90	Cover Image, Volume 8, Issue 3. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1368.	14.6	1

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91	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.	2.8	1
92	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
93	ANHARMONIC VIBRATIONAL SPECTROSCOPY ON METAL TRANSITION COMPLEXES. , 2014, , .		0
94	ACCURATE ANHARMONIC IR SPECTRA FROM INTEGRATED CC/DFT APPROACH. , 2014, , .		0
95	SIMULATION OF ACCURATE VIBRATIONALLY RESOLVED ELECTRONIC SPECTRA: THE INTEGRATED TIME-DEPENDENT AND TIME-INDEPENDENT FRAMEWORK. , 2014, , .		0
96	ANHARMONIC IR SPECTRA OF BIOMOLECULES: NUCLEOBASES AND THEIR OLIGOMERS. , 2014, , .		0
97	Modulation of Ï€ character upon complexation captured by molecular rotation spectra. Physical Chemistry Chemical Physics, 2022, , .	2.8	0