Fabrizio Santoro

List of Publications by Year
in descending order

152	7,725	57719	58549
papers	citations	44 h-index	82 g-index

162	162	162	4723
all docs	docs citations	times ranked	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.	1.2	523
2	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
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.	2.3	406
4	Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases. Chemical Reviews, 2016, 116, 3540-3593.	23.0	375
5	Effective method to compute vibrationally resolved optical spectra of large molecules at finite temperature in the gas phase and in solution. Journal of Chemical Physics, 2007, 126, 184102.	1.2	303
6	Tracking the excited-state time evolution of the visual pigment with multiconfigurational quantum chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7764-7769.	3.3	266
7	General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra. Journal of Chemical Theory and Computation, 2010, 6, 1256-1274.	2.3	253
8	Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation. Journal of Chemical Theory and Computation, 2013, 9, 2072-2082.	2.3	194
9	Comparison of vertical and adiabatic harmonic approaches for the calculation of the vibrational structure of electronic spectra. Physical Chemistry Chemical Physics, 2012, 14, 13549.	1.3	189
10	Going beyond the vertical approximation with timeâ€dependent density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 460-486.	6.2	174
11	Ab Initio Calculations of Absorption Spectra of Large Molecules in Solution: Coumarin C153. Angewandte Chemie - International Edition, 2007, 46, 405-408.	7.2	164
12	Solvent Effect on the Singlet Excited-State Lifetimes of Nucleic Acid Bases:Â A Computational Study of 5-Fluorouracil and Uracil in Acetonitrile and Water. Journal of the American Chemical Society, 2006, 128, 16312-16322.	6.6	149
13	Influence of base stacking on excited-state behavior of polyadenine in water, based on time-dependent density functional calculations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9931-9936.	3.3	124
14	Excited States Decay of the Aâ^'T DNA: A PCM/TD-DFT Study in Aqueous Solution of the (9-Methyl-adenine)2Â·(1-methyl-thymine)2 Stacked Tetramer. Journal of the American Chemical Society, 2009, 131, 15232-15245.	6.6	101
15	Excited-State Behavior of trans and cis Isomers of Stilbene and Stiff Stilbene:Â A TD-DFT Study. Journal of Physical Chemistry A, 2005, 109, 10058-10067.	1.1	97
16	An artificial molecular switch that mimics the visual pigment and completes its photocycle in picoseconds. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 17642-17647.	3.3	89
17	Computing the inhomogeneous broadening of electronic transitions in solution: a first-principle quantum mechanical approach. Physical Chemistry Chemical Physics, 2011, 13, 17007.	1.3	89
18	First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogenous broadening. Computational and Theoretical Chemistry, 2014, 1040-1041, 328-337.	1.1	88

#	Article	IF	Citations
19	Chirality Amplified: Long, Discrete Helicene Nanoribbons. Journal of the American Chemical Society, 2021, 143, 983-991.	6.6	85
20	Vibronically Resolved Electronic Circular Dichroism Spectra of (R)-(+)-3-Methylcyclopentanone: A Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 12401-12411.	1.1	78
21	Effective Time-Independent Calculations of Vibrational Resonance Raman Spectra of Isolated and Solvated Molecules Including Duschinsky and Herzbergâ€“Teller Effects. Journal of Chemical Theory and Computation, 2011, 7, 1824-1839.	2.3	77
22	Vibronic coupling in electronic transitions with significant Duschinsky effect. International Journal of Quantum Chemistry, 1997, 63, 233-244.	1.0	71
23	Amplification of Chirality in Monodisperse, Enantiopure Alleneâ€Acetylenic Oligomers. Angewandte Chemie - International Edition, 2010, 49, 2247-2250.	7.2	71
24	Twoâ€Photon Absorption Circular Dichroism: A New Twist in Nonlinear Spectroscopy. Chemistry - A European Journal, 2010, 16, 3504-3509.	1.7	69
25	The Decay from the Dark nÏ€* Excited State in Uracil: An Integrated CASPT2/CASSCF and PCM/TD-DFT Study in the Gas Phase and in Water. Journal of Physical Chemistry B, 2008, 112, 10769-10772.	1.2	67
26	Computational approach to the study of the lineshape of absorption and electronic circular dichroism spectra. International Journal of Quantum Chemistry, 2010, 110, 476-486.	1.0	67
27	Quantum Dynamics of the Ultrafast Ï€Ï€*/nÏ€* Population Transfer in Uracil and 5-Fluoro-Uracil in Water and Acetonitrile. Journal of Physical Chemistry B, 2009, 113, 14491-14503.	1.2	66
28	Vibrationally Resolved Absorption and Emission Spectra of Dithiophene in the Gas Phase and in Solution by First-Principle Quantum Mechanical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4483-4493.	2.3	66
29	Modeling Solvent Broadening on the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models. Journal of Chemical Theory and Computation, 2015, 11, 5810-5825.	2.3	66
30	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
31	Harmonic Models in Cartesian and Internal Coordinates to Simulate the Absorption Spectra of Carotenoids at Finite Temperatures. Journal of Chemical Theory and Computation, 2013, 9, 4947-4958.	2.3	62
32	Duschinsky, Herzbergâ€“Teller, and Multiple Electronic Resonance Interferential Effects in Resonance Raman Spectra and Excitation Profiles. The Case of Pyrene. Journal of Chemical Theory and Computation, 2013, 9, 3597-3611.	2.3	60
33	Can TDâ€DFT calculations accurately describe the excited states behavior of stacked nucleobases? The cytosine dimer as a test case. Journal of Computational Chemistry, 2008, 29, 957-964.	1.5	59
34	Vibronic Coupling Explains the Different Shape of Electronic Circular Dichroism and of Circularly Polarized Luminescence Spectra of Hexahelicenes. Journal of Chemical Theory and Computation, 2016, 12, 2799-2819.	2.3	59
35	Accurate Steady-State and Zero-Time Fluorescence Spectra of Large Molecules in Solution by a First-Principle Computational Method. Journal of Physical Chemistry B, 2007, 111, 14080-14082.	1.2	58
36	Vibronic Model for the Quantum Dynamical Study of the Competition between Bright and Charge-Transfer Excited States in Single-Strand Polynucleotides: The Adenine Dimer Case. Journal of Physical Chemistry A, 2009, 113, 15346-15354.	1.1	56

#	Article	IF	Citations
37	Enantiomerically Pure Alenoâ€“Acetylenic Macrocycles: Synthesis, Solidâ€State Structures, Chiroptical Properties, and Electron Localization Function Analysis. Chemistry - A European Journal, 2010, 16, 9796-9807.	1.7	51
38	A Tiny Excited-State Barrier Can Induce a Multiexponential Decay of the Retinal Chromophore: A Quantum Dynamics Investigation. Angewandte Chemie - International Edition, 2005, 44, 5118-5121.	7.2	50
39	Absorption and Emission Spectral Shapes of a Prototype Dye in Water by Combining Classical/Dynamical and Quantum/Static Approaches. Journal of Physical Chemistry A, 2015, 119, 5426-5438.	1.1	50
40	Adiabatic-Molecular Dynamics Generalized Vertical Hessian Approach: A Mixed Quantum Classical Method To Compute Electronic Spectra of Flexible Molecules in the Condensed Phase. Journal of Chemical Theory and Computation, 2020, 16, 1215-1231.	2.3	50
41	Theory for Vibrationally Resolved Two-Photon Circular Dichroism Spectra. Application to (R)-(+)-3-Methylcyclopentanone. Journal of Physical Chemistry A, 2009, 113, 4198-4207.	1.1	49
42	Vibronically-induced change in the chiral response of molecules revealed by electronic circular dichroism spectroscopy. Chemical Physics Letters, 2008, 464, 144-149.	1.2	47
43	The excited electronic states of adenine-guanine stacked dimers in aqueous solution: a PCM/TD-DFT study. Physical Chemistry Chemical Physics, 2010, 12, 4934.	1.3	46
44	Hierarchical transformation of Hamiltonians with linear and quadratic couplings for nonadiabatic quantum dynamics: Application to the Ï€Ï€*/nÏ€* internal conversion in thymine. Journal of Chemical Physics, 2012, 136, 244104.	1.2	44
45	The Interplay between Ï€Ï€*/nÏ€* Excited States in Gasâ€Phase Thymine: A Quantum Dynamical Study. ChemPhysChem, 2011, 12, 1957-1968.	1.0	43
46	Trajectory-Surface-Hopping Study of the Rennerâˆ’Teller Effect in the N(2D) + H2 Reaction. Journal of Physical Chemistry A, 2002, 106, 8276-8284.	1.1	42
47	A Theoretical Study on the Factors Influencing Cyanine Photoisomerization:Â The Case of Thiacyanine in Gas Phase and in Methanol. Journal of Chemical Theory and Computation, 2005, 1, 215-229.	2.3	42
48	Quantum-classical effective-modes dynamics of the Ï€Ï€* â†’ nÏ€* decay in 9H-adenine. A quadratic vibronic coupling model. Faraday Discussions, 2013, 163, 223.	1.6	42
49	Nonadiabatic wave packet dynamics of NO2 on the XÌƒâ€Š2Aâ€²/Ãƒâ€Š2Aâ€² conical intersection. Journal of Chemical Physics, 1999, 110, 4419-4427.	1.2	41
50	Time dependent DFT investigation on the two lowest 1Bu states of the trans isomer of stilbene and stiff-stilbenes. Chemical Physics Letters, 2004, 387, 509-516.	1.2	41
51	Revisiting Vertical Models To Simulate the Line Shape of Electronic Spectra Adopting Cartesian and Internal Coordinates. Journal of Chemical Theory and Computation, 2016, 12, 4970-4985.	2.3	41
52	Absorption Spectrum of Aâ€“T DNA Unraveled by Quantum Mechanical Calculations in Solution on the (dA)₂â‹…(dT)₂ Tetramer. ChemPhysChem, 2008, 9, 2531-2537.	1.0	39
53	Chemical Selectivity through Control of Excitedâ€State Dynamics. Angewandte Chemie - International Edition, 2008, 47, 6322-6325.	7.2	39
54	Relative Stability of the L_a and L_b Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra. Journal of Physical Chemistry Letters, 2014, 5, 1806-1811.	2.1	36

#	Article	IF	Citations
55	Vibronic Coupling Dominates the Electronic Circular Dichroism of the Benzene Chromophore ¹L_b band. Journal of Organic Chemistry, 2013, 78, 7398-7405.	1.7	35
56	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. Journal of Chemical Physics, 2020, 152, 054107.	1.2	35
57	Ultrafast Dynamics of the Two Lowest Bright Excited States of Cytosine and 1-Methylcytosine: A Quantum Dynamical Study. Journal of Chemical Theory and Computation, 2020, 16, 5792-5808.	2.3	34
58	Ab Initio Prediction of the Emission Color in Phosphorescent Iridium(III) Complexes for OLEDs. Journal of Physical Chemistry B, 2008, 112, 13181-13183.	1.2	32
59	Barrierless photoisomerisation of the â€œsimplest cyanineâ€: Joining computational and femtosecond optical spectroscopies to trace the full reaction path. Physical Chemistry Chemical Physics, 2012, 14, 13350.	1.3	32
60	A simple dimeric model accounts for the vibronic ECD spectra of chiral polythiophenes in their aggregated states. RSC Advances, 2016, 6, 37938-37943.	1.7	31
61	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The <i>Ï€Ï€<</i>*/nÏ€* Decay of Thymine in Water as a Test Case. Journal of Chemical Theory and Computation, 2018, 14, 820-832.	2.3	31
62	Computational Challenges in Simulating and Analyzing Experimental Linear and Nonlinear Circular Dichroism Spectra.R-(+)-1,1â€²-Bis(2-naphthol) as a Prototype Case. Journal of Physical Chemistry B, 2011, 115, 811-824.	1.2	29
63	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. Journal of Chemical Physics, 2017, 147, 164116.	1.2	29
64	Femtosecond photoelectron spectroscopy of trans-stilbene above the reaction barrier. Chemical Physics, 2005, 310, 201-211.	0.9	28
65	Femtosecond study on the isomerization dynamics of NK88. I. Ground-state dynamics after photoexcitation. Journal of Chemical Physics, 2006, 125, 044512.	1.2	28
66	Femtosecond study on the isomerization dynamics of NK88. II. Excited-state dynamics. Journal of Chemical Physics, 2006, 125, 044513.	1.2	28
67	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. Physical Chemistry Chemical Physics, 2015, 17, 11401-11411.	1.3	28
68	On the controversial nature of the 1â€‰B1u and 2â€‰B1u states of trans-stilbene: The n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2009, 130, 174307.	1.2	27
69	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part II: Solution Phase. ChemPhysChem, 2014, 15, 3246-3257.	1.0	27
70	Optical Properties of Diarylethenes with TD-DFT: 0â€“0 Energies, Fluorescence, Stokes Shifts, and Vibronic Shapes. Journal of Chemical Theory and Computation, 2014, 10, 3944-3957.	2.3	26
71	The excited state behavior of cytosine in the gas phase: A TD-DFT study. Computational and Theoretical Chemistry, 2014, 1040-1041, 186-194.	1.1	25
72	Quantumâ€Classical Calculation of the Absorption and Emission Spectral Shapes of Oligothiophenes at Low and Room Temperature by Firstâ€Principle Calculations. ChemPhysChem, 2014, 15, 3320-3333.	1.0	25

#	Article	IF	Citations
73	Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
74	Unveiling Excited-State Chirality of Binaphthols by Femtosecond Circular Dichroism and Quantum Chemical Calculations. Journal of Physical Chemistry Letters, 2019, 10, 4089-4094.	2.1	25
75	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. Journal of Chemical Physics, 2019, 151, 064107.	1.2	24
76	UV Absorption and Magnetic Circular Dichroism Spectra of Purine, Adenine, and Guanine: A Coupled Cluster Study in Vacuo and in Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1242-1254.	2.3	24
77	Electronic Circular Dichroism in Exciton-Coupled Dimers: Vibronic Spectra from a General All-Coordinates Quantum-Dynamical Approach. Journal of Physical Chemistry A, 2013, 117, 3355-3368.	1.1	23
78	Nonadiabatic Absorption Spectra and Ultrafast Dynamics of DNA and RNA Photoexcited Nucleobases. Molecules, 2021, 26, 1743.	1.7	23
79	Differences in Twoâ€Photon and Oneâ€Photon Absorption Profiles Induced by Vibronic Coupling: The Case of Dioxaborine Heterocyclic Dye. ChemPhysChem, 2011, 12, 3392-3403.	1.0	22
80	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. Physical Chemistry Chemical Physics, 2021, 23, 8181-8199.	1.3	22
81	Intermolecular exciton coupling and vibronic effects in solid-state circular dichroism: a case study. Physical Chemistry Chemical Physics, 2013, 15, 795-802.	1.3	21
82	TD-DFT Investigation of the Magnetic Circular Dichroism Spectra of Some Purine and Pyrimidine Bases of Nucleic Acids. Journal of Physical Chemistry A, 2015, 119, 5476-5489.	1.1	21
83	Vibronic Spectra of Ï€-Conjugated Systems with a Multitude of Coupled States: A Protocol Based on Linear Vibronic Coupling Models and Quantum Dynamics Tested on Hexahelicene. Journal of Chemical Theory and Computation, 2021, 17, 1691-1700.	2.3	21
84	Parameterization of a linear vibronic coupling model with multiconfigurational electronic structure methods to study the quantum dynamics of photoexcited pyrene. Journal of Chemical Physics, 2021, 154, 104106.	1.2	20
85	Twoâ€photon absorption circularâ€linear dichroism on axial enantiomers. Chirality, 2010, 22, E202-10.	1.3	19
86	First Principles Studies of the Vibrationally Resolved Magnetic Circular Dichroism Spectra of Biphenylene. Journal of Chemical Theory and Computation, 2013, 9, 1557-1567.	2.3	19
87	Quantum-Classical Calculation of Vibronic Spectra along a Reaction Path: The Case of the ECD of Easily Interconvertible Conformers with Opposite Chiral Responses. Journal of Physical Chemistry Letters, 2016, 7, 4891-4897.	2.1	19
88	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. Chemical Physics, 2018, 515, 452-463.	0.9	19
89	Excitonic Model for Strongly Coupled Multichromophoric Systems: The Electronic Circular Dichroism Spectra of Guanine Quadruplexes as Test Cases. Journal of Chemical Theory and Computation, 2021, 17, 405-415.	2.3	19
90	Nucleic Acids as a Playground for the Computational Study of the Photophysics and Photochemistry of Multichromophore Assemblies. Accounts of Chemical Research, 2022, 55, 2077-2087.	7.6	19

#	Article	IF	Citations
91	Ab initio study of NO2. VII. Ãƒâ€˜2B2â†Xìƒâ€˜2A1 nonadiabatic Franckâ€“Condon absorption spectrum. Chemical Physics, 1997, 225, 55-62.	0.9	18
92	Three-dimensional diabatic models for the Ï€Ï€*Âå†' nï€* excited-state decay of uracil derivatives in solution. Theoretical Chemistry Accounts, 2009, 123, 273-286.	0.5	18
93	Combination of Transient 2D-IR Experiments and Ab Initio Computations Sheds Light on the Formation of the Charge-Transfer State in Photoexcited Carbonyl Carotenoids. Journal of Physical Chemistry B, 2014, 118, 9613-9630.	1.2	17
94	Distinct Helical Molecular Orbitals through Conformational Lock**. Chemistry - A European Journal, 2020, 26, 17342-17349.	1.7	17
95	Accounting for Vibronic Features through a Mixed Quantum-Classical Scheme: Structure, Dynamics, and Absorption Spectra of a Perylene Diimide Dye in Solution. Journal of Chemical Theory and Computation, 2020, 16, 7061-7077.	2.3	17
96	Origin of Chiroptic Amplification in Perylene-Diimide Helicenes. Journal of Physical Chemistry C, 2021, 125, 2554-2564.	1.5	17
97	Fragment Diabatization Linear Vibronic Coupling Model for Quantum Dynamics of Multichromophoric Systems: Population of the Charge-Transfer State in the Photoexcited Guanineâ€“Cytosine Pair. Journal of Chemical Theory and Computation, 2021, 17, 4660-4674.	2.3	17
98	Statistical analysis of the computed Xìƒâ€‰2A1/Ãƒâ€‰2B2 spectrum of NO2: Some insights into the causes of its irregularity. Journal of Chemical Physics, 1998, 109, 1824-1832.	1.2	16
99	The interplay between neutral exciton and charge transfer states in single-strand polyadenine: a quantum dynamical investigation. Photochemical and Photobiological Sciences, 2013, 12, 1527.	1.6	16
100	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part I: Gas Phase. ChemPhysChem, 2014, 15, 3236-3245.	1.0	16
101	Time- and frequency-resolved spontaneous emission: Theory and application to the NO2 Xìƒâ€Š2Aâ€²/Ãƒâ€Š2Aâ€² conical intersection. Journal of Chemical Physics, 2000, 113, 4073-4082.	1.2	15
102	Combined use of three forms of chiroptical spectroscopies in the study of the absolute configuration and conformational properties of 3-phenylcyclopentanone, 3-phenylcyclohexanone, and 3-phenylcycloheptanone. Tetrahedron, 2013, 69, 10752-10762.	1.0	15
103	A Combined Experimentalâ€“Computational Investigation to Uncover the Puzzling (Chiroâ€)optical Response of Pyridocyclophanes: Oneâ€•and Twoâ€Photon Spectra. Chemistry - A European Journal, 2015, 21, 12136-12147.	1.7	15
104	Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution. Photochemical and Photobiological Sciences, 2017, 16, 1415-1423.	1.6	15
105	Excited-State Absorption of Uracil in the Gas Phase: Mapping the Main Decay Paths by Different Electronic Structure Methods. Journal of Chemical Theory and Computation, 2021, 17, 1638-1652.	2.3	15
106	Complex excited dynamics around a plateau on a retinal-like potential surface: chaos, multi-exponential decays and quantum/classical differences. Theoretical Chemistry Accounts, 2007, 117, 1061-1072.	0.5	14
107	Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. Physical Chemistry Chemical Physics, 2016, 18, 22889-22905.	1.3	14
108	Timeâ€dependent and timeâ€independent approaches for the computation of absorption spectra of Uracil derivatives in solution. International Journal of Quantum Chemistry, 2010, 110, 624-636.	1.0	13

#	Article	IF	Citations
109	Ultrafast resonance energy transfer in the umbelliferoneâ€“alizarin bichromophore. Physical Chemistry Chemical Physics, 2014, 16, 10059-10074.	1.3	12
110	A computational study of the vibronic effects on the electronic spectra and the photophysics of aza[7]helicene. Physical Chemistry Chemical Physics, 2021, 23, 16551-16563.	1.3	12
111	How the Interplay among Conformational Disorder, Solvation, Local, and Charge-Transfer Excitations Affects the Absorption Spectrum and Photoinduced Dynamics of Perylene Diimide Dimers: A Molecular Dynamics/Quantum Vibronic Approach. Journal of Chemical Theory and Computation, 2022, 18, 3718-3736.	2.3	12
112	Nonadiabatic radiative lifetimes and fluorescence spectra of NO2. Journal of Chemical Physics, 1999, 111, 9651-9657.	1.2	11
113	Quantum and semiclassical dynamics of the Franckâ€“Condon wave packet on the coupled potential surfaces of the conical intersection. Chemical Physics, 2000, 259, 193-200.	0.9	11
114	Comparison of the results of a mean-field mixed quantum/classical method with full quantum predictions for nonadiabatic dynamics: application to the $$pi pi ^*/npi ^*$$ Ï€ Ï€ â^— / n Ï€ â^— decay of thymine. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	11
115	Controlling Photochemistry via Isotopomers and IR Pre-excitation. Journal of the American Chemical Society, 2018, 140, 926-931.	6.6	11
116	Highâ€Resolution Absorption and Electronic Circular Dichroism Spectra of (R)â€(+)â€1â€Phenylethanol. Confident Interpretation Based on the Synergy between Experiments and Computations. ChemPhysChem, 2018, 19, 715-723.	1.0	11
117	Quantum dynamics of the Ï€Ï€*/nÏ€* decay of the epigenetic nucleobase 1,5-dimethyl-cytosine in the gas phase. Physical Chemistry Chemical Physics, 2020, 22, 26525-26535.	1.3	11
118	Excited state properties of sizable molecules in solution: from structure to reactivity. Theoretical Chemistry Accounts, 2007, 117, 1073-1084.	0.5	10
119	In Vivo Absorption Spectra of the Two Stable States of the Euglena Photoreceptor Photocycle. Photochemistry and Photobiology, 2009, 85, 304-312.	1.3	10
120	Vibrationally resolved circular dichroism spectra of a molecule with isotopically engendered chirality. Physical Chemistry Chemical Physics, 2012, 14, 3669.	1.3	10
121	Excitation Dynamics in Heteroâ€bichromophoric Calixarene Systems. ChemPhysChem, 2016, 17, 1686-1706.	1.0	10
122	Toward a general mixed quantum/classical method for the calculation of the vibronic ECD of a flexible dye molecule with different stable conformers: Revisiting the case of 2,2,2â€trifluoroâ€anthrylethanol. Chirality, 2018, 30, 730-743.	1.3	10
123	A computational study of the vibrationally-resolved electronic circular dichroism spectra of single-chain transoid and cisoid oligothiophenes in chiral conformations. Physical Chemistry Chemical Physics, 2018, 20, 21864-21880.	1.3	10
124	The role of intramolecular charge transfer and symmetry breaking in the photophysics of pyrrolo[3,2-b]pyrrole-dione. Physical Chemistry Chemical Physics, 2018, 20, 22260-22271.	1.3	9
125	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. ChemPhotoChem, 2019, 3, 846-855.	1.5	9
126	A Fermi Golden Rule, Liouville-space approach to the study of intramolecular electron transfer rate in solution. Journal of Chemical Physics, 1997, 106, 94-108.	1.2	8

#	Article	IF	Citations
127	The Intriguing Case of the Oneâ€Photon and Twoâ€Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Waveâ€Function Methods. ChemPhotoChem, 2019, 3, 778-793.	1.5	8
128	On the energy dependence of the hyperfine interaction in excited states of NO2. Journal of Chemical Physics, 2001, 115, 8868-8875.	1.2	7
129	UV-vis spectra of p-benzoquinone anion radical in solution by a TD-DFT/PCM approach. Theoretical Chemistry Accounts, 2007, 118, 143-148.	0.5	7
130	Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
131	The shape of the electronic circular dichroism spectrum of (2,6-dimethylphenyl)(phenyl)methanol: interplay between conformational equilibria and vibronic effects. Physical Chemistry Chemical Physics, 2017, 19, 32349-32360.	1.3	7
132	Excited state absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study. Physical Chemistry Chemical Physics, 2022, 24, 4987-5000.	1.3	7
133	Analysis of the Electronic Circular Dichroism Spectrum of (âˆ')â€“[9](2,5)Pyridinophane. Chirality, 2012, 24, 994-1004.	1.3	6
134	On the geometry of 3-amino-sydnones. Computational and Theoretical Chemistry, 1998, 433, 291-299.	1.5	5
135	The absorption and emission spectra in solution of oligothiophene-based pushâ€“pull biomarkers: a PCM/TD-DFT vibronic study. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	5
136	The Ultrafast Quantum Dynamics of Photoexcited Adenineâ€“Thymine Basepair Investigated with a Fragment-based Diabatization and a Linear Vibronic Coupling Model. Journal of Physical Chemistry A, 2021, 125, 8912-8924.	1.1	5
137	the <mml:math altimg="si11.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/x	0.4	4
138	Stable laser control of complex multilevel systems using a weak-intensity multicolor gaussian pulse. Chemical Physics, 2002, 277, 297-312.	0.9	4
139	Robust control by a multicolor weak laser pulse of the fluorescence of NO2 from the X2Aâ€²/A2Aâ€² conical intersection. Chemical Physics, 2003, 287, 237-251.	0.9	4
140	Weak-field laser control of systems experiencing dissipation and decoherence. An application to the enhancement of the coherent fluorescence of the B850 ring in light harvesting complexes. Chemical Physics Letters, 2004, 384, 86-93.	1.2	4
141	Effective time-independent studies on resonance Raman spectroscopy of trans-stilbene including the Duschinsky effect. Molecular Physics, 2013, 111, 1511-1525.	0.8	4
142	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanineâ€“Cytosine stacked dimer in water solution. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4
143	Solvent effect on the energetics of proton coupled electron transfer in guanine-cytosine pair in chloroform by mixed explicit and implicit solvation models. Chemical Physics, 2018, 515, 493-501.	0.9	4
144	ON/OFF Spiroconjugation through Peripheral Functionalization: Impact on the Reactivity and Chiroptical Properties of Spirobifluorenes. ChemPlusChem, 2022, 87, e202100554.	1.3	3

#	Article	IF	Citations
145	Towards the Understanding of the Excited State Dynamics of Nucleic Acids: Solvent and Stacking Effect on the Photophysical Behavior of Nucleobases. AIP Conference Proceedings, 2007, , .	0.3	2
146	Chemisorption of silyl radicals onto Pd(100) surface: A computational DFT study. Surface Science, 2007, 601, 255-261.	0.8	2
147	Quantum Dynamics of Ultrafast Photoinduced Processes in Biological Molecules. AIP Conference Proceedings, 2007, , .	0.3	1
148	XËœ 2 Aâ€²/Ãƒ 2 Aâ€² conical intersection effects on the fluorescence of NO 2. Theoretical Chemistry Accounts, 2000, 104, 203-206.	0.5	0
149	Infrared pre-excitation grants isotopomer-specific photochemistry. EPJ Web of Conferences, 2019, 205, 03001.	0.1	0
150	The role of chlorine position in the electronic circular dichroism of chlorophenylâ€ethanol investigated by vibronic calculations. Chirality, 2020, 32, 932-948.	1.3	0
151	A METHOD FOR ROBUST SOLUTIONS IN THE WEAK-INTENSITY LASER CONTROL OF MULTILEVEL SYSTEMS. , 2002, , .		0
152	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