Fabrizio Santoro

List of Publications by Year in Descending Order

153 papers	6,508 citations	42 h-index	76 g-index
162 ext. papers	7,179 ext. citations	5 avg, IF	6.12 L-index

#	Paper	IF	Citations
153	Excited state absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	1
152	ON/OFF Spiroconjugation through Peripheral Functionalization: Impact on the Reactivity and Chiroptical Properties of Spirobifluorenes.. *ChemPlusChem*, **2022**, e202100554	2.8	0
151	The Ultrafast Quantum Dynamics of Photoexcited Adenine-Thymine Basepair Investigated with a Fragment-based Diabatization and a Linear Vibronic Coupling Model. *Journal of Physical Chemistry A*, **2021**, 125, 8912-8924	2.8	1
150	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	6.4	9
149	Chirality Amplified: Long, Discrete Helicene Nanoribbons. *Journal of the American Chemical Society*, **2021**, 143, 983-991	16.4	33
148	Nonadiabatic Absorption Spectra and Ultrafast Dynamics of DNA and RNA Photoexcited Nucleobases. *Molecules*, **2021**, 26,	4.8	8
147	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	3.9	6
146	Fragment Diabatization Linear Vibronic Coupling Model for Quantum Dynamics of Multichromophoric Systems: Population of the Charge-Transfer State in the Photoexcited Guanine-Cytosine Pair. *Journal of Chemical Theory and Computation*, **2021**, 17, 4660-4674	6.4	8
145	Origin of Chiroptic Amplification in Perylene-Diimide Helicenes. *Journal of Physical Chemistry C*, **2021**, 125, 2554-2564	3.8	7
144	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	3.6	5
143	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	6.4	6
142	Vibronic Spectra of □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	6.4	12
141	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. *Physical Chemistry Chemical Physics*, **2021**, 23, 8181-8199	3.6	7
140	The role of chlorine position in the electronic circular dichroism of chlorophenyl-ethanol investigated by vibronic calculations. *Chirality*, **2020**, 32, 932-948	2.1	
139	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	3.9	18
138	Quantum dynamics of the □/n□ decay of the epigenetic nucleobase 1,5-dimethyl-cytosine in the gas phase. *Physical Chemistry Chemical Physics*, **2020**, 22, 26525-26535	3.6	4
137	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	6.4	23

136	Distinct Helical Molecular Orbitals through Conformational Lock*. *Chemistry - A European Journal*, **2020**, 26, 17342-17349	4.8	8
135	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	6.4	17
134	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	6.4	7
133	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. *ChemPhotoChem*, **2019**, 3, 846-855	3.3	6
132	The Intriguing Case of the One-Photon and Two-Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Wave-Function Methods. *ChemPhotoChem*, **2019**, 3, 778-793	3.3	5
131	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	3.9	18
130	Infrared pre-excitation grants isotopomer-specific photochemistry. *EPJ Web of Conferences*, **2019**, 205, 03001	0.3	
129	Unveiling Excited-State Chirality of Binaphthols by Femtosecond Circular Dichroism and Quantum Chemical Calculations. *Journal of Physical Chemistry Letters*, **2019**, 10, 4089-4094	6.4	14
128	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	6.4	16
127	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 ^*) decay of thymine. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
126	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 2,2,2-trifluoro-anthrylethanol. *Chirality*, **2018**, 30, 730-743	2.1	7
125	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	3.6	9
124	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	2.3	2
123	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. *Chemical Physics*, **2018**, 515, 452-463	2.3	15
122	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	3.6	5
121	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The □/n□ Decay of Thymine in Water as a Test Case. *Journal of Chemical Theory and Computation* , **2018**, 14, 820-832	6.4	20
120	Controlling Photochemistry via Isotopomers and IR Pre-excitation. *Journal of the American Chemical Society*, **2018**, 140, 926-931	16.4	6
119	High-Resolution Absorption and Electronic Circular Dichroism Spectra of (R)-(+)-1-Phenylethanol. Confident Interpretation Based on the Synergy between Experiments and Computations. *ChemPhysChem*, **2018**, 19, 715-723	3.2	8

118	Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution. *Photochemical and Photobiological Sciences*, **2017**, 16, 1415-1423	4.2	10
117	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	3.6	6
116	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. *Journal of Chemical Physics*, **2017**, 147, 164116	3.9	17
115	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanine□Cytosine stacked dimer in water solution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
114	Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. *Physical Chemistry Chemical Physics*, **2016**, 18, 22889-905	3.6	13
113	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	6.4	15
112	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	1.9	7
111	The absorption and emission spectra in solution of oligothiophene-based push□pull biomarkers: a PCM/TD-DFT vibronic study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	5
110	Going beyond the vertical approximation with time-dependent density functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 460-486	7.9	137
109	Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases. *Chemical Reviews*, **2016**, 116, 3540-93	68.1	291
108	Excitation Dynamics in Hetero-bichromophoric Calixarene Systems. *ChemPhysChem*, **2016**, 17, 1686-706	3.2	10
107	A simple dimeric model accounts for the vibronic ECD spectra of chiral polythiophenes in their aggregated states. *RSC Advances*, **2016**, 6, 37938-37943	3.7	24
106	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	1.9	18
105	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, 2799-819	6.4	40
104	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	6.4	26
103	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. *Physical Chemistry Chemical Physics*, **2015**, 17, 11401-11	3.6	25
102	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, 5426-38	2.8	45
101	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, 5810-25	6.4	54

100	A Combined Experimental-Computational Investigation to Uncover the Puzzling (Chiro-)optical Response of Pyridocyclophanes: One- and Two-Photon Spectra. *Chemistry - A European Journal*, **2015**, 21, 12136-47	4.8	13
99	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, 5476-89	2.8	18
98	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	2	77
97	The excited state behavior of cytosine in the gas phase: A TD-DFT study. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 186-194	2	24
96	Optical Properties of Diarylethenes with TD-DFT: 0-0 Energies, Fluorescence, Stokes Shifts, and Vibronic Shapes. *Journal of Chemical Theory and Computation*, **2014**, 10, 3944-57	6.4	22
95	Ultrafast resonance energy transfer in the umbelliferone-alizarin bichromophore. *Physical Chemistry Chemical Physics*, **2014**, 16, 10059-74	3.6	8
94	Relative Stability of the La and Lb Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra. *Journal of Physical Chemistry Letters*, **2014**, 5, 1806-11	6.4	34
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, 9613-30	3.4	15
92	Quantum-classical calculation of the absorption and emission spectral shapes of oligothiophenes at low and room temperature by first-principle calculations. *ChemPhysChem*, **2014**, 15, 3320-33	3.2	22
91	The lineshape of the electronic spectrum of the green fluorescent protein chromophore, part I: gas phase. *ChemPhysChem*, **2014**, 15, 3236-45	3.2	13
90	The lineshape of the electronic spectrum of the green fluorescent protein chromophore, part II: solution phase. *ChemPhysChem*, **2014**, 15, 3246-57	3.2	19
89	Vibronic coupling dominates the electronic circular dichroism of the benzene chromophore □L(b) band. *Journal of Organic Chemistry*, **2013**, 78, 7398-405	4.2	34
88	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	2.4	15
87	The interplay between neutral exciton and charge transfer states in single-strand polyadenine: a quantum dynamical investigation. *Photochemical and Photobiological Sciences*, **2013**, 12, 1527-43	4.2	16
86	Intermolecular exciton coupling and vibronic effects in solid-state circular dichroism: a case study. *Physical Chemistry Chemical Physics*, **2013**, 15, 795-802	3.6	18
85	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, 4947-58	6.4	47
84	Quantum-classical effective-modes dynamics of the pipi* --> npi* decay in 9H-adenine. A quadratic vibronic coupling model. *Faraday Discussions*, **2013**, 163, 223-42; discussion 243-75	3.6	38
83	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, 2072-82	6.4	166

82	Electronic circular dichroism in exciton-coupled dimers: vibronic spectra from a general all-coordinates quantum-dynamical approach. *Journal of Physical Chemistry A*, **2013**, 117, 3355-68	2.8	20
81	Duschinsky, Herzberg-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, 3597-611	6.4	51
80	First Principles Studies of the Vibrationally Resolved Magnetic Circular Dichroism Spectra of Biphenylene. *Journal of Chemical Theory and Computation*, **2013**, 9, 1557-67	6.4	14
79	Effective time-independent studies on resonance Raman spectroscopy of trans-stilbene including the Duschinsky effect. *Molecular Physics*, **2013**, 111, 1511-1525	1.7	4
78	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		
77	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, 4483-93	6.4	58
76	Barrierless photoisomerisation of the "simplest cyanine": joining computational and femtosecond optical spectroscopies to trace the full reaction path. *Physical Chemistry Chemical Physics*, **2012**, 14, 13350-64	3.6	28
75	Vibrationally resolved circular dichroism spectra of a molecule with isotopically engendered chirality. *Physical Chemistry Chemical Physics*, **2012**, 14, 3669-80	3.6	10
74	Hierarchical transformation of Hamiltonians with linear and quadratic couplings for nonadiabatic quantum dynamics: application to the □□□ internal conversion in thymine. *Journal of Chemical Physics*, **2012**, 136, 244104	3.9	38
73	Analysis of the electronic circular dichroism spectrum of (-)-[9](2,5)Pyridinophane. *Chirality*, **2012**, 24, 994-1004	2.1	6
72	Comparison of vertical and adiabatic harmonic approaches for the calculation of the vibrational structure of electronic spectra. *Physical Chemistry Chemical Physics*, **2012**, 14, 13549-63	3.6	137
71	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	1.9	63
70	Time-Independent Approaches to Simulate Electronic Spectra Lineshapes: From Small Molecules to Macrosystems **2011**, 361-443		55
69	Computing the inhomogeneous broadening of electronic transitions in solution: a first-principle quantum mechanical approach. *Physical Chemistry Chemical Physics*, **2011**, 13, 17007-12	3.6	81
68	Effective Time-Independent Calculations of Vibrational Resonance Raman Spectra of Isolated and Solvated Molecules Including Duschinsky and Herzberg-Teller Effects. *Journal of Chemical Theory and Computation*, **2011**, 7, 1824-39	6.4	69
67	The interplay between □/n□ excited states in gas-phase thymine: a quantum dynamical study. *ChemPhysChem*, **2011**, 12, 1957-68	3.2	39
66	Differences in two-photon and one-photon absorption profiles induced by vibronic coupling: the case of dioxaborine heterocyclic dye. *ChemPhysChem*, **2011**, 12, 3392-403	3.2	19
65	Computational challenges in simulating and analyzing experimental linear and nonlinear circular dichroism spectra. R-(+)-1,1'-bis(2-naphthol) as a prototype case. *Journal of Physical Chemistry B*, **2011**, 115, 811-24	3.4	28

64	Time-Dependent Approaches to Calculation of Steady-State Vibronic Spectra: From Fully Quantum to Classical Approaches **2011**, 475-516		24
63	General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra. *Journal of Chemical Theory and Computation*, **2010**, 6, 1256-1274	6.4	225
62	The excited electronic states of adenine-guanine stacked dimers in aqueous solution: a PCM/TD-DFT study. *Physical Chemistry Chemical Physics*, **2010**, 12, 4934-48	3.6	43
61	Two-photon absorption circular-linear dichroism on axial enantiomers. *Chirality*, **2010**, 22 Suppl 1, E202-10	2.1	19
60	Two-photon absorption circular dichroism: a new twist in nonlinear spectroscopy. *Chemistry - A European Journal*, **2010**, 16, 3504-9	4.8	59
59	Enantiomerically pure alleno-acetylenic macrocycles: synthesis, solid-state structures, chiroptical properties, and electron localization function analysis. *Chemistry - A European Journal*, **2010**, 16, 9796-807	4.8	48
58	Amplifikation der Chiralit□t in monodispersen, enantiomerenreinen Allen-Acetylen-Oligomeren. *Angewandte Chemie*, **2010**, 122, 2296-2300	3.6	30
57	Amplification of chirality in monodisperse, enantiopure alleno-acetylenic oligomers. *Angewandte Chemie - International Edition*, **2010**, 49, 2247-50	16.4	65
56	Time-dependent and time-independent approaches for the computation of absorption spectra of Uracil derivatives in solution. *International Journal of Quantum Chemistry*, **2010**, 110, 624-636	2.1	12
55	Computational approach to the study of the lineshape of absorption and electronic circular dichroism spectra. *International Journal of Quantum Chemistry*, **2010**, 110, 476-486	2.1	62
54	Theory for vibrationally resolved two-photon circular dichroism spectra. Application to (R)-(+)-3-methylcyclopentanone. *Journal of Physical Chemistry A*, **2009**, 113, 4198-207	2.8	47
53	Three-dimensional diabatic models for the □ -> n□ excited-state decay of uracil derivatives in solution. *Theoretical Chemistry Accounts*, **2009**, 123, 273-286	1.9	16
52	In vivo absorption spectra of the two stable states of the Euglena photoreceptor photocycle. *Photochemistry and Photobiology*, **2009**, 85, 304-12	3.6	8
51	Quantum dynamics of the ultrafast pi pi*/n pi* population transfer in uracil and 5-fluoro-uracil in water and acetonitrile. *Journal of Physical Chemistry B*, **2009**, 113, 14491-503	3.4	58
50	Fully Integrated Approach to Compute Vibrationally Resolved Optical Spectra: From Small Molecules to Macrosystems. *Journal of Chemical Theory and Computation*, **2009**, 5, 540-54	6.4	353
49	Excited states decay of the A-T DNA: A PCM/TD-DFT study in aqueous solution of the (9-methyl-adenine)(2).(1-methyl-thymine)(2) stacked tetramer. *Journal of the American Chemical Society*, **2009**, 131, 15232-45	16.4	99
48	On the controversial nature of the 1 1B(u) and 2 1B(u) states of trans-stilbene: the n-electron valence state perturbation theory approach. *Journal of Chemical Physics*, **2009**, 130, 174307	3.9	25
47	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, 15346-54	2.8	54

46	Vibronically resolved electronic circular dichroism spectra of (R)-(+)-3-methylcyclopentanone: a theoretical study. *Journal of Physical Chemistry A*, **2008**, 112, 12401-11	2.8	73
45	Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzberg-Teller effect: the Qx band of porphyrin as a case study. *Journal of Chemical Physics*, **2008**, 128, 224311	3.9	418
44	Ab initio prediction of the emission color in phosphorescent iridium(III) complexes for OLEDs. *Journal of Physical Chemistry B*, **2008**, 112, 13181-3	3.4	32
43	The decay from the dark npi* 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, 10769-72	3.4	61
42	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, 17642-7	11.5	78
41	Absorption spectrum of A-T DNA unraveled by quantum mechanical calculations in solution on the (dA)2 x (dT)2 tetramer. *ChemPhysChem*, **2008**, 9, 2531-7	3.2	36
40	Can TD-DFT calculations accurately describe the excited states behavior of stacked nucleobases? The cytosine dimer as a test case. *Journal of Computational Chemistry*, **2008**, 29, 957-64	3.5	56
39	Chemical selectivity through control of excited-state dynamics. *Angewandte Chemie - International Edition*, **2008**, 47, 6322-5	16.4	38
38	Chemische Selektivit□t durch Kontrolle der Dynamik angeregter Zust□nde. *Angewandte Chemie*, **2008**, 120, 6420-6424	3.6	8
37	Vibronically-induced change in the chiral response of molecules revealed by electronic circular dichroism spectroscopy. *Chemical Physics Letters*, **2008**, 464, 144-149	2.5	45
36	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, 14080-2	3.4	53
35	Ab initio calculations of absorption spectra of large molecules in solution: coumarin C153. *Angewandte Chemie - International Edition*, **2007**, 46, 405-8	16.4	157
34	Ab Initio Calculations of Absorption Spectra of Large Molecules in Solution: Coumarin C153. *Angewandte Chemie*, **2007**, 119, 409-412	3.6	19
33	Chemisorption of silyl radicals onto Pd(100) surface: A computational DFT study. *Surface Science*, **2007**, 601, 255-261	1.8	1
32	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	1.9	14
31	Excited state properties of sizable molecules in solution: from structure to reactivity. *Theoretical Chemistry Accounts*, **2007**, 117, 1073-1084	1.9	9
30	UV-vis spectra of p-benzoquinone anion radical in solution by a TD-DFT/PCM approach. *Theoretical Chemistry Accounts*, **2007**, 118, 143-148	1.9	6
29	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, 7764-9	11.5	239

28	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, 9931-6	11.5	119
27	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	2
26	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	3.9	271
25	Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. *Journal of Chemical Physics*, **2007**, 126, 084509	3.9	398
24	Femtosecond study on the isomerization dynamics of NK88. I. Ground-state dynamics after photoexcitation. *Journal of Chemical Physics*, **2006**, 125, 44512	3.9	25
23	Femtosecond study on the isomerization dynamics of NK88. II. Excited-state dynamics. *Journal of Chemical Physics*, **2006**, 125, 44513	3.9	26
22	Solvent effect on the singlet excited-state lifetimes of nucleic acid bases: A computational study of 5-fluorouracil and uracil in acetonitrile and water. *Journal of the American Chemical Society*, **2006**, 128, 16312-22	16.4	142
21	Excited-state behavior of trans and cis isomers of stilbene and stiff stilbene: a TD-DFT study. *Journal of Physical Chemistry A*, **2005**, 109, 10058-67	2.8	88
20	A Theoretical Study on the Factors Influencing Cyanine Photoisomerization: The Case of Thiacyanine in Gas Phase and in Methanol. *Journal of Chemical Theory and Computation*, **2005**, 1, 215-29	6.4	38
19	Femtosecond photoelectron spectroscopy of trans-stilbene above the reaction barrier. *Chemical Physics*, **2005**, 310, 201-211	2.3	27
18	A tiny excited-state barrier can induce a multiexponential decay of the retinal chromophore: a quantum dynamics investigation. *Angewandte Chemie - International Edition*, **2005**, 44, 5118-21	16.4	48
17	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	2.5	4
16	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	2.5	39
15	Robust control by a multicolor weak laser pulse of the fluorescence of NO2 from the X2A?/A2A? conical intersection. *Chemical Physics*, **2003**, 287, 237-251	2.3	4
14	Stable laser control of complex multilevel systems using a weak-intensity multicolor gaussian pulse. *Chemical Physics*, **2002**, 277, 297-312	2.3	4
13	Trajectory-Surface-Hopping Study of the Renner□Teller Effect in the N(2D) + H2 Reaction□*Journal of Physical Chemistry A*, **2002**, 106, 8276-8284	2.8	40
12	On the energy dependence of the hyperfine interaction in excited states of NO2. *Journal of Chemical Physics*, **2001**, 115, 8868-8875	3.9	7
11	Lanczos calculation of the X□A1/A□B2 nonadiabatic Franck-Condon absorption spectrum of NO2. *Advances in Quantum Chemistry*, **2000**, 36, 323-340	1.4	3

10	Quantum and semiclassical dynamics of the Franck□Condon wave packet on the coupled potential surfaces of the X2A?/A2A? conical intersection. *Chemical Physics*, **2000**, 259, 193-200	2.3	11
9	X□2A?/□□2A? conical intersection effects on the fluorescence of NO2. *Theoretical Chemistry Accounts*, **2000**, 104, 203-206	1.9	
8	Time- and frequency-resolved spontaneous emission: Theory and application to the NO2 X 2A?/□□2A? conical intersection. *Journal of Chemical Physics*, **2000**, 113, 4073-4082	3.9	15
7	Nonadiabatic wave packet dynamics of NO2 on the X 2A?/□□2A? conical intersection. *Journal of Chemical Physics*, **1999**, 110, 4419-4427	3.9	40
6	Nonadiabatic radiative lifetimes and fluorescence spectra of NO2. *Journal of Chemical Physics*, **1999**, 111, 9651-9657	3.9	11
5	On the geometry of 3-amino-sydnones. *Computational and Theoretical Chemistry*, **1998**, 433, 291-299		3
4	Statistical analysis of the computed X 2A1/□□2B2 spectrum of NO2: Some insights into the causes of its irregularity. *Journal of Chemical Physics*, **1998**, 109, 1824-1832	3.9	16
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