Marco Garavelli

List of Publications by Year in Descending Order

195 papers	8,943 citations	49 h-index	89 g-index
228 ext. papers	9,946 ext. citations	7.2 avg, IF	5.97 L-index

#	Paper	IF	Citations
195	Unified Description of Ultrafast Excited State Decay Processes in Epigenetic Deoxycytidine Derivatives. *Journal of Physical Chemistry Letters*, **2021**, 12, 11070-11077	6.4	1
194	Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 77-142	0.7	0
193	In Silico Ultrafast Nonlinear Spectroscopy Meets Experiments: The Case of Perylene Bisimide Dye. *Journal of Chemical Theory and Computation*, **2021**, 17, 7134-7145	6.4	2
192	Control of Protonated Schiff Base Excited State Decay within Visual Protein Mimics: A Unified Model for Retinal Chromophores. *Chemistry - A European Journal*, **2021**, 27, 16389-16400	4.8	1
191	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
190	Polymerization Isomerism in Co-M (M = Cu, Ag, Au) Carbonyl Clusters: Synthesis, Structures and Computational Investigation. *Molecules*, **2021**, 26,	4.8	2
189	Unveiling the spatial distribution of molecular coherences at conical intersections by covariance X-ray diffraction signals. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	7
188	Nonadiabatic Molecular Dynamics Study of the Relaxation Pathways of Photoexcited Cyclooctatetraene. *Journal of Physical Chemistry Letters*, **2021**, 12, 5716-5722	6.4	1
187	QM/MM Nonadiabatic Dynamics: the SHARC/COBRAMM Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 4639-4647	6.4	8
186	Bimetallic Co$_2$M (M = Cu, Ag, and Au) Carbonyl Complexes Supported by N-Heterocyclic Carbene Ligands: Synthesis, Structures, Computational Investigation, and Catalysis for Ammonia Borane Dehydrogenation. *Organometallics*, **2021**, 40, 2724-2735	3.8	2
185	Tailored Coumarin Dyes for Photoredox Catalysis: Calculation, Synthesis, and Electronic Properties. *ChemCatChem*, **2021**, 13, 981-989	5.2	3
184	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. *Molecules*, **2021**, 26,	4.8	1
183	On the origin of controlled anisotropic growth of monodisperse gold nanobipyramids. *Nanoscale*, **2021**, 13, 15292-15300	7.7	2
182	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
181	iSPECTRON: A simulation interface for linear and nonlinear spectra with ab-initio quantum chemistry software. *Journal of Computational Chemistry*, **2021**, 42, 644-659	3.5	6
180	Manipulating Core Excitations in Molecules by X-Ray Cavities. *Physical Review Letters*, **2021**, 126, 053201	7.4	3
179	Diffractive Imaging of Conical Intersections Amplified by Resonant Infrared Fields. *Journal of the American Chemical Society*, **2021**, 143, 13806-13815	16.4	2

178	Imaging conical intersection dynamics during azobenzene photoisomerization by ultrafast X-ray diffraction. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	14
177	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time.. *Nature Communications*, **2021**, 12, 7285	17.4	3
176	Conical Intersection Passages of Molecules Probed by X-ray Diffraction and Stimulated Raman Spectroscopy.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12300-12309	6.4	1
175	Simulating Plasmon Resonances of Gold Nanoparticles with Bipyramidal Shapes by Boundary Element Methods. *Journal of Chemical Theory and Computation*, **2020**, 16, 3807-3815	6.4	9
174	Photoinduced Forward and Backward Pedalo-Type Motion of a Molecular Switch. *Journal of Physical Chemistry Letters*, **2020**, 11, 4741-4746	6.4	1
173	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
172	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. *Physical Chemistry Chemical Physics*, **2020**, 22, 15496-15508	3.6	6
171	Boron-Doped Polycyclic Aromatic Hydrocarbons: A Molecular Set Revealing the Interplay between Topology and Singlet Fission Propensity. *Journal of Physical Chemistry Letters*, **2020**, 11, 1390-1396	6.4	13
170	Ultrafast Spectroscopy: State of the Art and Open Challenges. *Journal of the American Chemical Society*, **2020**, 142, 3-15	16.4	73
169	A Unified Experimental/Theoretical Description of the Ultrafast Photophysics of Single and Double Thionated Uracils. *Chemistry - A European Journal*, **2020**, 26, 336-343	4.8	17
168	A novel spectroscopic window on conical intersections in biomolecules. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 26553-26555	11.5	3
167	Spectral Tuning and Photoisomerization Efficiency in Push-Pull Azobenzenes: Designing Principles. *Journal of Physical Chemistry A*, **2020**, 124, 9513-9523	2.8	8
166	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. *Angewandte Chemie - International Edition*, **2020**, 59, 20619-20627	16.4	1
165	Tailoring Spectral and Photochemical Properties of Bioinspired Retinal Mimics by in Silico Engineering. *Angewandte Chemie*, **2020**, 132, 20800-20808	3.6	
164	Ultrafast Spectroscopy of Photoactive Molecular Systems from First Principles: Where We Stand Today and Where We Are Going. *Journal of the American Chemical Society*, **2020**, 142, 16117-16139	16.4	23
163	UV-light induced vibrational coherences explain Kasha rule violation in frans-azobenzene. *EPJ Web of Conferences*, **2019**, 205, 09016	0.3	
162	Intersystem crossing in thiobases proceeds by a dark intermediate state. *EPJ Web of Conferences*, **2019**, 205, 10005	0.3	1
161	Conical intersection dynamics of pyrimidine nucleosides tracked with sub-20-fs UV pulses. *EPJ Web of Conferences*, **2019**, 205, 10007	0.3	

160	X-ray linear and non-linear spectroscopy of the ESCA molecule. *Journal of Chemical Physics*, **2019**, 151, 114110	3.9	10
159	Pyrene, a Test Case for Deep-Ultraviolet Molecular Photophysics. *Journal of Physical Chemistry Letters*, **2019**, 10, 3481-3487	6.4	22
158	Ternary Complex Formation and Photoactivation of a Photoenzyme Results in Altered Protein Dynamics. *Journal of Physical Chemistry B*, **2019**, 123, 7372-7384	3.4	2
157	Quantum Chemical Modeling of the Photoinduced Activity of Multichromophoric Biosystems. *Chemical Reviews*, **2019**, 119, 9361-9380	68.1	51
156	Multidimensional Potential Energy Surfaces Resolved at the RASPT2 Level for Accurate Photoinduced Isomerization Dynamics of Azobenzene. *Journal of Chemical Theory and Computation*, **2019**, 15, 6813-6823	6.4	23
155	Exploring the capabilities of optical pump X-ray probe NEXAFS spectroscopy to track photo-induced dynamics mediated by conical intersections. *Faraday Discussions*, **2019**, 221, 245-264	3.6	12
154	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. *Chemical Science*, **2019**, 10, 9907-9921	9.4	24
153	QM/MM Photodynamics of Retinal in the Channelrhodopsin Chimera C1C2 with OM3/MRCI. *ChemPhotoChem*, **2019**, 3, 107-116	3.3	7
152	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. *Topics in Current Chemistry Collections*, **2019**, 63-112	1.8	3
151	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. *Faraday Discussions*, **2019**, 221, 219-244	3.6	17
150	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
149	UV-Light-Induced Vibrational Coherences: The Key to Understand Kasha Rule Violation in trans-Azobenzene. *Journal of Physical Chemistry Letters*, **2018**, 9, 1534-1541	6.4	76
148	Evolution of the Excitonic State of DNA Stacked Thymines: Intrabase □ -> S Decay Paths Account for Ultrafast (Subpicosecond) and Longer (>100 ps) Deactivations. *Journal of Physical Chemistry Letters*, **2018**, 9, 2373-2379	6.4	15
147	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. *Journal of Chemical Theory and Computation*, **2018**, 14, 2570-2585	6.4	12
146	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. *Physical Chemistry Chemical Physics*, **2018**, 20, 6877-6890	3.6	32
145	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. *Photochemical and Photobiological Sciences*, **2018**, 17, 323-331	4.2	8
144	Converging many-body correlation energies by means of sequence extrapolation. *Journal of Chemical Physics*, **2018**, 148, 034107	3.9	5
143	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. *Faraday Discussions*, **2018**, 207, 233-250	3.6	10

142	Photoinduced formation mechanism of the thymine-thymine (6-4) adduct in DNA; a QM(CASPT2//CASSCF):MM(AMBER) study. *Faraday Discussions*, **2018**, 207, 375-387	3.6	15
141	Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Two-Dimensional Electronic Spectroscopy. *Chemistry - A European Journal*, **2018**, 24, 12084-12092	4.8	1
140	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. *Journal of Physical Chemistry B*, **2018**, 122, 7668-7681	3.4	7
139	Linear absorption spectra of solvated thiouracils resolved at the hybrid RASPT2/MM level. *Chemical Physics*, **2018**, 515, 643-653	2.3	13
138	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. *Topics in Current Chemistry*, **2018**, 376, 24	7.2	16
137	Semiclassical Path Integral Calculation of Nonlinear Optical Spectroscopy. *Journal of Chemical Theory and Computation*, **2018**, 14, 856-866	6.4	24
136	Observation of the Sub-100 Femtosecond Population of a Dark State in a Thiobase Mediating Intersystem Crossing. *Journal of the American Chemical Society*, **2018**, 140, 16087-16093	16.4	39
135	COBRAMM 2.0 - A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. *Journal of Molecular Modeling*, **2018**, 24, 271	2	29
134	Relationship between Excited State Lifetime and Isomerization Quantum Yield in Animal Rhodopsins: Beyond the One-Dimensional Landau-Zener Model. *Journal of Physical Chemistry Letters*, **2018**, 9, 3315-3322	6.4	20
133	Photophysics of Deoxycytidine and 5-Methyldeoxycytidine in Solution: A Comprehensive Picture by Quantum Mechanical Calculations and Femtosecond Fluorescence Spectroscopy. *Journal of the American Chemical Society*, **2017**, 139, 7780-7791	16.4	49
132	A Quantum Chemical Interpretation of Two-Dimensional Electronic Spectroscopy of Light-Harvesting Complexes. *Journal of the American Chemical Society*, **2017**, 139, 7558-7567	16.4	58
131	Photochemistry: Caught in the act. *Nature Chemistry*, **2017**, 9, 506-507	17.6	2
130	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. *Journal of Physical Chemistry Letters*, **2017**, 8, 1777-1783	6.4	43
129	On the Simulation of Two-dimensional Electronic Spectroscopy of Indole-containing Peptides. *Photochemistry and Photobiology*, **2017**, 93, 1368-1380	3.6	10
128	Fine Tuning of Retinal Photoinduced Decay in Solution. *Journal of Physical Chemistry Letters*, **2017**, 8, 4407-4412	6.4	14
127	Multiple Electronic and Structural Factors Control Cyclobutane Pyrimidine Dimer and 6-4 Thymine-Thymine Photodimerization in a DNA Duplex. *Chemistry - A European Journal*, **2017**, 23, 15177-15188	4.8	32
126	Analysis of the vibronic structure of the trans-stilbene fluorescence and excitation spectra: the S and S PES along the C[double bond, length as m-dash]C and C-C torsions. *Physical Chemistry Chemical Physics*, **2017**, 19, 25095-25104	3.6	5
125	Theoretical mechanistic study of self-sensitized photo-oxygenation and singlet oxygen thermal release in a dimethyldihydropyrene derivative. *Journal of Photochemistry and Photobiology A: Chemistry*, **2017**, 333, 156-164	4.7	12

124	Computing the Absorption and Emission Spectra of 5-Methylcytidine in Different Solvents: A Test-Case for Different Solvation Models. *Journal of Chemical Theory and Computation*, **2016**, 12, 4430-9	6.4	30
123	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Coordination Polymers. *Journal of the American Chemical Society*, **2016**, 138, 15234-15242	16.4	19
122	Multiple Decay Mechanisms and 2D-UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenine-Uracil Monophosphate. *Chemistry - A European Journal*, **2016**, 22, 7497-507	4.8	26
121	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
120	Intramolecular photo-induced charge transfer in visual retinal chromophore mimics: electron density-based indices at the TD-DFT and post-HF levels. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	11
119	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
118	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	24
117	Photoelectrochromism in the Retinal Protonated Schiff Base Chromophore: Photoisomerization Speed and Selectivity under a Homogeneous Electric Field at Different Operational Regimes. *Journal of Chemical Theory and Computation*, **2016**, 12, 4460-75	6.4	5
116	Excited state evolution of DNA stacked adenines resolved at the CASPT2//CASSCF/Amber level: from the bright to the excimer state and back. *Physical Chemistry Chemical Physics*, **2015**, 17, 7291-302	3.6	31
115	Multiconfigurational Second-Order Perturbation Theory with Frozen Natural Orbitals Extended to the Treatment of Photochemical Problems. *Journal of Chemical Theory and Computation*, **2015**, 11, 3772-84	6.4	36
114	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. *Photochemical and Photobiological Sciences*, **2015**, 14, 213-28	4.2	27
113	Photochemical reaction paths of cis-dienes studied with RASSCF: the changing balance between ionic and covalent excited states. *Molecular Physics*, **2015**, 113, 1978-1990	1.7	10
112	Two-Dimensional Electronic Spectroscopy of Benzene, Phenol, and Their Dimer: An Efficient First-Principles Simulation Protocol. *Journal of Chemical Theory and Computation*, **2015**, 11, 3755-71	6.4	23
111	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. *Faraday Discussions*, **2015**, 177, 345-62	3.6	27
110	Ultra-broadband 2D electronic spectroscopy of carotenoid-bacteriochlorophyll interactions in the LH1 complex of a purple bacterium. *Journal of Chemical Physics*, **2015**, 142, 212433	3.9	21
109	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. *Journal of Chemical Physics*, **2015**, 142, 212443	3.9	37
108	Tetrapeptide unfolding dynamics followed by core-level spectroscopy: a first-principles approach. *Physical Chemistry Chemical Physics*, **2015**, 17, 11269-76	3.6	3
107	A multi-addressable switch based on the dimethyldihydropyrene photochrome with remarkable proton-triggered photo-opening efficiency. *Chemistry - A European Journal*, **2015**, 21, 455-67	4.8	35

106	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. *Frontiers in Chemistry*, **2015**, 3, 29	5	23
105	Spectral lineshapes in nonlinear electronic spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 30925-36	3.6	34
104	Rationalization and Design of Enhanced Photoinduced Cycloreversion in Photochromic Dimethyldihydropyrenes by Theoretical Calculations. *Journal of Physical Chemistry A*, **2015**, 119, 6024-32	2.8	19
103	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. *Journal of Physical Chemistry Letters*, **2015**, 6, 576-80	6.4	40
102	Wavepacket splitting and two-pathway deactivation in the photoexcited visual pigment isorhodopsin. *Angewandte Chemie - International Edition*, **2014**, 53, 2504-7	16.4	39
101	Modelling retinal chromophores photoisomerization: from minimal models in vacuo to ultimate bidimensional spectroscopy in rhodopsins. *Physical Chemistry Chemical Physics*, **2014**, 16, 16865-79	3.6	30
100	Modelling time-resolved two-dimensional electronic spectroscopy of the primary photoisomerization event in rhodopsin. *Journal of Physical Chemistry B*, **2014**, 118, 8396-405	3.4	27
99	Disentangling Peptide Configurations via Two-Dimensional Electronic Spectroscopy: Ab Initio Simulations Beyond the Frenkel Exciton Hamiltonian. *Journal of Physical Chemistry Letters*, **2014**, 5, 767-771	6.4	31
98	Aufspaltung des Wellenpakets und Doppelpfad-Desaktivierung im photoangeregten Sehpigment Isorhodopsin. *Angewandte Chemie*, **2014**, 126, 2537-2541	3.6	3
97	Microjoule-level, tunable sub-10 fs UV pulses by broadband sum-frequency generation. *Optics Letters*, **2014**, 39, 3849-52	3	36
96	Tracking conformational dynamics of polypeptides by nonlinear electronic spectroscopy of aromatic residues: a first-principles simulation study. *ChemPhysChem*, **2014**, 15, 3282-90	3.2	22
95	Bidimensional electronic spectroscopy on indole in gas phase and in water from first principles. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 295-303	2	20
94	Ab initio simulations of two-dimensional electronic spectra: The SOS//QM/MM approach. *International Journal of Quantum Chemistry*, **2014**, 114, 85-93	2.1	34
93	Tracking the stilbene photoisomerization in the S(1) state using RASSCF. *Physical Chemistry Chemical Physics*, **2013**, 15, 19763-73	3.6	27
92	Photoinduced formation mechanism of the thymine-thymine (6-4) adduct. *Journal of Physical Chemistry B*, **2013**, 117, 1999-2004	3.4	42
91	Computational Evidence for the Catalytic Mechanism of Human Glutathione S-Transferase A3-3: A QM/MM Investigation. *ACS Catalysis*, **2012**, 2, 280-286	13.1	13
90	Sampling excited state dynamics: influence of HOOP mode excitations in a retinal model. *Physical Chemistry Chemical Physics*, **2012**, 14, 14299-305	3.6	27
89	Modelling vibrational coherence in the primary rhodopsin photoproduct. *Journal of Chemical Physics*, **2012**, 137, 22A523	3.9	18

88	Product formation in rhodopsin by fast hydrogen motions. *Physical Chemistry Chemical Physics*, **2011**, 13, 3645-8	3.6	66
87	On the role of the triplet state in the cis/trans isomerization of rhodopsin: A CASPT2//CASSCF study of a model chromophore. *International Journal of Quantum Chemistry*, **2011**, 111, 3431-3437	2.1	9
86	Conical intersection dynamics of the primary photoisomerization event in vision. *Nature*, **2010**, 467, 440-3	30.4	651
85	Aborted double bicycle-pedal isomerization with hydrogen bond breaking is the primary event of bacteriorhodopsin proton pumping. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 20172-7	11.5	74
84	Spectroscopic Properties of Formaldehyde in Aqueous Solution: Insights from Car-Parrinello and TDDFT/CASPT2 Calculations. *Journal of Chemical Theory and Computation*, **2010**, 6, 3403-9	6.4	7
83	Adenine deactivation in DNA resolved at the CASPT2//CASSCF/ AMBER level. *Physical Chemistry Chemical Physics*, **2010**, 12, 5016-23	3.6	71
82	Probing and Modeling the Absorption of Retinal Protein Chromophores in Vacuo. *Angewandte Chemie*, **2010**, 122, 1834-1837	3.6	14
81	Significance of a Zwitterionic State for Fulgide Photochromism: Implications for the Design of Mimics. *Angewandte Chemie*, **2010**, 122, 2975-2978	3.6	7
80	Probing and modeling the absorption of retinal protein chromophores in vacuo. *Angewandte Chemie - International Edition*, **2010**, 49, 1790-3	16.4	68
79	Significance of a zwitterionic state for fulgide photochromism: implications for the design of mimics. *Angewandte Chemie - International Edition*, **2010**, 49, 2913-6	16.4	48
78	Deciphering low energy deactivation channels in adenine. *Journal of the American Chemical Society*, **2009**, 131, 16108-18	16.4	67
77	Electrostatic control of the photoisomerization efficiency and optical properties in visual pigments: on the role of counterion quenching. *Journal of the American Chemical Society*, **2009**, 131, 5172-86	16.4	116
76	Multistate photo-induced relaxation and photoisomerization ability of fumaramide threads: a computational and experimental study. *Journal of the American Chemical Society*, **2009**, 131, 104-17	16.4	24
75	Deciphering intrinsic deactivation/isomerization routes in a phytochrome chromophore model. *Journal of Physical Chemistry B*, **2009**, 113, 15067-73	3.4	27
74	Catalytic Mechanism of Diaminopimelate Epimerase: A QM/MM Investigation. *Journal of Chemical Theory and Computation*, **2009**, 5, 1915-30	6.4	11
73	Computational DFT investigation of vicinal amide group anchimeric assistance in ether cleavage. *Journal of Organic Chemistry*, **2008**, 73, 2066-73	4.2	9
72	Triplet pathways in diarylethene photochromism: photophysical and computational study of dyads containing ruthenium(II) polypyridine and 1,2-bis(2-methylbenzothiophene-3-yl)maleimide units. *Journal of the American Chemical Society*, **2008**, 130, 7286-99	16.4	150
71	The catalytic activity of proline racemase: a quantum mechanical/molecular mechanical study. *Journal of Physical Chemistry B*, **2008**, 112, 1057-9	3.4	13

70	Modeling the photophysics and photochromic potential of 1,2-dihydronaphthalene (DHN): a combined CASPT2//CASSCF-topological and MMVB-dynamical investigation. *Journal of Physical Chemistry A*, **2008**, 112, 10096-107	2.8	14
69	Computational evidence for the catalytic mechanism of glutaminyl cyclase. A DFT investigation. *Proteins: Structure, Function and Bioinformatics*, **2008**, 73, 527-38	4.2	19
68	nano□A calculus for the modeling and simulation of nano devices. *Theoretical Computer Science*, **2008**, 408, 17-30	1.1	8
67	A new formulation of the phase change approach in the theory of conical intersections. *Chemical Physics*, **2008**, 347, 46-56	2.3	10
66	The different photoisomerization efficiency of azobenzene in the lowest n pi* and pi pi* singlets: the role of a phantom state. *Journal of the American Chemical Society*, **2008**, 130, 5216-30	16.4	159
65	The role of the intersection space in the photochemistry of tricyclo[3.3.0.0(2,6)]octa-3,7-diene. *Journal of Physical Chemistry A*, **2007**, 111, 2830-8	2.8	6
64	Substituent-controlled photoisomerization in retinal chromophore models: Fluorinated and methoxy-substituted protonated Schiff bases. *Journal of Photochemistry and Photobiology A: Chemistry*, **2007**, 190, 258-273	4.7	8
63	Cyclohexenylphenyldiazene: a simple surrogate of the azobenzene photochromic unit. *Journal of the American Chemical Society*, **2007**, 129, 3198-210	16.4	33
62	Structure of the Conical Intersections Driving the cis□rans Photoisomerization of Conjugated Molecules¶. *Photochemistry and Photobiology*, **2007**, 76, 622-633	3.6	3
61	Light driven molecular switches: exploring and tuning their photophysical and photochemical properties. *Theoretical Chemistry Accounts*, **2007**, 117, 1041-1059	1.9	17
60	About the intrinsic photochemical properties of the 11-cis retinal chromophore: computational clues for a trap state and a lever effect in Rhodopsin catalysis. *Theoretical Chemistry Accounts*, **2007** , 118, 173-183	1.9	30
59	A tunable QM/MM approach to chemical reactivity, structure and physico-chemical properties prediction. *Theoretical Chemistry Accounts*, **2007**, 118, 219-240	1.9	73
58	A Computational Strategy for Organic Photochemistry. *Reviews in Computational Chemistry*, **2007**, 87-146		106
57	COBRAMM: A Tunable QM/MM Approach to Complex Molecular Architectures. Modelling the Excited and Ground State Properties of Sized Molecular Systems. *AIP Conference Proceedings*, **2007**,	0	4
56	An ab initio Study of Decay Mechanism of Adenine: the Facile Path of the Amino NH Bond Cleavage. *AIP Conference Proceedings*, **2007**,	0	2
55	Computational clues for a new mechanism in the glycosylase activity of the human DNA repair protein hOGG1. A generalized paradigm for purine-repairing systems?. *Journal of Physical Chemistry B*, **2007**, 111, 6557-70	3.4	29
54	Computational Organic Photochemistry: Strategy, Achievements and Perspectives. *Theoretical Chemistry Accounts*, **2006**, 116, 87-105	1.9	78
53	Substituent controlled spectroscopy and excited state topography of retinal chromophore models: fluorinated and methoxy-substituted protonated Schiff bases. *Molecular Physics*, **2006**, 104, 915-924	1.7	10

52	Spectral Tuning and Photochemical Reactivity Control in Biological Chromophores **2006**, 1292-1292		
51	Computation of Photochemical Reaction Mechanisms in Organic Chemistry. *Theoretical and Computational Chemistry*, **2005**, 16, 191-223		9
50	Solvent effects on the vibrational activity and photodynamics of the green fluorescent protein chromophore: a quantum-chemical study. *Journal of the American Chemical Society*, **2005**, 127, 3952-63	16.4	127
49	Structure, spectroscopy, and spectral tuning of the gas-phase retinal chromophore: the beta-ionone "handle" and alkyl group effect. *Journal of Physical Chemistry A*, **2005**, 109, 6597-605	2.8	79
48	Photoisomerization mechanism of 11-cis-locked artificial retinal chromophores: acceleration and primary photoproduct assignment. *Journal of the American Chemical Society*, **2005**, 127, 2433-42	16.4	25
47	Iridium cyclometalated complexes with axial symmetry: time-dependent density functional theory investigation of trans-bis-cyclometalated complexes containing the tridentate ligand 2,6-diphenylpyridine. *Inorganic Chemistry*, **2005**, 44, 1282-9	5.1	83
46	The retinal chromophore/chloride ion pair: structure of the photoisomerization path and interplay of charge transfer and covalent states. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6255-60	11.5	99
45	On the mechanism of the cis-trans isomerization in the lowest electronic states of azobenzene: S0, S1, and T1. *Journal of the American Chemical Society*, **2004**, 126, 3234-43	16.4	380
44	A theoretical study of the lowest electronic states of azobenzene: the role of torsion coordinate in the cis□trans photoisomerization. *Theoretical Chemistry Accounts*, **2004**, 111, 363-372	1.9	119
43	Complete-active-space self-consistent-field/Amber parameterization of the Lys296□etinal□Glu113 rhodopsin chromophore-counterion system. *Theoretical Chemistry Accounts*, **2004**, 112, 335	1.9	54
42	Structure of the intersection space associated with ZIE photoisomerization of retinal in rhodopsin proteins. *Faraday Discussions*, **2004**, 127, 179-91	3.6	58
41	beta-Pseudopeptide foldamers. The homo-oligomers of (4R)-(2-oxo-1,3-oxazolidin-4-yl)-acetic acid (D-Oxac). *Organic and Biomolecular Chemistry*, **2004**, 2, 2181-7	3.9	16
40	Counterion controlled photoisomerization of retinal chromophore models: a computational investigation. *Journal of the American Chemical Society*, **2004**, 126, 16018-37	16.4	84
39	Can simple enones be useful partners for the catalytic stereoselective alkylation of indoles?. *Journal of Organic Chemistry*, **2004**, 69, 7511-8	4.2	68
38	A global investigation of excited state surfaces within time-dependent density-functional response theory. *Journal of Chemical Physics*, **2004**, 120, 1674-92	3.9	149
37	A simple approach for improving the hybrid MMVB force field: application to the photoisomerization of s-cis butadiene. *Journal of Computational Chemistry*, **2003**, 24, 1357-63	3.5	28
36	Pseudopeptide Foldamers □The Homo-Oligomers of Benzyl (4S,5R)-5-Methyl-2-oxo-1,3-oxazolidine-4-carboxylate. *European Journal of Organic Chemistry*, **2003**, 2003, 259-267	3.2	29
35	Unusual peptides containing the 2,6-diaminopimelic acid framework: Stereocontrolled synthesis, X-ray analysis, and computational modelling. Part 2. *Tetrahedron: Asymmetry*, **2003**, 14, 2639-2649		19

34	Can Diarylethene Photochromism Be Explained by a Reaction Path Alone? A CASSCF Study with Model MMVB Dynamics. *Journal of Physical Chemistry A*, **2003**, 107, 11139-11152	2.8	151
33	Development and conformational analysis of a pseudoproline-containing turn mimic. *Journal of Organic Chemistry*, **2003**, 68, 1982-93	4.2	22
32	Excited-state singlet manifold and oscillatory features of a nonatetraeniminium retinal chromophore model. *Journal of the American Chemical Society*, **2003**, 125, 12509-19	16.4	39
31	Computer simulation of photoinduced molecular motion and reactivity. *International Journal of Photoenergy*, **2002**, 4, 57-68	2.1	14
30	Pseudopeptide foldamers: the homo-oligomers of pyroglutamic acid. *Chemistry - A European Journal*, **2002**, 8, 2516-25	4.8	51
29	Exploring Organic Chemistry with DFT: Radical, Organo-metallic, and Bio-organic Applications. *QSAR and Combinatorial Science*, **2002**, 21, 128-148		24
28	A hypothetical mechanism for HIV-1 integrase catalytic action: DFT modelling of a bio-mimetic environment. *Chemical Physics Letters*, **2002**, 362, 1-7	2.5	24
27	Cyclooctatetraene computational photo- and thermal chemistry: a reactivity model for conjugated hydrocarbons. *Journal of the American Chemical Society*, **2002**, 124, 13770-89	16.4	60
26	Structure of the conical intersections driving the cis-trans photoisomerization of conjugated molecules. *Photochemistry and Photobiology*, **2002**, 76, 622-33	3.6	82
25	Reaction path analysis of the "tunable" photoisomerization selectivity of free and locked retinal chromophores. *Journal of the American Chemical Society*, **2002**, 124, 4124-34	16.4	64
24	Intrinsically Competitive Photoinduced Polycyclization and Double-Bond Shift through a Boatlike Conical Intersection. *Angewandte Chemie*, **2001**, 113, 1514-1516	3.6	1
23	Intrinsically Competitive Photoinduced Polycyclization and Double-Bond Shift through a Boatlike Conical Intersection. *Angewandte Chemie - International Edition*, **2001**, 40, 1466-1468	16.4	16
22	Reaction Path of a sub-200 fs Photochemical Electrocyclic Reaction. *Journal of Physical Chemistry A*, **2001**, 105, 4458-4469	2.8	141
21	Product Distribution in the Photolysis of s-cis Butadiene:A Dynamics Simulation. *Journal of Physical Chemistry A*, **2001**, 105, 11496-11504	2.8	49
20	Computational evidence in favor of a two-state, two-mode model of the retinal chromophore photoisomerization. *Proceedings of the National Academy of Sciences of the United States of America* , **2000**, 97, 9379-84	11.5	301
19	Relaxation Paths and Dynamics of Photoexcited Polyene Chains: Evidence for Creation and Annihilation of Neutral Soliton Pairs. *Journal of the American Chemical Society*, **2000**, 122, 5568-5581	16.4	39
18	CAS-SCF and MM-VB Dynamics: Applications to Organic Photochemistry. *Lecture Notes in Quantum Chemistry II*, **2000**, 150-155	0.6	
17	The short-chain acroleiniminium and pentadieniminium cations: towards a model for retinal photoisomerization. A CASSCF/PT2 study. *Computational and Theoretical Chemistry*, **1999**, 463, 59-64		43

16	Initial Excited-State Relaxation of the Isolated 11-cis Protonated Schiff Base of Retinal: Evidence for in-Plane Motion from ab Initio Quantum Chemical Simulation of the Resonance Raman Spectrum. *Journal of the American Chemical Society*, **1999**, 121, 1023-1029	16.4	96
15	Photochemistry of Highly Alkylated Dienes: Computational Evidence for a Concerted Formation of Bicyclobutane. *Journal of the American Chemical Society*, **1999**, 121, 1537-1545	16.4	28
14	Minimum energy paths in the excited and ground states of short protonated Schiff bases and of the analogous polyenes. *Journal of Photochemistry and Photobiology A: Chemistry*, **1998**, 114, 109-116	4.7	28
13	Photoisomerization Path for a Realistic Retinal Chromophore Model: The Nonatetraeniminium Cation. *Journal of the American Chemical Society*, **1998**, 120, 1285-1288	16.4	143
12	Potential-energy surfaces for ultrafast photochemistry Static and dynamic aspects. *Faraday Discussions*, **1998**, 110, 51-70	3.6	132
11	DFT Study of the Reactions between Singlet-Oxygen and a Carotenoid Model. *Journal of the American Chemical Society*, **1998**, 120, 10210-10222	16.4	50
10	Potential Energy Surfaces for Ultrafast Photochemistry: Short Chain Polyenes and Protonated Schiff Bases. *Springer Series in Chemical Physics*, **1998**, 612-614	0.3	
9	Relaxation Paths from a Conical Intersection: The Mechanism of Product Formation in the Cyclohexadiene/Hexatriene Photochemical Interconversion. *Journal of Physical Chemistry A*, **1997**, 101, 2023-2032	2.8	144
8	The C5H6NH2+Protonated Shiff Base: Anab InitioMinimal Model for Retinal Photoisomerization. *Journal of the American Chemical Society*, **1997**, 119, 6891-6901	16.4	259
7	Trans cis isomerization in long linear polyenes as beta-carotene models: a comparative CAS-PT2 and DFT study. *Molecular Physics*, **1997**, 92, 359-364	1.7	4
6	Ab Initio Photoisomerization Dynamics of a Simple Retinal Chromophore Model. *Journal of the American Chemical Society*, **1997**, 119, 12687-12688	16.4	172
5	Force Fields for Ultrafast Photochemistry: The S2 (1Bu) -> S1 (2Ag) -> S0 (1Ag) Reaction Path for all-trans-Hexa-1,3,5-triene. *Journal of the American Chemical Society*, **1997**, 119, 11487-11494	16.4	77
4	The Structure of the Nonadiabatic Photochemical Trans -> Cis Isomerization Channel in All-Trans Octatetraene. *Journal of the American Chemical Society*, **1996**, 118, 11656-11657	16.4	49
3	Molecular "Trigger" for the Radiationless Deactivation of Photoexcited Conjugated Hydrocarbons. *Journal of the American Chemical Society*, **1995**, 117, 11584-11585	16.4	95
2	Geometry optimisation on a hypersphere. Application to finding reaction paths from a conical intersection. *Chemical Physics Letters*, **1995**, 243, 1-8	2.5	103
1	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time		3