Marco Garavelli

List of Publications by Citations

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	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
194	Conical intersection dynamics of the primary photoisomerization event in vision. *Nature*, **2010**, 467, 440-3	30.4	651
193	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
192	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
191	The C5H6NH2+Protonated Shiff Base:Anab InitioMinimal Model for Retinal Photoisomerization. *Journal of the American Chemical Society*, **1997**, 119, 6891-6901	16.4	259
190	Ab Initio Photoisomerization Dynamics of a Simple Retinal Chromophore Model. *Journal of the American Chemical Society*, **1997**, 119, 12687-12688	16.4	172
189	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
188	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
187	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
186	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
185	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
184	Photoisomerization Path for a Realistic Retinal Chromophore Model: The Nonatetraeniminium Cation. *Journal of the American Chemical Society*, **1998**, 120, 1285-1288	16.4	143
183	Reaction Path of a sub-200 fs Photochemical Electrocyclic Reaction. *Journal of Physical Chemistry A*, **2001**, 105, 4458-4469	2.8	141
182	Potential-energy surfaces for ultrafast photochemistry Static and dynamic aspects. *Faraday Discussions*, **1998**, 110, 51-70	3.6	132
181	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
180	A theoretical study of the lowest electronic states of azobenzene: the role of torsion coordinate in the cistrans photoisomerization. *Theoretical Chemistry Accounts*, **2004**, 111, 363-372	1.9	119
179	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

178	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
177	A Computational Strategy for Organic Photochemistry. *Reviews in Computational Chemistry*, **2007**, 87-146		106
176	Geometry optimisation on a hypersphere. Application to finding reaction paths from a conical intersection. *Chemical Physics Letters*, **1995**, 243, 1-8	2.5	103
175	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
174	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
173	Molecular "Trigger" for the Radiationless Deactivation of Photoexcited Conjugated Hydrocarbons. *Journal of the American Chemical Society*, **1995**, 117, 11584-11585	16.4	95
172	Counterion controlled photoisomerization of retinal chromophore models: a computational investigation. *Journal of the American Chemical Society*, **2004**, 126, 16018-37	16.4	84
171	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
170	Structure of the conical intersections driving the cis-trans photoisomerization of conjugated molecules. *Photochemistry and Photobiology*, **2002**, 76, 622-33	3.6	82
169	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
168	Computational Organic Photochemistry: Strategy, Achievements and Perspectives. *Theoretical Chemistry Accounts*, **2006**, 116, 87-105	1.9	78
167	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
166	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
165	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
164	A tunable QM/MM approach to chemical reactivity, structure and physico-chemical properties prediction. *Theoretical Chemistry Accounts*, **2007**, 118, 219-240	1.9	73
163	Ultrafast Spectroscopy: State of the Art and Open Challenges. *Journal of the American Chemical Society*, **2020**, 142, 3-15	16.4	73
162	Adenine deactivation in DNA resolved at the CASPT2//CASSCF/ AMBER level. *Physical Chemistry Chemical Physics*, **2010**, 12, 5016-23	3.6	71
161	Probing and modeling the absorption of retinal protein chromophores in vacuo. *Angewandte Chemie - International Edition*, **2010**, 49, 1790-3	16.4	68

160	Can simple enones be useful partners for the catalytic stereoselective alkylation of indoles?. *Journal of Organic Chemistry*, **2004**, 69, 7511-8	4.2	68
159	Deciphering low energy deactivation channels in adenine. *Journal of the American Chemical Society*, **2009**, 131, 16108-18	16.4	67
158	Product formation in rhodopsin by fast hydrogen motions. *Physical Chemistry Chemical Physics*, **2011**, 13, 3645-8	3.6	66
157	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
156	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
155	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
154	Structure of the intersection space associated with ZIE photoisomerization of retinal in rhodopsin proteins. *Faraday Discussions*, **2004**, 127, 179-91	3.6	58
153	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
152	Quantum Chemical Modeling of the Photoinduced Activity of Multichromophoric Biosystems. *Chemical Reviews*, **2019**, 119, 9361-9380	68.1	51
151	Pseudopeptide foldamers: the homo-oligomers of pyroglutamic acid. *Chemistry - A European Journal*, **2002**, 8, 2516-25	4.8	51
150	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
149	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
148	Product Distribution in the Photolysis of s-cis Butadiene:□A Dynamics Simulation. *Journal of Physical Chemistry A*, **2001**, 105, 11496-11504	2.8	49
147	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
146	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
145	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. *Journal of Physical Chemistry Letters*, **2017**, 8, 1777-1783	6.4	43
144	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
143	Photoinduced formation mechanism of the thymine-thymine (6-4) adduct. *Journal of Physical Chemistry B*, **2013**, 117, 1999-2004	3.4	42

142	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. *Journal of Physical Chemistry Letters*, **2015**, 6, 576-80	6.4	40
141	Wavepacket splitting and two-pathway deactivation in the photoexcited visual pigment isorhodopsin. *Angewandte Chemie - International Edition*, **2014**, 53, 2504-7	16.4	39
140	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
139	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
138	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
137	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. *Journal of Chemical Physics*, **2015**, 142, 212443	3.9	37
136	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
135	Microjoule-level, tunable sub-10 fs UV pulses by broadband sum-frequency generation. *Optics Letters*, **2014**, 39, 3849-52	3	36
134	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
133	Spectral lineshapes in nonlinear electronic spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 30925-36	3.6	34
132	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
131	Cyclohexenylphenyldiazene: a simple surrogate of the azobenzene photochromic unit. *Journal of the American Chemical Society*, **2007**, 129, 3198-210	16.4	33
130	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
129	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
128	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
127	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
126	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
125	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

124	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
123	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
122	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
121	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
120	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
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118	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
117	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. *Photochemical and Photobiological Sciences*, **2015**, 14, 213-28	4.2	27
116	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. *Faraday Discussions*, **2015**, 177, 345-62	3.6	27
115	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
114	Tracking the stilbene photoisomerization in the S(1) state using RASSCF. *Physical Chemistry Chemical Physics*, **2013**, 15, 19763-73	3.6	27
113	Sampling excited state dynamics: influence of HOOP mode excitations in a retinal model. *Physical Chemistry Chemical Physics*, **2012**, 14, 14299-305	3.6	27
112	Deciphering intrinsic deactivation/isomerization routes in a phytochrome chromophore model. *Journal of Physical Chemistry B*, **2009**, 113, 15067-73	3.4	27
111	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
110	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
109	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
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107	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

106	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	24
105	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. *Chemical Science*, **2019**, 10, 9907-9921	9.4	24
104	Semiclassical Path Integral Calculation of Nonlinear Optical Spectroscopy. *Journal of Chemical Theory and Computation*, **2018**, 14, 856-866	6.4	24
103	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
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101	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. *Frontiers in Chemistry*, **2015**, 3, 29	5	23
100	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
99	Pyrene, a Test Case for Deep-Ultraviolet Molecular Photophysics. *Journal of Physical Chemistry Letters*, **2019**, 10, 3481-3487	6.4	22
98	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
97	Development and conformational analysis of a pseudoproline-containing turn mimic. *Journal of Organic Chemistry*, **2003**, 68, 1982-93	4.2	22
96	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
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
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93	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Coordination Polymers. *Journal of the American Chemical Society*, **2016**, 138, 15234-15242	16.4	19
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83	Intrinsically Competitive Photoinduced Polycyclization and Double-Bond Shift through a Boatlike Conical Intersection. *Angewandte Chemie - International Edition*, **2001**, 40, 1466-1468	16.4	16
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81	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
80	Fine Tuning of Retinal Photoinduced Decay in Solution. *Journal of Physical Chemistry Letters*, **2017**, 8, 4407-4412	6.4	14
79	Probing and Modeling the Absorption of Retinal Protein Chromophores in Vacuo. *Angewandte Chemie*, **2010**, 122, 1834-1837	3.6	14
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75	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
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69	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
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54	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
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48	Significance of a Zwitterionic State for Fulgide Photochromism: Implications for the Design of Mimics. *Angewandte Chemie*, **2010**, 122, 2975-2978	3.6	7
47	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
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