Christel M Marian

List of Publications by Citations

214 papers	8,471 citations	47 h-index	82 g-index
227 ext. papers	9,440 ext. citations	3.8 avg, IF	6.69 L-index

#	Paper	IF	Citations
214	A mean-field spin-orbit method applicable to correlated wavefunctions. *Chemical Physics Letters*, **1996**, 251, 365-371	2.5	871
213	Spin□orbit coupling and intersystem crossing in molecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 187-203	7.9	471
212	Spin-Vibronic Mechanism for Intersystem Crossing. *Chemical Reviews*, **2018**, 118, 6975-7025	68.1	377
211	A new pathway for the rapid decay of electronically excited adenine. *Journal of Chemical Physics*, **2005**, 122, 104314	3.9	211
210	The guanine tautomer puzzle: quantum chemical investigation of ground and excited states. *Journal of Physical Chemistry A*, **2007**, 111, 1545-53	2.8	162
209	Performance of the Density Functional Theory/Multireference Configuration Interaction Method on Electronic Excitation of Extended □Systems. *Journal of Chemical Theory and Computation*, **2008**, 4, 1501-15	6.4	152
208	Quantum chemical investigation of the electronic spectra of the keto, enol, and keto-imine tautomers of cytosine. *Journal of Physical Chemistry A*, **2005**, 109, 8410-8	2.8	133
207	Spin-orbit coupling of DFT/MRCI wavefunctions: method, test calculations, and application to thiophene. *Journal of Computational Chemistry*, **2002**, 23, 824-33	3.5	126
206	Calculation of spin-forbidden radiative transitions using correlated wavefunctions: Lifetimes of b1□, a1□states in O2, S2 and SO. *Chemical Physics*, **1984**, 89, 223-236	2.3	124
205	Ultrafast deactivation mechanism of the excited singlet in the light-induced spin crossover of [Fe(2,2□bipyridine)3]2+. *Chemistry - A European Journal*, **2013**, 19, 17541-51	4.8	123
204	A new mean-field and ECP-based spin-orbit method. Applications to Pt and PtH. *Chemical Physics Letters*, **1996**, 251, 357-364	2.5	116
203	Mechanism of the Triplet-to-Singlet Upconversion in the Assistant Dopant ACRXTN. *Journal of Physical Chemistry C*, **2016**, 120, 3715-3721	3.8	111
202	Time-dependent approaches for the calculation of intersystem crossing rates. *Journal of Chemical Physics*, **2011**, 134, 154105	3.9	106
201	Intersystem crossing driven by vibronic spin-orbit coupling: a case study on psoralen. *Physical Chemistry Chemical Physics*, **2007**, 9, 5209-21	3.6	103
200	The generalized active space concept for the relativistic treatment of electron correlation. I. Kramers-restricted two-component configuration interaction. *Journal of Chemical Physics*, **2001**, 114, 4775-4790	3.9	101
199	Protonation effect on the electronic spectrum of tryptophan in the gas phase. *Physical Chemistry Chemical Physics*, **2004**, 6, 2633	3.6	99
198	Parallel multireference configuration interaction calculations on mini-beta-carotenes and beta-carotene. *Journal of Chemical Physics*, **2009**, 130, 044708	3.9	97

197	Singlet and triplet excited states and intersystem crossing in free-base porphyrin: TDDFT and DFT/MRCI study. *ChemPhysChem*, **2008**, 9, 282-92	3.2	97
196	Intersystem crossing and characterization of dark states in the pyrimidine nucleobases uracil, thymine, and 1-methylthymine. *Journal of Physical Chemistry A*, **2009**, 113, 11809-16	2.8	96
195	The photophysics of flavins: What makes the difference between gas phase and aqueous solution?. *Journal of Photochemistry and Photobiology A: Chemistry*, **2008**, 198, 221-231	4.7	88
194	The electronic spectrum of protonated adenine: theory and experiment. *Physical Chemistry Chemical Physics*, **2005**, 7, 3306-16	3.6	85
193	SPOCK.CI: a multireference spin-orbit configuration interaction method for large molecules. *Journal of Chemical Physics*, **2006**, 124, 124101	3.9	85
192	Redesign of the DFT/MRCI Hamiltonian. *Journal of Chemical Physics*, **2016**, 144, 034104	3.9	81
191	Electronic excitation and singlet-triplet coupling in uracil tautomers and uracil-water complexes. *European Physical Journal D*, **2002**, 20, 357-367	1.3	80
190	Spin-Orbit Coupling in Molecules. *Reviews in Computational Chemistry*, **2001**, 99-204		80
189	Excited states of thiophene: ring opening as deactivation mechanism. *Physical Chemistry Chemical Physics*, **2008**, 10, 380-92	3.6	78
188	Ab initio CI calculation of O2 + predissociation phenomena induced by a spin-orbit coupling mechanism. *Molecular Physics*, **1982**, 46, 779-810	1.7	75
187	Cyclic (Amino)(aryl)carbenes Enter the Field of Chromophore Ligands: Expanded π System Leads to Unusually Deep Red Emitting Cu Compounds. *Journal of the American Chemical Society*, **2020**, 142, 8897-8909	16.4	73
186	Efficient generation of matrix elements for one-electron spin□orbit operators. *Chemical Physics*, **2005**, 311, 71-79	2.3	70
185	Rotationally Assisted Spin-State Inversion in Carbene-Metal-Amides Is an Artifact. *Journal of Physical Chemistry Letters*, **2017**, 8, 5643-5647	6.4	65
184	Theoretical investigation of the energies and geometries of photoexcited uranyl(VI) ion: a comparison between wave-function theory and density functional theory. *Journal of Chemical Physics*, **2007**, 127, 214302	3.9	63
183	Intersystem-crossing and phosphorescence rates in fac-Ir(III)(ppy)3: a theoretical study involving multi-reference configuration interaction wavefunctions. *Journal of Chemical Physics*, **2015**, 142, 094301	3.9	61
182	The DFT/MRCI method. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1394	7.9	61
181	Time-dependent approach to spin-vibronic coupling: implementation and assessment. *Journal of Chemical Physics*, **2014**, 140, 114104	3.9	57
180	UV excitation and radiationless deactivation of imidazole. *Journal of Chemical Physics*, **2009**, 130, 034305	3.9	57

179	QM/MM calculation of solvent effects on absorption spectra of guanine. *Journal of Computational Chemistry*, **2010**, 31, 90-106	3.5	57
178	On the molecular mechanism of non-radiative decay of nitrobenzene and the unforeseen challenges this simple molecule holds for electronic structure theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 12393-406	3.6	56
177	Tautomers and electronic states of jet-cooled 2-aminopurine investigated by double resonance spectroscopy and theory. *Physical Chemistry Chemical Physics*, **2005**, 7, 3021-6	3.6	56
176	Spin□Orbit Coupling Patterns Induced by Twist and Pyramidalization Modes in C2H4:□A Quantitative Study and a Qualitative Analysis. *Journal of Physical Chemistry A*, **1998**, 102, 5923-5936	2.8	56
175	Electronic coherence provides a direct proof for energy-level crossing in photoexcited lutein and beta-carotene. *Physical Review Letters*, **2009**, 103, 108302	7.4	55
174	Photophysical properties of structurally and electronically modified flavin derivatives determined by spectroscopy and theoretical calculations. *Journal of Physical Chemistry A*, **2009**, 113, 9365-75	2.8	55
173	Empirical two-body potential for solid silicon nitride, boron nitride, and borosilazane modifications. *Physical Review B*, **2000**, 62, 3117-3124	3.3	55
172	Deactivation via ring opening: A quantum chemical study of the excited states of furan and comparison to thiophene. *Chemical Physics*, **2008**, 349, 269-277	2.3	53
171	AB initio calculation of the zero-field splittings of the X3g□and B3□g,i states of the S2 molecule. *Chemical Physics*, **1982**, 71, 79-85	2.3	49
170	Ab initio investigation of the methylation and hydration effects on the electronic spectra of uracil and thymine. *Physical Chemistry Chemical Physics*, **2010**, 12, 4915-23	3.6	48
169	Phosphorescence or Thermally Activated Delayed Fluorescence? Intersystem Crossing and Radiative Rate Constants of a Three-Coordinate Copper(I) Complex Determined by Quantum-Chemical Methods. *Inorganic Chemistry*, **2016**, 55, 7508-16	5.1	47
168	Spin-free relativistic no-pair ab initio core model potentials and valence basis sets for the transition metal elements Sc to Hg. Part I. *Journal of Chemical Physics*, **1999**, 110, 3678-3686	3.9	47
167	Determination of the radiative lifetimes of the b1□ and a1□states in NH by ab initio methods. *Chemical Physics*, **1985**, 95, 213-223	2.3	47
166	Influence of the LOV domain on low-lying excited states of flavin: a combined quantum-mechanics/molecular-mechanics investigation. *Journal of Physical Chemistry B*, **2009**, 113, 15610-8	3.4	46
165	On the performance of approximate spin□orbit Hamiltonians in light conjugated molecules: the fine-structure splitting of HC6H+, NC5H+, and NC4N+. *Chemical Physics Letters*, **1999**, 313, 351-357	2.5	46
164	On the photophysics of carotenoids: a multireference DFT study of peridinin. *Journal of Physical Chemistry B*, **2013**, 117, 13808-15	3.4	45
163	Climbing up the Ladder: Intermediate Triplet States Promote the Reverse Intersystem Crossing in the Efficient TADF Emitter ACRSA. *Journal of Physical Chemistry C*, **2017**, 121, 21145-21153	3.8	44
162	The resolution of the identity approximation for calculations of spin-spin contribution to zero-field splitting parameters. *Journal of Chemical Physics*, **2010**, 132, 144111	3.9	44

161	Vibronic absorption, fluorescence, and phosphorescence spectra of psoralen: a quantum chemical investigation. *Physical Chemistry Chemical Physics*, **2006**, 8, 2133-44	3.6	44
160	Structure analyses of Ba-silicate glasses. *Journal of Non-Crystalline Solids*, **2002**, 297, 37-54	3.9	43
159	Ultrafast dynamics in thiophene investigated by femtosecond pump probe photoelectron spectroscopy and theory. *Physical Chemistry Chemical Physics*, **2008**, 10, 393-404	3.6	42
158	Thioxanthone in apolar solvents: ultrafast internal conversion precedes fast intersystem crossing. *Physical Chemistry Chemical Physics*, **2016**, 18, 6637-47	3.6	41
157	Efficient calculation of electron paramagnetic resonance g-tensors by multireference configuration interaction sum-over-state expansions, using the atomic mean-field spin□orbit method. *Journal of Chemical Physics*, **2003**, 118, 9552-9562	3.9	41
156	Ab initio study of the vibronic and spin□orbit coupling in the X 2□u state of C2H+2. *Journal of Chemical Physics*, **1995**, 102, 7142-7149	3.9	39
155	Internal heavy atom effects in phenothiazinium dyes: enhancement of intersystem crossing via vibronic spin-orbit coupling. *Physical Chemistry Chemical Physics*, **2015**, 17, 11350-8	3.6	38
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152	Cu-F Interactions between Cationic Linear N-Heterocyclic Carbene Copper(I) Pyridine Complexes and Their Counterions Greatly Enhance Blue Luminescence Efficiency. *Inorganic Chemistry*, **2019**, 58, 5433-5445	5.1	37
151	Carotenoids and light-harvesting: from DFT/MRCI to the Tamm-Dancoff approximation. *Journal of Chemical Theory and Computation*, **2015**, 11, 655-66	6.4	37
150	AIScore chemically diverse empirical scoring function employing quantum chemical binding energies of hydrogen-bonded complexes. *Journal of Chemical Information and Modeling*, **2008**, 48, 1492-510	6.1	37
149	Understanding and Controlling Intersystem Crossing in Molecules. *Annual Review of Physical Chemistry*, **2021**, 72, 617-640	15.7	36
148	Chimeric behavior of excited thioxanthone in protic solvents: I. Experiments. *Journal of Physical Chemistry A*, **2014**, 118, 11696-707	2.8	35
147	Molecular design of two sterol 14alpha-demethylase homology models and their interactions with the azole antifungals ketoconazole and bifonazole. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 149-63	4.2	35
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145	Multireference and relativistic effects in NiH. *Journal of Chemical Physics*, **1989**, 91, 3589-3595	3.9	35
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142	Spin-free relativistic no-pair ab initio core model potentials and valence basis sets for the transition metal elements Sc to Hg. II. *Journal of Chemical Physics*, **1999**, 111, 10436-10443	3.9	34
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140	Adsorption of CO on TiO2 (110) studied by means of a cluster model surrounded by multipoles obtained from slab calculations. *Physical Review B*, **1996**, 54, 14812-14821	3.3	33
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137	Theoretical study of the spectra of CuH and CuD. *Journal of Chemical Physics*, **1991**, 94, 5574-5585	3.9	33
136	Investigation of electron correlation on the theoretical prediction of zero-field splittings of 2 molecular states. *Chemical Physics Letters*, **1982**, 89, 459-462	2.5	33
135	A quantum chemical investigation of the electronic structure of thionine. *Photochemical and Photobiological Sciences*, **2012**, 11, 397-408	4.2	31
134	An extrapolation scheme for spin orbit configuration interaction energies applied to the ground and excited electronic states of thallium hydride. *Chemical Physics*, **1997**, 225, 223-238	2.3	31
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129	Chimeric behavior of excited thioxanthone in protic solvents: II. Theory. *Journal of Physical Chemistry A*, **2014**, 118, 11708-17	2.8	29
128	Overruling the energy gap law: fast triplet formation in 6-azauracil. *Physical Chemistry Chemical Physics*, **2010**, 12, 15665-71	3.6	29
127	Theoretical study of the low-lying excited states of carotene isomers by a multireference configuration interaction method. *Chemical Physics*, **2010**, 373, 98-103	2.3	29
126	Calculation of potential energy curves for Rb2 including relativistic effects. *Molecular Physics*, **2003**, 101, 2381-2389	1.7	28

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124	Isolated and solvated thioxanthone: a photophysical study. *Journal of Physical Chemistry A*, **2011**, 115, 8589-96	2.8	26
123	Effects of protonation and deprotonation on the excitation energies of lumiflavin. *Chemical Physics Letters*, **2008**, 463, 400-404	2.5	26
122	Quantum-Chemical Studies on Excitation Energy Transfer Processes in BODIPY-Based Donor-Acceptor Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 4316-27	6.4	25
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117	On the performance of DFT/MRCI Hamiltonians for electronic excitations in transition metal complexes: The role of the damping function. *Journal of Chemical Physics*, **2018**, 149, 164106	3.9	24
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112	Computer-Aided Design of Luminescent Linear N-Heterocyclic Carbene Copper(I) Pyridine Complexes. *Inorganic Chemistry*, **2019**, 58, 5446-5456	5.1	22
111	Singlet Fission in Quinoidal Oligothiophenes. *Journal of Physical Chemistry C*, **2016**, 120, 13901-13910	3.8	22
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109	Quantum chemical investigation of hydrogen-bond strengths and partition into donor and acceptor contributions. *Journal of Computational Chemistry*, **2007**, 28, 1503-1515	3.5	22
108	The photophysics of 7H-adenine: A quantum chemical investigation including spin–orbit effects. *Chemical Physics*, **2008**, 347, 346-359	2.3	22

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106	Ab initio study of the vibronic and spin□orbit structure in the X 2□electronic state of CCCH. *Journal of Chemical Physics*, **2003**, 118, 4444-4451	3.9	22
105	The photophysics of pyranthione: a theoretical investigation focussing on spin-forbidden transitions. *Chemical Physics*, **2001**, 264, 245-254	2.3	22
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103	Comparison of the structure and spectra of the HNO+ and NOH+ ions using ab initio SCF and CI methods. *Molecular Physics*, **1977**, 33, 63-74	1.7	21
102	Electroabsorption Spectroscopy as a Tool for Probing Charge Transfer and State Mixing in Thermally Activated Delayed Fluorescence Emitters. *Journal of Physical Chemistry Letters*, **2019**, 10, 3205-3211	6.4	20
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100	Ab Initio Investigation of the Structure of the X2A?, A2A?(12□) Spectral System of HCO: Theoretical Treatment of the Vibronic and Spin-Orbit-Coupling. *Journal of Molecular Spectroscopy*, **1994**, 166, 406-422	1.3	19
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96	Ab initio prediction of 15N-NMR chemical shift in □boron nitride based on an analysis of connectivities. *Journal of Computational Chemistry*, **1998**, 19, 716-725	3.5	18
95	An Approach to the Calculation of □Splittings in Diatomic Molecules with Strongly Coupled Electronic States and its Application to NiH and NiD. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1995**, 99, 254-264		18
94	Structure-Emission Property Relationships in Cyclometalated Pt(II) □Diketonate Complexes. *Inorganic Chemistry*, **2019**, 58, 6123-6136	5.1	17
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91	On the dependence of correlation and relativity: The electron affinity of the copper atom. *Chemical Physics Letters*, **1990**, 173, 175-180	2.5	16
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89	Towards an understanding of the singlet-triplet splittings in conjugated hydrocarbons: azulene investigated by anion photoelectron spectroscopy and theoretical calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 23573-81	3.6	15
88	Spectroscopic and theoretical study on electronically modified chromophores in LOV domains: 8-bromo- and 8-trifluoromethyl-substituted flavins. *ChemBioChem*, **2013**, 14, 645-54	3.8	15
87	Quantitative structure-property relationships in boron nitrides: the 15N- and 11B chemical shifts. *Solid State Nuclear Magnetic Resonance*, **2001**, 19, 29-44	3.1	15
86	Understanding the luminescence properties of Cu(i) complexes: a quantum chemical perusal. *Physical Chemistry Chemical Physics*, **2020**, 22, 23530-23544	3.6	15
85	On the performance of DFT/MRCI-R and MR-MP2 in spin□orbit coupling calculations on diatomics and polyatomic organic molecules. *Molecular Physics*, **2017**, 115, 109-137	1.7	14
84	Accurate calculations of the ground state and low-lying excited states of the (RbBa)+molecular ion: a proposed system for ultracold reactive collisions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2010**, 43, 055101	1.3	14
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80	DFT/MRCI Hamiltonian for odd and even numbers of electrons. *Journal of Chemical Physics*, **2017**, 147, 194104	3.9	13
79	Charge-transfer contributions to the excitonic coupling matrix element in BODIPY-based energy transfer cassettes. *Chemical Physics*, **2017**, 482, 265-276	2.3	13
78	The Influence of Excess Ammonia on the Mechanism of the Reaction of Boron Trichloride with Ammonia-An Ab Initio Molecular Dynamics Study This work was supported by the Deutsche Forschungsgemeinschaft in the framework of the Sonderforschungsbereich 408 "Anorganische Festk□per ohne Translationssymmetrie". We thank Mauro Boero from the Joint Research Center	16.4	13
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66	Reverse intersystem crossing in rhodamines by near-infrared laser excitation. *Journal of Physical Chemistry A*, **2014**, 118, 6985-90	2.8	11
65	Dual Photochemical Reaction Pathway in Flavin-Based Photoreceptor LOV Domain: A Combined Quantum-Mechanics/Molecular-Mechanics Investigation. *Journal of Physical Chemistry B*, **2017**, 121, 9583-9596	3.4	11
64	Spin-forbidden transitions in flavone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 73, 1-5	4.4	11
63	Imaging spectroscopy of recombination fragments of. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1997**, 30, 4919-4933	1.3	11
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