Christel M Marian

List of Publications by Year in Descending Order

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	Linear Carbene Pyridine Copper Complexes with Sterically Demanding ,Q-Bis(trityl)imidazolylidene: Syntheses, Molecular Structures, and Photophysical Properties. *Inorganic Chemistry*, **2021**, 60, 18529-18543	5.1	7
213	Large Inverted Singlet-Triplet Energy Gaps Are Not Always Favorable for Triplet Harvesting: Vibronic Coupling Drives the (Reverse) Intersystem Crossing in Heptazine Derivatives. *Journal of Physical Chemistry A*, **2021**, 125, 10044-10051	2.8	5
212	Lowest Triplet and Singlet States in -Methylacridone and ,Q-Dimethylquinacridone: Theory and Experiment. *Journal of Physical Chemistry A*, **2021**, 125, 8777-8790	2.8	1
211	Understanding and Controlling Intersystem Crossing in Molecules. *Annual Review of Physical Chemistry*, **2021**, 72, 617-640	15.7	36
210	Acridones: Strongly Emissive HIGHrISC Fluorophores. *Journal of Physical Chemistry Letters*, **2021**, 12, 5708-5709	5.4	2
209	Intersystem crossing processes in the 2CzPN emitter: a DFT/MRCI study including vibrational spin-orbit interactions. *Physical Chemistry Chemical Physics*, **2021**, 23, 3668-3678	3.6	2
208	Internal conversion of singlet and triplet states employing numerical DFT/MRCI derivative couplings: Implementation, tests, and application to xanthone. *Journal of Chemical Physics*, **2021**, 155, 014102	3.9	3
207	Persistent Room Temperature Phosphorescence from Triarylboranes: A Combined Experimental and Theoretical Study. *Angewandte Chemie*, **2020**, 132, 17285-17292	3.6	6
206	Persistent Room Temperature Phosphorescence from Triarylboranes: A Combined Experimental and Theoretical Study. *Angewandte Chemie - International Edition*, **2020**, 59, 17137-17144	16.4	34
205	Theoretical spectroscopy in the early days of digital computing an homage to Sigrid D. Peyerimhoff. *Molecular Physics*, **2020**, 118, e1744755	1.7	
204	Visible Light-Induced Homolytic Cleavage of Perfluoroalkyl Iodides Mediated by Phosphines. *Molecules*, **2020**, 25,	4.8	6
203	On the photophysical properties of Ir, Pt, and Pd (phenylpyrazole) (phenyldipyrrin) complexes. *Physical Chemistry Chemical Physics*, **2020**, 22, 3217-3233	3.6	9
202	Understanding the luminescence properties of Cu(i) complexes: a quantum chemical perusal. *Physical Chemistry Chemical Physics*, **2020**, 22, 23530-23544	3.6	15
201	Cyclic (Amino)(aryl)carbenes Enter the Field of Chromophore Ligands: Expanded System Leads to Unusually Deep Red Emitting Cu Compounds. *Journal of the American Chemical Society*, **2020**, 142, 8897-8909	16.4	73
200	DFT/MRCI-R2018 study of the photophysics of the zinc(ii) tripyrrindione radical: non-Kasha emission?. *Physical Chemistry Chemical Physics*, **2019**, 21, 19857-19867	3.6	5
199	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
198	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

197	Computer-Aided Design of Luminescent Linear N-Heterocyclic Carbene Copper(I) Pyridine Complexes. *Inorganic Chemistry*, **2019**, 58, 5446-5456	5.1	22
196	Structure-Emission Property Relationships in Cyclometalated Pt(II) Diketonate Complexes. *Inorganic Chemistry*, **2019**, 58, 6123-6136	5.1	17
195	The UVA response of enolic dibenzoylmethane: beyond the static approach. *Photochemical and Photobiological Sciences*, **2019**, 18, 1324-1332	4.2	4
194	Vibronic and spin-orbit coupling effects in the absorption spectra of pyrazine: A quantum chemical approach. *Journal of the Serbian Chemical Society*, **2019**, 84, 819-836	0.9	4
193	The simulation of X-ray absorption spectra from ground and excited electronic states using core-valence separated DFT/MRCI. *Journal of Chemical Physics*, **2019**, 151, 144104	3.9	9
192	QM/MM Photodynamics of Retinal in the Channelrhodopsin Chimera C1C2 with OM3/MRCI. *ChemPhotoChem*, **2019**, 3, 107-116	3.3	7
191	The DFT/MRCI method. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1394	7.9	61
190	Spin-Vibronic Mechanism for Intersystem Crossing. *Chemical Reviews*, **2018**, 118, 6975-7025	68.1	377
189	Exciton energy transfer in organic light emitting diodes with thermally activated delayed fluorescence dopants. *Journal of Materials Chemistry C*, **2018**, 6, 6860-6868	7.1	8
188	Intersystem Crossing Processes in TADF Emitters **2018**, 257-296		4
187	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
186	Solvent mediated catalysis and proton-shuttling in the formation of 3-methylphthalide from a ketene intermediate. *Chemical Physics*, **2018**, 515, 750-756	2.3	
185	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
184	Nonadiabatic photodynamics and UV absorption spectrum of all-trans-octatetraene. *Physical Chemistry Chemical Physics*, **2017**, 19, 3937-3947	3.6	5
183	Modulation of the L/L Mixing in an Indole Derivative: A Position-Dependent Study Using 4-, 5-, and 6-Fluoroindole. *Journal of Physical Chemistry A*, **2017**, 121, 1597-1606	2.8	11
182	A theoretical study of low-lying singlet and triplet excited states of quinazoline, quinoxaline and phthalazine: insight into triplet formation. *Physical Chemistry Chemical Physics*, **2017**, 19, 13828-13837	3.6	7
181	Assessment of Interstate Spin-Orbit Couplings from Linear Response Amplitudes. *Journal of Chemical Theory and Computation*, **2017**, 13, 749-766	6.4	15
180	New Perspectives on an Old Issue: A Comparative MS-CASPT2 and OM2-MRCI Study of Polyenes and Protonated Schiff Bases. *Photochemistry and Photobiology*, **2017**, 93, 1345-1355	3.6	7

179	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
178	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
177	Protonation-State-Driven Photophysics in Phenothiazinium Dyes: Intersystem Crossing and Singlet-Oxygen Production. *ChemPhotoChem*, **2017**, 1, 459-469	3.3	4
176	DFT/MRCI Hamiltonian for odd and even numbers of electrons. *Journal of Chemical Physics*, **2017**, 147, 194104	3.9	13
175	Rotationally Assisted Spin-State Inversion in Carbene-Metal-Amides Is an Artifact. *Journal of Physical Chemistry Letters*, **2017**, 8, 5643-5647	6.4	65
174	Charge-transfer contributions to the excitonic coupling matrix element in BODIPY-based energy transfer cassettes. *Chemical Physics*, **2017**, 482, 265-276	2.3	13
173	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
172	Failure of the IDA in FRET Systems at Close Inter-Dye Distances Is Moderated by Frequent Low κ^2 Values. *Journal of Physical Chemistry B*, **2016**, 120, 8845-62	3.4	12
171	Singlet Fission in Quinoidal Oligothiophenes. *Journal of Physical Chemistry C*, **2016**, 120, 13901-13910	3.8	22
170	Solvent tunable photophysics of acridone: a quantum chemical perspective. *RSC Advances*, **2016**, 6, 18530-18537	3.7	37
169	Thioxanthone in apolar solvents: ultrafast internal conversion precedes fast intersystem crossing. *Physical Chemistry Chemical Physics*, **2016**, 18, 6637-47	3.6	41
168	Mechanism of the Triplet-to-Singlet Upconversion in the Assistant Dopant ACRXTN. *Journal of Physical Chemistry C*, **2016**, 120, 3715-3721	3.8	111
167	Redesign of the DFT/MRCI Hamiltonian. *Journal of Chemical Physics*, **2016**, 144, 034104	3.9	81
166	Ab Initio Benchmark Study of Nonadiabatic S1-S2 Photodynamics of cis- and trans-Hexatriene. *Journal of Physical Chemistry A*, **2016**, 120, 6541-56	2.8	6
165	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
164	Electron-Vibrational Coupling and Fluorescence Spectra of Tetra-, Penta-, and Hexacoordinated Chlorophylls c1 and c2. *Journal of Physical Chemistry B*, **2015**, 119, 10156-69	3.4	9
163	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
162	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

161	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
160	On the photophysics of four heteroleptic iridium(III) phenylpyridyl complexes investigated by relativistic multi-configuration methods. *Molecular Physics*, **2015**, 1-16	1.7	12
159	Intersystem crossing rates of S1 state keto-amino cytosine at low excess energy. *Journal of Chemical Physics*, **2015**, 143, 234301	3.9	26
158	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
157	Time-dependent approach to spin-vibronic coupling: implementation and assessment. *Journal of Chemical Physics*, **2014**, 140, 114104	3.9	57
156	Photophysics of flavin derivatives absorbing in the blue-green region: thioflavins as potential cofactors of photoswitches. *Journal of Physical Chemistry B*, **2014**, 118, 1743-53	3.4	16
155	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
154	Thermal and solvent effects on the triplet formation in cinnoline. *Physical Chemistry Chemical Physics*, **2014**, 16, 4740-51	3.6	38
153	Reverse intersystem crossing in rhodamines by near-infrared laser excitation. *Journal of Physical Chemistry A*, **2014**, 118, 6985-90	2.8	11
152	Chimeric behavior of excited thioxanthone in protic solvents: II. Theory. *Journal of Physical Chemistry A*, **2014**, 118, 11708-17	2.8	29
151	Chimeric behavior of excited thioxanthone in protic solvents: I. Experiments. *Journal of Physical Chemistry A*, **2014**, 118, 11696-707	2.8	35
150	On the photophysics of carotenoids: a multireference DFT study of peridinin. *Journal of Physical Chemistry B*, **2013**, 117, 13808-15	3.4	45
149	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
148	Photophysics of xanthone: a quantum chemical perusal. *Journal of Physical Chemistry A*, **2013**, 117, 3935-44	2.8	30
147	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
146	In search of the dark state of 5-methyl-2-hydroxypyrimidine using a numerical DFT/MRCI gradient. *Molecular Physics*, **2012**, 110, 2429-2438	1.7	5
145	A theoretical study of thionine: spin-orbit coupling and intersystem crossing. *Photochemical and Photobiological Sciences*, **2012**, 11, 1860-7	4.2	22
144	A quantum chemical investigation of the electronic structure of thionine. *Photochemical and Photobiological Sciences*, **2012**, 11, 397-408	4.2	31

143	Spin□rbit coupling and intersystem crossing in molecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 187-203	7.9	471
142	Time-dependent approaches for the calculation of intersystem crossing rates. *Journal of Chemical Physics*, **2011**, 134, 154105	3.9	106
141	On the photophysics of 1,6-diphenyl-1,3,5-hexatriene isomers and rotamers. *ChemPhysChem*, **2011**, 12, 1872-9	3.2	7
140	T1, T2 state energies and electron affinities of small □□diphenylpolyenes investigated by anion photodetachment photoelectron spectroscopy and excited-state theory. *ChemPhysChem*, **2011**, 12, 1948-56	3.2	2
139	Throwing light on dark states of □oligothiophenes of chain lengths 2 to 6: radical anion photoelectron spectroscopy and excited-state theory. *Physical Chemistry Chemical Physics*, **2011**, 13, 10350-63	3.6	33
138	Isolated and solvated thioxanthone: a photophysical study. *Journal of Physical Chemistry A*, **2011**, 115, 8589-96	2.8	26
137	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
136	Diphenylhexatrienes as photoprotective agents for ultrasensitive fluorescence detection. *Journal of Physical Chemistry A*, **2010**, 114, 4099-108	2.8	17
135	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
134	Thioxanthone: on the shape of the first absorption band. *Physical Chemistry Chemical Physics*, **2010**, 12, 9320-7	3.6	12
133	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
132	Overruling the energy gap law: fast triplet formation in 6-azauracil. *Physical Chemistry Chemical Physics*, **2010**, 12, 15665-71	3.6	29
131	QM/MM calculation of solvent effects on absorption spectra of guanine. *Journal of Computational Chemistry*, **2010**, 31, 90-106	3.5	57
130	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
129	Excited state relaxation dynamics and electronic properties of a quinoid carotenoid. *Chemical Physics*, **2010**, 373, 137-144	2.3	5
128	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
127	Calculating electron paramagnetic resonance g-matrices for triplet state molecules from multireference spin-orbit configuration interaction wave functions. *Journal of Chemical Physics*, **2009**, 130, 154106	3.9	14
126	Spin-forbidden transitions in flavone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2009**, 73, 1-5	4.4	11

125	Transient spectroscopy of UV excited flavone: Triplet–triplet absorption and comparison with theory. *Chemical Physics Letters*, **2009**, 473, 167-170	2.5	4
124	The photophysics of alloxazine: a quantum chemical investigation in vacuum and solution. *Photochemical and Photobiological Sciences*, **2009**, 8, 1655-66	4.2	30
123	Four-component relativistic coupled cluster and configuration interaction calculations on the ground and excited states of the RbYb molecule. *Journal of Physical Chemistry A*, **2009**, 113, 12607-14	2.8	34
122	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
121	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
120	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
119	Photophysics of phenalenone: quantum-mechanical investigation of singlet-triplet intersystem crossing. *Physical Chemistry Chemical Physics*, **2009**, 11, 1688-96	3.6	25
118	Parallel multireference configuration interaction calculations on mini-beta-carotenes and beta-carotene. *Journal of Chemical Physics*, **2009**, 130, 044708	3.9	97
117	Spectroscopic properties of phenolic and quinoid carotenoids: a combined theoretical and experimental study. *Photochemical and Photobiological Sciences*, **2009**, 8, 270-8	4.2	18
116	UV excitation and radiationless deactivation of imidazole. *Journal of Chemical Physics*, **2009**, 130, 034305	3.9	57
115	Performance of the Density Functional Theory/Multireference Configuration Interaction Method on Electronic Excitation of Extended π-Systems. *Journal of Chemical Theory and Computation*, **2008**, 4, 1501-15	6.4	152
114	Electron spin-spin coupling from multireference configuration interaction wave functions. *Journal of Chemical Physics*, **2008**, 129, 044102	3.9	24
113	Ultrafast dynamics in thiophene investigated by femtosecond pump probe photoelectron spectroscopy and theory. *Physical Chemistry Chemical Physics*, **2008**, 10, 393-404	3.6	42
112	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	4.1	37
111	The photophysics of 7H-adenine: A quantum chemical investigation including spin–orbit effects. *Chemical Physics*, **2008**, 347, 346-359	2.3	22
110	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
109	Stepwise conversion of a single source precursor into crystalline AlN by transamination reaction. *Journal of Solid State Chemistry*, **2008**, 181, 530-538	3.3	5
108	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

107	Spin□rbit coupling in keto-porphyrins. *Chemical Physics Letters*, **2008**, 458, 190-194	2.5	7
106	Effects of protonation and deprotonation on the excitation energies of lumiflavin. *Chemical Physics Letters*, **2008**, 463, 400-404	2.5	26
105	The g-tensor of AlO: Principal problems and first approaches. *Chemical Physics*, **2008**, 343, 258-269	2.3	22
104	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
103	Excited states of thiophene: ring opening as deactivation mechanism. *Physical Chemistry Chemical Physics*, **2008**, 10, 380-92	3.6	78
102	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
101	Intersystem crossing driven by vibronic spin-orbit coupling: a case study on psoralen. *Physical Chemistry Chemical Physics*, **2007**, 9, 5209-21	3.6	103
100	The guanine tautomer puzzle: quantum chemical investigation of ground and excited states. *Journal of Physical Chemistry A*, **2007**, 111, 1545-53	2.8	162
99	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
98	Reverse Monte Carlo modelling of amorphous Si3B3N7using scattering and15N NMR data. *Journal of Physics Condensed Matter*, **2007**, 19, 056201	1.8	2
97	The 15N chemical shifts in mixed NB2Si and NBSi2 environments of Si3B3N7--a theoretical investigation. *Solid State Nuclear Magnetic Resonance*, **2006**, 30, 16-28	3.1	4
96	The UV/Vis Spectrum of Potassium Heptacyanovanadate(III): A Theoretical Multi-Reference Configuration Interaction Study Combined with Low-Temperature Experiments. *European Journal of Inorganic Chemistry*, **2006**, 2006, 1588-1593	2.3	2
95	Electronically excited states of tryptamine and its microhydrated complex. *Journal of Chemical Physics*, **2006**, 125, 124309	3.9	25
94	SPOCK.CI: a multireference spin-orbit configuration interaction method for large molecules. *Journal of Chemical Physics*, **2006**, 124, 124101	3.9	85
93	Fully automated flexible docking of ligands into flexible synthetic receptors using forward and inverse docking strategies. *Journal of Chemical Information and Modeling*, **2006**, 46, 903-11	6.1	23
92	Vibronic absorption, fluorescence, and phosphorescence spectra of psoralen: a quantum chemical investigation. *Physical Chemistry Chemical Physics*, **2006**, 8, 2133-44	3.6	44
91	The electronic spectrum of protonated adenine: theory and experiment. *Physical Chemistry Chemical Physics*, **2005**, 7, 3306-16	3.6	85
90	Carboborosilazane ceramics: initial reactions between TSDE and methylamine □a combined quantum chemical and first principles molecular dynamics study. *Journal of Non-Crystalline Solids*, **2005**, 351, 1113-1120	3.9	

89	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
88	A new pathway for the rapid decay of electronically excited adenine. *Journal of Chemical Physics*, **2005**, 122, 104314	3.9	211
87	Efficient generation of matrix elements for one-electron spin□orbit operators. *Chemical Physics*, **2005**, 311, 71-79	2.3	70
86	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
85	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
84	Electronic excitation spectra and singlet□triplet coupling in psoralen and its sulfur and selenium analogs. *Journal of Photochemistry and Photobiology A: Chemistry*, **2004**, 167, 201-212	4.7	19
83	Protonation effect on the electronic spectrum of tryptophan in the gas phase. *Physical Chemistry Chemical Physics*, **2004**, 6, 2633	3.6	99
82	Quantum Chemical Investigation of Spin-Forbidden Transitions in Dithiosuccinimide. *Zeitschrift Fur Physikalische Chemie*, **2003**, 217, 205-230	3.1	5
81	Charged-particle potential for boron nitrides, silicon nitrides, and borosilazane ceramics: Derivation of parameters and probing of capabilities. *Physical Review B*, **2003**, 68,	3.3	14
80	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
79	Calculation of potential energy curves for Rb2 including relativistic effects. *Molecular Physics*, **2003**, 101, 2381-2389	1.7	28
78	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
77	Kramers-Type Splitting in the X2□and a4□States of CH and CD Calculated in a Hund□s Case (a) Basis. *Journal of Molecular Spectroscopy*, **2002**, 211, 179-188	1.3	9
76	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
75	Electronic excitation and singlet-triplet coupling in uracil tautomers and uracil-water complexes. *European Physical Journal D*, **2002**, 20, 357-367	1.3	80
74	Quantum Chemical Investigation of Initial Reactions between the Molecular Precursor TADB and Ammonia. 1. Gas-Phase Reactions. *Journal of Physical Chemistry A*, **2002**, 106, 4205-4216	2.8	6
73	Structure analyses of Ba-silicate glasses. *Journal of Non-Crystalline Solids*, **2002**, 297, 37-54	3.9	43
72	The photophysics of pyranthione: a theoretical investigation focussing on spin-forbidden transitions. *Chemical Physics*, **2001**, 264, 245-254	2.3	22

71	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
70	Der Einfluss eines Ammoniak□berschusses auf den Mechanismus der Reaktion von Bortrichlorid mit Ammoniak □eine Ab-initio-Molek□□dynamik-Untersuchung. *Angewandte Chemie*, **2001**, 113, 3795-3797	3.6	5
69	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 for Atom Technology, Tsukuba (Japan) for the reoptimization of the Martins-Troullier pseudopotentials for boron and chlorine, as well as the John-von-Neum. *Angewandte Chemie - International Edition*, **2001**, 40, 3683-3685	16.4	13
68	Spin-Orbit Coupling in Molecules. *Reviews in Computational Chemistry*, **2001**, 99-204		80
67	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
66	Simulation of the Solid State Vibrational Spectra of Aminodichloroborane and Ammonia Boron Trichloride. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2000**, 626, 1871-1880	1.3	3
65	A systematic theoretical study of molecular Si/N, B/N, and Si/B/N(H) compounds and parameterisation of a force-field for molecules and solids. *Computational and Theoretical Chemistry*, **2000**, 506, 107-129		8
64	Empirical two-body potential for solid silicon nitride, boron nitride, and borosilazane modifications. *Physical Review B*, **2000**, 62, 3117-3124	3.3	55
63	Ground and excited states of PtCH2+: assessment of the no-pair Douglas□Kroll ab initio model potential method. *Physical Chemistry Chemical Physics*, **2000**, 2, 2481-2488	3.6	23
62	Reactions in the initial stage of the CVD of BN□ quantum chemical investigation. *Physical Chemistry Chemical Physics*, **2000**, 2, 955-963	3.6	12
61	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
60	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
59	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
58	[(Trichlorosilyl)dichloroboryl]ethane: Synthesis and Characterisation by Means of Experiment and Theory. *European Journal of Inorganic Chemistry*, **1999**, 1999, 75-81	2.3	9
57	Theoretical investigation of the Renner-Teller effect in □electronic states of tetra-atomic molecules. 1. Variational calculation of vibronic structure in the 11□ state of B2H2. *Molecular Physics*, **1999**, 97, 731-742	1.7	9
56	Calculation of predissociation rates in O22+ by ab initio MRD-CI methods. *Chemical Physics*, **1998**, 229, 203-216	2.3	18
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