Mario Barbatti

List of Publications by Year in Descending Order

178 papers	7,379 citations	46 h-index	80 g-index
201 ext. papers	8,234 ext. citations	5 avg, IF	6.62 L-index

#	Paper	IF	Citations
178	Electron delocalisation in conjugated sulfur heterocycles probed by resonant Auger spectroscopy.. *Physical Chemistry Chemical Physics*, **2022**, 24, 8477-8487	3.6	0
177	Simulations of molecular photodynamics in long timescales.. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2022**, 380, 20200382	3	5
176	MLatom 2: An Integrative Platform for Atomistic Machine Learning. *Topics in Current Chemistry Collections*, **2022**, 13-53	1.8	0
175	Towards developing novel and sustainable molecular light-to-heat converters.. *Chemical Science*, **2021**, 12, 15239-15252	9.4	2
174	How the Size and Density of Charge-Transfer Excitons Depend on Heterojunction Architecture. *Journal of Physical Chemistry C*, **2021**, 125, 5458-5474	3.8	3
173	Velocity Adjustment in Surface Hopping: Ethylene as a Case Study of the Maximum Error Caused by Direction Choice. *Journal of Chemical Theory and Computation*, **2021**, 17, 3010-3018	6.4	12
172	Molecular excited states through a machine learning lens. *Nature Reviews Chemistry*, **2021**, 5, 388-405	34.6	38
171	MLatom 2: An Integrative Platform for Atomistic Machine Learning. *Topics in Current Chemistry*, **2021**, 379, 27	7.2	15
170	Mechanistic Aspects of the Photophysics of UVA Filters Based on Meldrum Derivatives. *Journal of Physical Chemistry A*, **2021**, 125, 5499-5508	2.8	2
169	New Generation UV-A Filters: Understanding Their Photodynamics on a Human Skin Mimic. *Journal of Physical Chemistry Letters*, **2021**, 12, 337-344	6.4	7
168	Choosing the right molecular machine learning potential. *Chemical Science*, **2021**, 12, 14396-14413	9.4	21
167	Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. *Journal of Chemical Physics*, **2021**, 154, 044306	3.9	6
166	Simulation of Excitation by Sunlight in Mixed Quantum-Classical Dynamics. *Journal of Chemical Theory and Computation*, **2020**, 16, 4849-4856	6.4	8
165	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
164	Time-Dependent Density Functional Theory **2020**, 13-46		6
163	Machine Learning for Absorption Cross Sections. *Journal of Physical Chemistry A*, **2020**, 124, 7199-7210	2.8	27
162	Nonadiabatic dynamics in multidimensional complex potential energy surfaces. *Chemical Science*, **2020**, 11, 9827-9835	9.4	6

161	On the origin of the shift between vertical excitation and band maximum in molecular photoabsorption. *Journal of Molecular Modeling*, **2020**, 26, 107	2	22
160	Nonadiabatic Dynamics of Charge-Transfer States Using the Anthracene-Tetracyanoethylene Complex as a Prototype. *Journal of Physical Chemistry A*, **2020**, 124, 3347-3357	2.8	8
159	Modulating Electron Transfer in an Organic Reaction via Chemical Group Modification of the Photocatalyst. *Journal of Physical Chemistry Letters*, **2019**, 10, 5634-5639	6.4	3
158	Dynamics of benzene excimer formation from the parallel-displaced dimer. *Physical Chemistry Chemical Physics*, **2019**, 21, 13916-13924	3.6	16
157	Ultrafast Photoinduced Dynamics of 1,3-Cyclohexadiene Using XMS-CASPT2 Surface Hopping. *Journal of Chemical Theory and Computation*, **2019**, 15, 3929-3940	6.4	30
156	Promoting Intersystem Crossing of a Fluorescent Molecule via Single Functional Group Modification. *Journal of Physical Chemistry Letters*, **2019**, 10, 1388-1393	6.4	9
155	Mechanism of Spin-Exchange Internal Conversion: Practical Proxies for Diabatic and Nonadiabatic Couplings. *Journal of Chemical Theory and Computation*, **2019**, 15, 1503-1513	6.4	6
154	Photoinduced Formation of H-Bonded Ion Pair in HCFC-133a. *Journal of Physical Chemistry A*, **2019**, 123, 1953-1961	2.8	6
153	Stereoselective Excited-State Isomerization and Decay Paths in -Cyclobiazobenzene. *Journal of Physical Chemistry A*, **2019**, 123, 6144-6151	2.8	1
152	On-the-fly dynamics simulations of transient anions. *Journal of Chemical Physics*, **2019**, 151, 224104	3.9	9
151	Nuclear Ensemble Approach with Importance Sampling. *Journal of Chemical Theory and Computation*, **2018**, 14, 3173-3183	6.4	14
150	The effect of hydrogen bonding on the nonadiabatic dynamics of a thymine-water cluster. *Chemical Physics*, **2018**, 515, 472-479	2.3	7
149	Photochemistry of CFCl: Quenching of Charged Fragments Is Caused by Nonadiabatic Effects. *Journal of Chemical Theory and Computation*, **2018**, 14, 4844-4855	6.4	7
148	Multireference Approaches for Excited States of Molecules. *Chemical Reviews*, **2018**, 118, 7293-7361	68.1	181
147	Intersystem crossing dynamics in singly substituted thiouracil studied by time-resolved photoelectron spectroscopy: Micro-environmental effects due to sulfur position. *Chemical Physics*, **2018**, 515, 572-579	2.3	12
146	High-Resolution Near-Edge X-ray Absorption Fine Structure Study of Condensed Polyacenes. *Journal of Physical Chemistry C*, **2018**, 122, 28692-28701	3.8	7
145	Nonadiabatic dynamics simulations of photoexcited urocanic acid. *Chemical Physics*, **2018**, 515, 521-534	2.3	8
144	Nonadiabatic Excited-State Dynamics with Machine Learning. *Journal of Physical Chemistry Letters*, **2018**, 9, 5660-5663	6.4	87

143	Mechanism of enhanced triplet decay of thionucleobase by glycosylation and rate-modulating strategies. *Physical Chemistry Chemical Physics*, **2018**, 20, 16428-16436	3.6	5
142	Recent Advances and Perspectives on Nonadiabatic Mixed Quantum-Classical Dynamics. *Chemical Reviews*, **2018**, 118, 7026-7068	68.1	270
141	Model Systems for Dynamics of π-Conjugated Biomolecules in Excited States **2017**, 1697-1739		1
140	Tailoring the Schiff base photoswitching - a non-adiabatic molecular dynamics study of substituent effect on excited state proton transfer. *Physical Chemistry Chemical Physics*, **2017**, 19, 5318-5325	3.6	25
139	On the decay of the triplet state of thionucleobases. *Physical Chemistry Chemical Physics*, **2017**, 19, 12674-12682	3.6	28
138	The photophysics of naphthalene dimers controlled by sulfur bridge oxidation. *Chemical Science*, **2017**, 8, 4941-4950	9.4	11
137	Evaluation of Spin-Orbit Couplings with Linear-Response Time-Dependent Density Functional Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 515-524	6.4	152
136	Spatial Factors for Triplet Fusion Reaction of Singlet Oxygen Photosensitization. *Journal of Physical Chemistry Letters*, **2017**, 8, 5456-5460	6.4	9
135	Divide-to-Conquer: A Kinetic Model for Singlet Oxygen Photosensitization. *Journal of Chemical Theory and Computation*, **2017**, 13, 5528-5538	6.4	11
134	Hot and Cold Charge-Transfer Mechanisms in Organic Photovoltaics: Insights into the Excited States of Donor/Acceptor Interfaces. *Journal of Physical Chemistry Letters*, **2017**, 8, 4727-4734	6.4	30
133	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. *Journal of Chemical Theory and Computation*, **2017**, 13, 5846-5860	6.4	33
132	A three-state model for the photo-Fries rearrangement. *Physical Chemistry Chemical Physics*, **2017**, 19, 19103-19108	3.6	5
131	Insights on the Auxochromic Properties of the Guanidinium Group. *Journal of Physical Chemistry A*, **2016**, 120, 7088-100	2.8	13
130	Why Replacing Different Oxygens of Thymine with Sulfur Causes Distinct Absorption and Intersystem Crossing. *Journal of Physical Chemistry A*, **2016**, 120, 6342-50	2.8	36
129	Photochemistry of CH3Cl: Dissociation and CH···Cl Hydrogen Bond Formation. *Journal of the American Chemical Society*, **2016**, 138, 272-80	16.4	21
128	Unveiling the Role of Hot Charge-Transfer States in Molecular Aggregates via Nonadiabatic Dynamics. *Journal of the American Chemical Society*, **2016**, 138, 4502-11	16.4	32
127	Surface Hopping Dynamics with DFT Excited States. *Topics in Current Chemistry*, **2016**, 368, 415-44		48
126	Model Systems for Dynamics of π-Conjugated Biomolecules in Excited States **2016**, 1-43		

125	New Insights into the State Trapping of UV-Excited Thymine. *Molecules*, **2016**, 21,	4.8	23
124	Effects of different initial condition samplings on photodynamics and spectrum of pyrrole. *International Journal of Quantum Chemistry*, **2016**, 116, 762-771	2.1	90
123	UV-photoexcitation and ultrafast dynamics of HCFC-132b (CF2 ClCH2 Cl). *Journal of Computational Chemistry*, **2016**, 37, 675-83	3.5	4
122	UV excitations of halons. *Journal of Chemical Physics*, **2016**, 145, 184306	3.9	6
121	Steady and Time-Resolved Photoelectron Spectra Based on Nuclear Ensembles. *Journal of Chemical Theory and Computation*, **2016**, 12, 5037-5049	6.4	27
120	Photochemistry of methyl hypobromite (CH3OBr): excited states and photoabsorption spectrum. *RSC Advances*, **2015**, 5, 97003-97015	3.7	2
119	Excited-State Proton Transfer Can Tune the Color of Protein Fluorescent Markers. *ChemPhysChem*, **2015**, 16, 3444-9	3.2	17
118	Modeling ultrafast exciton deactivation in oligothiophenes via nonadiabatic dynamics. *Physical Chemistry Chemical Physics*, **2015**, 17, 7787-99	3.6	38
117	Why water makes 2-aminopurine fluorescent?. *Physical Chemistry Chemical Physics*, **2015**, 17, 15452-9	3.6	24
116	Stepwise double excited-state proton transfer is not possible in 7-azaindole dimer. *Chemical Science*, **2015**, 6, 5762-5767	9.4	42
115	Absorption and fluorescence spectra of poly(p-phenylenevinylene) (PPV) oligomers: an ab initio simulation. *Journal of Physical Chemistry A*, **2015**, 119, 1787-95	2.8	17
114	Photoinduced Phenomena in Nucleic Acids II. *Topics in Current Chemistry*, **2015**,		10
113	Photoinduced processes in nucleic acids. *Topics in Current Chemistry*, **2015**, 355, 1-32		27
112	Electronic structure of fullerene-squaraine complexes for photovoltaic devices. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 237-242	2	5
111	Computational reference data for the photochemistry of cyclobutane pyrimidine dimers. *ChemPhysChem*, **2014**, 15, 3342-54	3.2	18
110	Photo-stability of peptide-bond aggregates: N-methylformamide dimers. *Physical Chemistry Chemical Physics*, **2014**, 16, 18877-87	3.6	17
109	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1395-405	6.4	139
108	Structure□unction Relationships of High-Electron Mobility Naphthalene Diimide Copolymers Prepared Via Direct Arylation. *Chemistry of Materials*, **2014**, 26, 6233-6240	9.6	94

107	Effects of the second hydration shell on excited-state multiple proton transfer: dynamics simulations of 7-azaindole:(H2O)15 clusters in the gas phase. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	10
106	Photorelaxation induced by water-chromophore electron transfer. *Journal of the American Chemical Society*, **2014**, 136, 10246-9	16.4	75
105	Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 26-33	7.9	280
104	Photochemical deactivation process of HCFC-133a (C2H2F3Cl): a nonadiabatic dynamics study. *Journal of Physical Chemistry A*, **2014**, 118, 12041-9	2.8	13
103	Guanidine and guanidinium cation in the excited state--theoretical investigation. *Journal of Chemical Physics*, **2014**, 141, 074307	3.9	4
102	Nonadiabatic dynamics study of methaniminium with ORMAS: Challenges of incomplete active spaces in dynamics simulations. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 158-166	2	6
101	Spectrum simulation and decomposition with nuclear ensemble: formal derivation and application to benzene, furan and 2-phenylfuran. *Highlights in Theoretical Chemistry*, **2014**, 89-102		2
100	Electronic states of porphycene-O2 complex and photoinduced singlet O2 production. *Journal of Chemical Physics*, **2013**, 139, 074307	3.9	6
99	Theoretical study on excited-state intermolecular proton transfer reactions of 1H-pyrrolo[3,2-h]quinoline with water and methanol. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	11
98	Interfacial States in Donor-Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions. *Journal of Chemical Theory and Computation*, **2013**, 9, 533-42	6.4	36
97	Dynamics simulations of excited-state triple proton transfer in 7-azaindole complexes with water, water–methanol and methanol. *Journal of Photochemistry and Photobiology A: Chemistry*, **2013**, 266, 28-36	4.7	14
96	Photochemical steps in the prebiotic synthesis of purine precursors from HCN. *Angewandte Chemie - International Edition*, **2013**, 52, 8000-3	16.4	27
95	Nonadiabatic photodynamics of a retinal model in polar and nonpolar environment. *Journal of Physical Chemistry A*, **2013**, 117, 2790-9	2.8	50
94	Photochemistry of N-methylformamide: matrix isolation and nonadiabatic dynamics. *ChemPhysChem*, **2013**, 14, 827-36	3.2	12
93	Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. *Molecular Physics*, **2013**, 111, 2439-2450	1.7	37
92	Photochemical Steps in the Prebiotic Synthesis of Purine Precursors from HCN. *Angewandte Chemie*, **2013**, 125, 8158-8161	3.6	9
91	Electronically excited states and photodynamics: a continuing challenge. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	69
90	Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine. *Journal of Chemical Physics*, **2012**, 137, 22A503	3.9	90

89	Theoretical characterization of absorption and emission spectra of an asymmetric porphycene. *Journal of Physical Chemistry A*, **2012**, 116, 3366-76	2.8	9
88	Electronic spectra of nitroethylene. *International Journal of Quantum Chemistry*, **2012**, 112, 1225-1232	2.1	9
87	Does the H+5 hydrogen cluster exist in dense interstellar clouds?. *International Journal of Quantum Chemistry*, **2012**, 112, 3169-3173	2.1	1
86	Model Systems for Dynamics of Conjugated Biomolecules in Excited States **2012**, 1175-1213		1
85	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2'-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 9016-25	3.6	60
84	Spectrum simulation and decomposition with nuclear ensemble: formal derivation and application to benzene, furan and 2-phenylfuran. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	175
83	Cis-transphotoisomerization of azobenzene upon excitation to the S1state: an ab initio molecular dynamics and QM/MM study **2012**,		1
82	Experimental and theoretical investigations on photoabsorption and photoionization of trimethylphosphate in the vacuum-ultraviolet energy range. *Journal of Chemical Physics*, **2012**, 137, 184305	3.9	7
81	Surface hopping dynamics using a locally diabatic formalism: charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. *Journal of Chemical Physics*, **2012**, 137, 22A514	3.9	139
80	Electronically excited states and photodynamics: a continuing challenge **2012**, 147-160		1
79	Computational and Methodological Elements for Nonadiabatic Trajectory Dynamics Simulations of Molecules. *Advanced Series in Physical Chemistry*, **2011**, 415-462		16
78	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. *Physical Chemistry Chemical Physics*, **2011**, 13, 6145-55	3.6	79
77	Nonadiabatic dynamics of uracil: population split among different decay mechanisms. *Journal of Physical Chemistry A*, **2011**, 115, 5247-55	2.8	77
76	The decay mechanism of photoexcited guanine - a nonadiabatic dynamics study. *Journal of Chemical Physics*, **2011**, 134, 014304	3.9	66
75	Nonadiabatic molecular dynamics study of the cis-trans photoisomerization of azobenzene excited to the S1 state. *Journal of Physical Chemistry A*, **2011**, 115, 11136-43	2.8	97
74	Nonadiabatic dynamics with trajectory surface hopping method. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 620-633	7.9	302
73	Theoretical study of the excitation spectrum of azomethane. *Chemical Physics*, **2011**, 380, 9-16	2.3	13
72	Influence of the active space on CASSCF nonadiabatic dynamics simulations. *International Journal of Quantum Chemistry*, **2011**, 111, 3307-3315	2.1	17

71	Ultrafast dynamics of UV-excited imidazole. *ChemPhysChem*, **2011**, 12, 3365-75	3.2	32
70	The role of tautomers in the UV absorption of urocanic acid. *Physical Chemistry Chemical Physics*, **2011**, 13, 4686-92	3.6	26
69	Ionization potentials of adenine along the internal conversion pathways. *Physical Chemistry Chemical Physics*, **2011**, 13, 15492-500	3.6	25
68	Excited-state intermolecular proton transfer reactions of 7-azaindole(MeOH)(n) (n = 1-3) clusters in the gas phase: on-the-fly dynamics simulation. *Journal of Physical Chemistry A*, **2011**, 115, 14129-36	2.8	39
67	Cr(CO)6 photochemistry: semi-classical study of UV absorption spectral intensities and dynamics of photodissociation. *Journal of Chemical Physics*, **2011**, 134, 164305	3.9	24
66	Texture Evolution during Cold Rolling and Annealing in Dual Phase Steels. *Materials Science Forum*, **2011**, 702-703, 778-781	0.4	2
65	TORSIONAL POTENTIALS AND FULL-DIMENSIONAL SIMULATION OF ELECTRONIC ABSORPTION SPECTRA OF para-PHENYLENEVINYLENE OLIGOMERS USING SEMIEMPIRICAL HAMILTONIANS. *Journal of Theoretical and Computational Chemistry*, **2010**, 09, 249-263	1.8	13
64	Does stacking restrain the photodynamics of individual nucleobases?. *Journal of the American Chemical Society*, **2010**, 132, 8261-3	16.4	64
63	Photodynamics of azomethane: a nonadiabatic surface-hopping study. *Journal of Physical Chemistry A*, **2010**, 114, 8778-85	2.8	29
62	Azomethane: nonadiabatic photodynamical simulations in solution. *Journal of Physical Chemistry A*, **2010**, 114, 12585-90	2.8	39
61	Nonadiabatic excited-state dynamics with hybrid ab initio quantum-mechanical/molecular-mechanical methods: solvation of the pentadieniminium cation in apolar media. *Journal of Physical Chemistry A*, **2010**, 114, 6757-65	2.8	67
60	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 21453-8	11.5	323
59	The UV absorption of nucleobases: semi-classical ab initio spectra simulations. *Physical Chemistry Chemical Physics*, **2010**, 12, 4959-67	3.6	179
58	The effect of C5 substitution on the photochemistry of uracil. *Physical Chemistry Chemical Physics*, **2010**, 12, 4924-33	3.6	19
57	Effect of substituents on the excited-state dynamics of the modified DNA bases 2,4-diaminopyrimidine and 2,6-diaminopurine. *Physical Chemistry Chemical Physics*, **2010**, 12, 5375-88	3.6	25
56	Matrix-controlled photofragmentation of formamide: dynamics simulation in argon by nonadiabatic QM/MM method. *Physical Chemistry Chemical Physics*, **2010**, 12, 12719-26	3.6	26
55	Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 77-106	0.7	6
54	The photodynamics of 2,4-diaminopyrimidine in comparison with 4-aminopyrimidine: The effect of amino-substitution. *Chemical Physics Letters*, **2010**, 497, 129-134	2.5	14

53	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. *Chemical Physics*, **2010**, 375, 26-34	2.3	115
52	Dynamics starting at a conical intersection: application to the photochemistry of pyrrole. *Journal of Chemical Physics*, **2009**, 131, 024312	3.9	48
51	Excited-state diproton transfer in [2,2'-bipyridyl]-3,3'-diol: the mechanism is sequential, not concerted. *Journal of Physical Chemistry A*, **2009**, 113, 8490-9	2.8	96
50	The electronically excited states of RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine): Vertical excitations. *International Journal of Quantum Chemistry*, **2009**, 109, 2348-2355	2.1	25
49	Optimization of mixed quantum-classical dynamics: Time-derivative coupling terms and selected couplings. *Chemical Physics*, **2009**, 356, 147-152	2.3	90
48	Is the photoinduced isomerization in retinal protonated Schiff bases a single- or double-torsional process?. *Journal of Physical Chemistry A*, **2009**, 113, 11907-18	2.8	37
47	Photodynamics simulations of thymine: relaxation into the first excited singlet state. *Journal of Physical Chemistry A*, **2009**, 113, 12686-93	2.8	82
46	Excited-state non-adiabatic dynamics simulations of pyrrole. *Molecular Physics*, **2009**, 107, 845-854	1.7	64
45	Ultrafast internal conversion pathway and mechanism in 2-(2'-hydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems. *Physical Chemistry Chemical Physics*, **2009**, 11, 1406-15	3.6	154
44	UV excitation and radiationless deactivation of imidazole. *Journal of Chemical Physics*, **2009**, 130, 034305	3.9	57
43	Nonadiabatic deactivation of 9H-adenine: a comprehensive picture based on mixed quantum-classical dynamics. *Journal of the American Chemical Society*, **2008**, 130, 6831-9	16.4	178
42	Torsional potentials and full-dimensional simulation of electronic absorption and fluorescence spectra of para-phenylene oligomers using the semiempirical self-consistent charge density-functional tight binding approach. *Journal of Chemical Physics*, **2008**, 129, 164905	3.9	20
41	Mechanism of Ultrafast Photodecay in Restricted Motions in Protonated Schiff Bases: The Pentadieniminium Cation. *Journal of Chemical Theory and Computation*, **2008**, 4, 1189-99	6.4	30
40	Photophysics and deactivation pathways of thymine. *Journal of Physical Chemistry A*, **2008**, 112, 8273-9	2.8	66
39	Nonadiabatic excited-state dynamics of polar pi-systems and related model compounds of biological relevance. *Physical Chemistry Chemical Physics*, **2008**, 10, 482-94	3.6	76
38	Nonadiabatic Excited-State Dynamics of Aromatic Heterocycles: Toward the Time-Resolved Simulation of Nucleobases. *Challenges and Advances in Computational Chemistry and Physics*, **2008**, 209-235	0.7	4
37	Quantum chemical calculations of electronically excited states: formamide, its protonated form and alkali cation complexes as case studies. *Monatshefte Fü Chemie*, **2008**, 139, 319-328	1.4	19
36	Ab initio study of the photochemistry of aminopyrimidine. *International Journal of Quantum Chemistry*, **2008**, 108, 1266-1276	2.1	12

35	The effect of protonation on the photodissociation processes in formamide An ab initio surface hopping dynamics study. *Chemical Physics*, **2008**, 349, 308-318	2.3	20
34	Sensitivity of femtosecond quantum dynamics and control with respect to non-adiabatic couplings: Model simulations for the cis trans isomerization of the dideuterated methaniminium cation. *Chemical Physics*, **2008**, 350, 145-153	2.3	15
33	Theoretical investigation of the mode-specific induced non-radiative decay in 2-pyridone. *Chemical Physics*, **2008**, 349, 278-286	2.3	15
32	The interplay of skeletal deformations and ultrafast excited-state intramolecular proton transfer: Experimental and theoretical investigation of 10-hydroxybenzo[h]quinoline. *Chemical Physics*, **2008**, 347, 446-461	2.3	82
31	Simulation of the photodeactivation of formamide in the nO-pi* and pi-pi* states: an ab initio on-the-fly surface-hopping dynamics study. *Journal of Chemical Physics*, **2007**, 127, 234303	3.9	42
30	Can the nonadiabatic photodynamics of aminopyrimidine be a model for the ultrafast deactivation of adenine?. *Journal of Physical Chemistry A*, **2007**, 111, 2852-8	2.8	61
29	An ab initio study of the excited States, isomerization energy profiles and conical intersections of a chiral cyclohexylidene derivative. *Journal of Physical Chemistry A*, **2007**, 111, 238-43	2.8	16
28	Experimental and theoretical study of S 2p and C 1s spectroscopy in CS2. *Journal of Electron Spectroscopy and Related Phenomena*, **2007**, 156-158, 158-163	1.7	4
27	Experimental and theoretical study of S 2p and C 1s generalized oscillator strengths in CS2. *Journal of Electron Spectroscopy and Related Phenomena*, **2007**, 155, 21-27	1.7	3
26	The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems. *Journal of Photochemistry and Photobiology A: Chemistry*, **2007**, 190, 228-240	4.7	366
25	Nonadiabatic Ab Initio Surface-Hopping Dynamics Calculation in a Grid Environment First Experiences **2007**, 281-294		1
24	Excited-state properties and environmental effects for protonated schiff bases: a theoretical study. *ChemPhysChem*, **2006**, 7, 2089-96	3.2	42
23	Automerization reaction of cyclobutadiene and its barrier height: an ab initio benchmark multireference average-quadratic coupled cluster study. *Journal of Chemical Physics*, **2006**, 125, 64310	3.9	87
22	Ultrafast two-step process in the non-adiabatic relaxation of the CH2 molecule. *Molecular Physics*, **2006**, 104, 1053-1060	1.7	60
21	The nonadiabatic deactivation paths of pyrrole. *Journal of Chemical Physics*, **2006**, 125, 164323	3.9	99
20	Multiple pathways in the photodynamics of a polar bond: A case study of silaethylene. *Chemical Physics Letters*, **2006**, 418, 377-382	2.5	30
19	A multireference configuration interaction investigation of the excited-state energy surfaces of fluoroethylene (C2H3F). *Journal of Physical Chemistry A*, **2005**, 109, 5168-75	2.8	34
18	The photodynamics of ethylene: a surface-hopping study on structural aspects. *Journal of Chemical Physics*, **2005**, 122, 174307	3.9	68

17	High-Level Quantum Chemical Methods for the Study of Photochemical Processes. *Lecture Notes in Computer Science*, **2005**, 1004-1011	0.9	5
16	Semiempirical molecular dynamics investigation of the excited state lifetime of ethylene. *Chemical Physics Letters*, **2005**, 401, 276-281	2.5	65
15	Young-type interference pattern in molecular inner-shell excitations by electron impact. *Physical Review A*, **2005**, 72,	2.6	6
14	Generalized oscillator strength for core excitations of nitrous oxide. *Chemical Physics*, **2004**, 299, 83-88	2.3	9
13	Photochemistry of ethylene: a multireference configuration interaction investigation of the excited-state energy surfaces. *Journal of Chemical Physics*, **2004**, 121, 11614-24	3.9	150
12	Vibrational analysis of small Hn+ hydrogen clusters. *Journal of Chemical Physics*, **2003**, 119, 5444-5448	3.9	22
11	On the formation mechanisms of hydrogen ionic clusters. *Brazilian Journal of Physics*, **2003**, 33, 792-797	1.2	5
10	Generalized oscillator strengths for C 1s excitation of acetylene and ethylene. *Journal of Electron Spectroscopy and Related Phenomena*, **2002**, 123, 303-314	1.7	16
9	Clustering of Hydrogen Molecules around a Molecular Cation: The Li3+(H2)n Clusters (n = 1 6). *Journal of Physical Chemistry A*, **2002**, 106, 551-555	2.8	17
8	The structure and the thermochemical properties of the H3+(H2)n clusters (n=8 12). *Journal of Chemical Physics*, **2001**, 114, 7066-7072	3.9	24
7	Event-by-event analysis of collision-induced cluster-ion fragmentation: sequential monomer evaporation versus fission reactions. *Physical Review Letters*, **2001**, 86, 4263-6	7.4	10
6	The effects of the presence of an alkaline atomic cation in a molecular hydrogen environment. *Journal of Chemical Physics*, **2001**, 114, 2213-2218	3.9	55
5	Isomeric structures and energies of Hn+ clusters (n=13, 15, and 17). *Journal of Chemical Physics*, **2000**, 113, 4230-4237	3.9	42
4	Collisional fragmentation of fast HeH+ ions: The He2++H channel. *Physical Review A*, **1999**, 59, 1988-1993	2.6	3
3	Dependence on the incident angle of the electronic energy loss of planarly channeled fast ions. *Nuclear Instruments & Methods in Physics Research B*, **1999**, 149, 425-432	1.2	2
2	Fewest switches surface hopping with Baeck-An couplings. *Open Research Europe*,1, 49		4
1	Fewest switches surface hopping with Baeck-An couplings. *Open Research Europe*,1, 49		2