Leticia Gonzalez

List of Publications by Year
in descending order

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341 papers	12,447 citations	26567 56 h-index	42291 92 g-index
374 all docs	374 docs citations	374 times ranked	8497 citing authors

#	Article	IF	Citations
1	Oxygenâ€Doped PAH Electrochromes: Difurano, Dipyrano, and Furanoâ€Pyrano Containing Naphthaleneâ€Cored Molecules. European Journal of Organic Chemistry, 2022, 2022, .	1.2	7
2	HFIP Mediates a Direct Câ^'C Coupling between Michael Acceptors and Eschenmoser's salt. Angewandte Chemie - International Edition, 2022, 61, .	7.2	10
3	Taming Disulfide Bonds with Laser Fields. Nonadiabatic Surface-Hopping Simulations in a Ruthenium Complex. Journal of Physical Chemistry Letters, 2022, 13, 1894-1900.	2.1	6
4	Solvation Effects on the Thermal Helix Inversion of Molecular Motors from QM/MM Calculations. Chemistry, 2022, 4, 185-195.	0.9	5
5	Sampling effects in quantum mechanical/molecular mechanics trajectory surface hopping non-adiabatic dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200381.	1.6	11
6	Unravelling the Turnâ€On Fluorescence Mechanism of a Fluoresceinâ€Based Probe in GABA_A Receptors. Angewandte Chemie - International Edition, 2022, 61, .	7.2	6
7	Deep learning study of tyrosine reveals that roaming can lead to photodamage. Nature Chemistry, 2022, 14, 914-919.	6.6	21
8	Back Cover: Unravelling the Turnâ€On Fluorescence Mechanism of a Fluoresceinâ€Based Probe in GABA_A Receptors (Angew. Chem. Int. Ed. 30/2022). Angewandte Chemie - International Edition, 2022, 61, .	7.2	0
9	RÃ¼cktitelbild: Unravelling the Turnâ€On Fluorescence Mechanism of a Fluoresceinâ€Based Probe in GABA_A Receptors (Angew. Chem. 30/2022). Angewandte Chemie, 2022, 134, .	1.6	0
10	Direct Stereodivergent Olefination of Carbonyl Compounds with Sulfur Ylides. Journal of the American Chemical Society, 2022, 144, 12536-12543.	6.6	19
11	Ultrafast Intersystem Crossing Dynamics of 6-Selenoguanine in Water. Jacs Au, 2022, 2, 1699-1711.	3.6	10
12	Resolving Femtosecond Solvent Reorganization Dynamics in an Iron Complex by Nonadiabatic Dynamics Simulations. Journal of the American Chemical Society, 2022, 144, 12861-12873.	6.6	11
13	Meyerâ€"Schuster-type rearrangement for the synthesis of Î±-selanyl-Î±,Î²-unsaturated thioesters. Chemical Communications, 2021, 57, 117-120.	2.2	4
14	Ultrafast photochemistry of a molybdenum carbonylâ€"nitrosyl complex with a triazacyclononane coligand. Physical Chemistry Chemical Physics, 2021, 23, 24187-24199.	1.3	2
15	Quantum Theory: The Challenge of Transition Metal Complexes. Physical Chemistry Chemical Physics, 2021, 23, 2533-2534.	1.3	5
16	The importance of finite temperature and vibrational sampling in the absorption spectrum of a nitro-functionalized Ru(<scp>ii</scp>) water oxidation catalyst. Physical Chemistry Chemical Physics, 2021, 23, 17724-17733.	1.3	2
17	Ultrafast and long-time excited state kinetics of an NIR-emissive vanadium(<scp>iii</scp>) complex II. Elucidating triplet-to-singlet excited-state dynamics. Chemical Science, 2021, 12, 10791-10801.	3.7	24
18	Excited-State Dynamics of [Ru(Sâ€"Sbpy)(bpy)2]2+ to Form Long-Lived Localized Triplet States. Inorganic Chemistry, 2021, 60, 1672-1682.	1.9	14

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19	Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex. Journal of Physical Chemistry B, 2021, 125, 1778-1789.	1.2	18
20	Validating fewest-switches surface hopping in the presence of laser fields. Journal of Chemical Physics, 2021, 154, 144102.	1.2	10
21	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. Catalysts, 2021, 11, 493.	1.6	8
22	The Role of Triplet States in the Photodissociation of a Platinum Azide Complex by a Density Matrix Renormalization Group Method. Journal of Physical Chemistry Letters, 2021, 12, 4876-4881.	2.1	7
23	QM/MM Nonadiabatic Dynamics: the SHARC/COBRAMM Approach. Journal of Chemical Theory and Computation, 2021, 17, 4639-4647.	2.3	24
24	Hydrogenâ€Bond Network Determines the Early Photoisomerization Processes of Cph1 and AnPixJ Phytochromes. Angewandte Chemie, 2021, 133, 18836-18841.	1.6	2
25	Photoâ€Initiated Cobaltâ€Catalyzed Radical Olefin Hydrogenation. Chemistry - A European Journal, 2021, 27, 16978-16989.	1.7	8
26	Hydrogenâ€Bond Network Determines the Early Photoisomerization Processes of Cph1 and AnPixJ Phytochromes. Angewandte Chemie - International Edition, 2021, 60, 18688-18693.	7.2	7
27	The Quest to Simulate Excited-State Dynamics of Transition Metal Complexes. Jacs Au, 2021, 1, 1116-1140.	3.6	30
28	A Ruthenium(II) Water Oxidation Catalyst Containing a pH-Responsive Ligand Framework. Inorganic Chemistry, 2021, 60, 13299-13308.	1.9	7
29	A Density Matrix Renormalization Group Study of the Lowâ€Lying Excited States of a Molybdenum Carbonylâ€Nitrosyl Complex. ChemPhysChem, 2021, 22, 2371-2377.	1.0	2
30	Spectral Signatures of Oxidation States in a Manganeseâ€Oxo Cubane Water Oxidation Catalyst. Chemistry - A European Journal, 2021, 27, 17078-17086.	1.7	4
31	Surface Hopping Dynamics on Vibronic Coupling Models. Accounts of Chemical Research, 2021, 54, 3760-3771.	7.6	32
32	On the population of triplet states of 2-seleno-thymine. Physical Chemistry Chemical Physics, 2021, 23, 5447-5454.	1.3	7
33	Activation by oxidation and ligand exchange in a molecular manganese vanadium oxide water oxidation catalyst. Chemical Science, 2021, 12, 12918-12927.	3.7	10
34	Flexibility Enhances Reactivity: Redox Isomerism and Jahnâ€“Teller Effects in a Bioinspired Mn₄O₄ Cubane Water Oxidation Catalyst. ACS Catalysis, 2021, 11, 13320-13329.	5.5	12
35	Jahnâ€Teller Effects in a Vanadateâ€Stabilized Manganeseâ€Oxo Cubane Water Oxidation Catalyst. Chemistry - A European Journal, 2021, 27, 17066-17077.	1.7	8
36	Strong Ligand Stabilization Based on Ï€â€Extension in a Series of Ruthenium Terpyridine Water Oxidation Catalysts. Chemistry - A European Journal, 2021, 27, 16871-16878.	1.7	12

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37	Simplified State Interaction for Matrix Product State Wave Functions. Journal of Chemical Theory and Computation, 2021, 17, 7477-7485.	2.3	4
38	Revealing Ultrafast Population Transfer between Nearly Degenerate Electronic States. Journal of Physical Chemistry Letters, 2020, 11, 1443-1449.	2.1	5
39	The Reactivity and Stability of Polyoxometalate Water Oxidation Electrocatalysts. Molecules, 2020, 25, 157.	1.7	47
40	Enhanced Rigidity Changes Ultraviolet Absorption: Effect of a Merocyanine Binder on G-Quadruplex Photophysics. Journal of Physical Chemistry Letters, 2020, 11, 10212-10218.	2.1	10
41	Î±â€Funktionalisierung von Ketonen durch metallfreie elektrophile Aktivierung. Angewandte Chemie, 2020, 132, 21121-21125.	1.6	5
42	The effect of N-heterocyclic carbene units on the absorption spectra of Fe(<scp>ii</scp>) complexes: a challenge for theory. Physical Chemistry Chemical Physics, 2020, 22, 27605-27616.	1.3	8
43	Excimer Intermediates en Route to Long-Lived Charge-Transfer States in Single-Stranded Adenine DNA as Revealed by Nonadiabatic Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 7483-7488.	2.1	21
44	Intersystem Crossing and Triplet Dynamics in an Iron(II) N-Heterocyclic Carbene Photosensitizer. Inorganic Chemistry, 2020, 59, 14666-14678.	1.9	23
45	Site-Specific Photo-oxidation of the Isolated Adenosine-5â€²-triphosphate Dianion Determined by Photoelectron Imaging. Journal of Physical Chemistry Letters, 2020, 11, 8195-8201.	2.1	9
46	Î±â€Functionalisation of Ketones Through Metalâ€Free Electrophilic Activation. Angewandte Chemie - International Edition, 2020, 59, 20935-20939.	7.2	29
47	Implementation of Coherent Switching with Decay of Mixing into the SHARC Program. Journal of Chemical Theory and Computation, 2020, 16, 3464-3475.	2.3	18
48	Spiropyran Meets Guanine Quadruplexes: Isomerization Mechanism and DNA Binding Modes of Quinolizidineâ€Substituted Spiropyran Probes. Chemistry - A European Journal, 2020, 26, 13039-13045.	1.7	13
49	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. Chemical Science, 2020, 11, 7685-7693.	3.7	9
50	Unveiling the reaction mechanism of novel copperN-alkylated tetra-azacyclophanes with outstanding superoxide dismutase activity. Chemical Communications, 2020, 56, 7511-7514.	2.2	9
51	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO)$$_3$$(Dmp)(His124)(Trp122)]$$^+$$ in Pseudomonas aeruginosa azurin: a nonadiabatic dynamics study. Theoretical Chemistry Accounts, 2020, 139, 65.	0.5	17
52	Electrochemical and Photophysical Properties of Ruthenium(II) Complexes Equipped with Sulfurated Bipyridine Ligands. Inorganic Chemistry, 2020, 59, 4972-4984.	1.9	21
53	Biological evaluation of novel thiomaltol-based organometallic complexes as topoisomerase IIÎ± inhibitors. Journal of Biological Inorganic Chemistry, 2020, 25, 451-465.	1.1	16
54	CASPT2 Potential Energy Curves for NO Dissociation in a Ruthenium Nitrosyl Complex. Molecules, 2020, 25, 2613.	1.7	15

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55	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
56	Early Relaxation Dynamics in the Photoswitchable Complex transâ€[RuCl(NO)(py)₄]²⁺. Chemistry - A European Journal, 2020, 26, 11522-11528.	1.7	23
57	A Vanadium(III) Complex with Blue and NIR-II Spin-Flip Luminescence in Solution. Journal of the American Chemical Society, 2020, 142, 7947-7955.	6.6	74
58	Molecular Photochemistry: Recent Developments in Theory. Angewandte Chemie - International Edition, 2020, 59, 16832-16846.	7.2	91
59	Molekulare Photochemie: Moderne Entwicklungen in der theoretischen Chemie. Angewandte Chemie, 2020, 132, 16976-16992.	1.6	1
60	Investigation of Complex Relaxation Dynamics of Nearly Degenerated Rydberg States in Acetone. , 2020, , .		0
61	Machine learning enables long time scale molecular photodynamics simulations. Chemical Science, 2019, 10, 8100-8107.	3.7	140
62	Strong Influence of Decoherence Corrections and Momentum Rescaling in Surface Hopping Dynamics of Transition Metal Complexes. Journal of Chemical Theory and Computation, 2019, 15, 5031-5045.	2.3	50
63	Reaction mechanism of nucleoside 2â€²-deoxyribosyltransferases: free-energy landscape supports an oxocarbenium ion as the reaction intermediate. Organic and Biomolecular Chemistry, 2019, 17, 7891-7899.	1.5	10
64	Unified Approach to the Chemoselective Î±-Functionalization of Amides with Heteroatom Nucleophiles. Journal of the American Chemical Society, 2019, 141, 18437-18443.	6.6	65
65	Directional and regioselective hole injection of spiropyran photoswitches intercalated into A/T-duplex DNA. Physical Chemistry Chemical Physics, 2019, 21, 17971-17977.	1.3	6
66	From Surface Hopping to Quantum Dynamics and Back. Finding Essential Electronic and Nuclear Degrees of Freedom and Optimal Surface Hopping Parameters. Journal of Physical Chemistry A, 2019, 123, 8321-8332.	1.1	24
67	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
68	Solvent reorganization triggers photo-induced solvated electron generation in phenol. Physical Chemistry Chemical Physics, 2019, 21, 14261-14269.	1.3	6
69	Highly efficient surface hopping dynamics using a linear vibronic coupling model. Physical Chemistry Chemical Physics, 2019, 21, 57-69.	1.3	81
70	A redox-neutral synthesis of ketones by coupling of alkenes and amides. Nature Communications, 2019, 10, 2327.	5.8	30
71	Nonadiabatic Dynamics Simulation Predict Intersystem Crossing in Nitroaromatic Molecules on a Picosecond Time Scale. ChemPhotoChem, 2019, 3, 833-845.	1.5	12
72	The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. Journal of Chemical Theory and Computation, 2019, 15, 3470-3480.	2.3	30

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73	Functional materials: making the world go round. Physical Chemistry Chemical Physics, 2019, 21, 8988-8991.	1.3	4
74	Curious Case of 2-Selenouracil: Efficient Population of Triplet States and Yet Photostable. Journal of Chemical Theory and Computation, 2019, 15, 3730-3742.	2.3	14
75	The 3s Rydberg state as a doorway state in the ultrafast dynamics of 1,1-difluoroethylene. Physical Chemistry Chemical Physics, 2019, 21, 4871-4878.	1.3	7
76	A XMS-CASPT2 non-adiabatic dynamics study on pyrrole. Computational and Theoretical Chemistry, 2019, 1155, 38-46.	1.1	20
77	DNA-binding mechanism of spiropyran photoswitches: the role of electrostatics. Physical Chemistry Chemical Physics, 2019, 21, 8614-8618.	1.3	6
78	Unconventional two-step spin relaxation dynamics of [Re(CO)₃(im)(phen)]⁺ in aqueous solution. Chemical Science, 2019, 10, 10405-10411.	3.7	35
79	Identification of important normal modes in nonadiabatic dynamics simulations by coherence, correlation, and frequency analyses. Journal of Chemical Physics, 2019, 151, 244115.	1.2	16
80	Finite-temperature Wigner phase-space sampling and temperature effects on the excited-state dynamics of 2-nitronaphthalene. Physical Chemistry Chemical Physics, 2019, 21, 13906-13915.	1.3	29
81	Exploring density functional subspaces with genetic algorithms. Monatshefte FÃ¼r Chemie, 2019, 150, 173-182.	0.9	8
82	The Role of Electronic Triplet States and Highâ€Lying Singlet States in the Deactivation Mechanism of the Parent BODIPY: An ADC(2) and CASPT2 Study. ChemPhotoChem, 2019, 3, 727-738.	1.5	21
83	Molecular light switch effect in Ru(II) complexes intercalated in DNA: a theoretical study. , 2019, , 778-779.		0
84	Solvent Effects on Electronically Excited States: QM/Continuum Versus QM/Explicit Models. Journal of Physical Chemistry B, 2018, 122, 2975-2984.	1.2	21
85	Computational Photophysics in the Presence of an Environment. Annual Review of Physical Chemistry, 2018, 69, 473-497.	4.8	47
86	Vibrational Sampling and Solvent Effects on the Electronic Structure of the Absorption Spectrum of 2-Nitronaphthalene. Journal of Chemical Theory and Computation, 2018, 14, 3205-3217.	2.3	21
87	Unusual mechanisms in Claisen rearrangements: an ionic fragmentation leading to a meta-selective rearrangement. Chemical Science, 2018, 9, 4124-4131.	3.7	28
88	Quantitative wave function analysis for excited states of transition metal complexes. Coordination Chemistry Reviews, 2018, 361, 74-97.	9.5	109
89	Mechanism of Ultrafast Intersystem Crossing in 2â€Nitronaphthalene. Chemistry - A European Journal, 2018, 24, 5379-5387.	1.7	50
90	Exciton Localization on Ru-Based Photosensitizers Induced by Binding to Lipid Membranes. Journal of Physical Chemistry Letters, 2018, 9, 683-688.	2.1	14

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91	Hydrative Aminoxylation of Ynamides: One Reaction, Two Mechanisms. Chemistry - A European Journal, 2018, 24, 2515-2519.	1.7	24
92	Frontispiece: A Valence-Delocalised Osmium Dimer capable of Dinitrogen Photocleavage: Ab Initio Insights into Its Electronic Structure. Chemistry - A European Journal, 2018, 24, .	1.7	0
93	Interstate vibronic coupling constants between electronic excited states for complex molecules. Journal of Chemical Physics, 2018, 148, 124119.	1.2	33
94	Visible light-induced cis/trans isomerization of dicarbonyl Fe(II) PNP pincer complexes. Polyhedron, 2018, 143, 94-98.	1.0	1
95	Stepwise photosensitized thymine dimerization mediated by an exciton intermediate. Monatshefte FÃ¼r Chemie, 2018, 149, 1-9.	0.9	14
96	A Valenceâ€Delocalised Osmium Dimer capable of Dinitrogen Photocleavage: Ab Initio Insights into Its Electronic Structure. Chemistry - A European Journal, 2018, 24, 5112-5123.	1.7	13
97	Assessing Configurational Sampling in the Quantum Mechanics/Molecular Mechanics Calculation of Temoporfin Absorption Spectrum and Triplet Density of States. Molecules, 2018, 23, 2932.	1.7	10
98	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. Frontiers in Chemistry, 2018, 6, 495.	1.8	28
99	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. Scientific Reports, 2018, 8, 17273.	1.6	32
100	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. Journal of Chemical Theory and Computation, 2018, 14, 6139-6148.	2.3	29
101	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. Molecules, 2018, 23, 2836.	1.7	28
102	Cover Image, Volume 8, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1400.	6.2	7
103	Enhancing the Stability of Photogenerated Benzophenone Triplet Radical Pairs through Supramolecular Assembly. Journal of the American Chemical Society, 2018, 140, 13064-13070.	6.6	15
104	Tribute to Manuel YÃ¡Ã±ez and Otilia MÃ³. Journal of Physical Chemistry A, 2018, 122, 5671-5672.	1.1	0
105	Hydrogen Bonding Regulates the Rigidity of Liposomeâ€Encapsulated Chlorin Photosensitizers. ChemistryOpen, 2018, 7, 475-483.	0.9	13
106	Shedding Light on the Nature of Photoinduced States Formed in a Hydrogen-Generating Supramolecular RuPt Photocatalyst by Ultrafast Spectroscopy. Journal of Physical Chemistry A, 2018, 122, 6396-6406.	1.1	8
107	Nonadiabatic dynamics: The SHARC approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1370.	6.2	274
108	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. Journal of Chemical Theory and Computation, 2018, 14, 4530-4540.	2.3	17

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109	Effect of DNA Environment on Electronically Excited States of Methylene Blue Evaluated by a Three-Layered QM/QM/MM ONIOM Scheme. Journal of Chemical Theory and Computation, 2018, 14, 4298-4308.	2.3	16
110	General Trajectory Surface Hopping Method for Ultrafast Nonadiabatic Dynamics. RSC Theoretical and Computational Chemistry Series, 2018, , 348-385.	0.7	3
111	An Asymmetric Redox Arylation: Chirality Transfer from Sulfur to Carbon through a Sulfonium [3,3]â€Sigmatropic Rearrangement. Angewandte Chemie - International Edition, 2017, 56, 2212-2215.	7.2	115
112	Impact of Lipid Environment on Photodamage Activation of Methylene Blue. ChemPhotoChem, 2017, 1, 178-182.	1.5	18
113	Asymmetrische Redoxarylierung: ChiralitÃtstransfer von Schwefel zu Kohlenstoff durch sigmatrope Sulfoniumâ€[3,3]â€Umlagerung. Angewandte Chemie, 2017, 129, 2248-2252.	1.6	38
114	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. Physical Chemistry Chemical Physics, 2017, 19, 5888-5894.	1.3	31
115	Sequential Proton-Coupled Electron Transfer Mediates Excited-State Deactivation of a Eumelanin Building Block. Journal of Physical Chemistry Letters, 2017, 8, 1004-1008.	2.1	26
116	Discrimination of 1,1-difluoroethylene nuclear spin isomers in the presence of non-adiabatic coupling terms. Chemical Physics Letters, 2017, 683, 205-210.	1.2	3
117	Direct Determination of Metal Complexesâ€™ Interaction with DNA by Atomic Telemetry and Multiscale Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 805-811.	2.1	21
118	Direct Regioselective Synthesis of Tetrazolium Salts by Activation of Secondary Amides under Mild Conditions. Organic Letters, 2017, 19, 2662-2665.	2.4	42
119	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	1.2	31
120	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 19756-19766.	1.3	58
121	Electronic delocalization, charge transfer and hypochromism in the UV absorption spectrum of polyadenine unravelled by multiscale computations and quantitative wavefunction analysis. Chemical Science, 2017, 8, 5682-5691.	3.7	79
122	Insights into the deactivation of 5-bromouracil after ultraviolet excitation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160202.	1.6	8
123	Excited-states of a rhenium carbonyl diimine complex: solvation models, spinâ€“orbit coupling, and vibrational sampling effects. Physical Chemistry Chemical Physics, 2017, 19, 27240-27250.	1.3	40
124	Detailed Wave Function Analysis for Multireference Methods: Implementation in the <scp>Molcas</scp> Program Package and Applications to Tetracene. Journal of Chemical Theory and Computation, 2017, 13, 5343-5353.	2.3	40
125	Publisher's Note: Molecular oxygen observed by direct photoproduction from carbon dioxide [Phys. Rev. A 95 , 011404(R) (2017)]. Physical Review A, 2017, 95, .	1.0	2
126	Ab initio molecular dynamics of thiophene: the interplay of internal conversion and intersystem crossing. Physical Chemistry Chemical Physics, 2017, 19, 25662-25670.	1.3	36

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127	Molecular oxygen observed by direct photoproduction from carbon dioxide. Physical Review A, 2017, 95, .	1.0	13
128	Intramolecular hydrogen bonding in conformationally semi-rigid Î±-acylmethane derivatives: a theoretical NMR study. Organic and Biomolecular Chemistry, 2017, 15, 7572-7579.	1.5	2
129	Trajectory Surface-Hopping Dynamics Including Intersystem Crossing in [Ru(bpy)₃]²⁺. Journal of Physical Chemistry Letters, 2017, 8, 3840-3845.	2.1	108
130	Assessing Excited State Energy Gaps with Time-Dependent Density Functional Theory on Ru(II) Complexes. Journal of Chemical Theory and Computation, 2017, 13, 4123-4145.	2.3	39
131	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. Journal of Chemical Physics, 2017, 147, 184109.	1.2	32
132	Linkage Photoisomerization Mechanism in a Photochromic Ruthenium Nitrosyl Complex: New Insights from an MS-CASPT2 Study. Journal of Chemical Theory and Computation, 2017, 13, 6120-6130.	2.3	33
133	Mechanistic Pathways in Amide Activation: Flexible Synthesis of Oxazoles and Imidazoles. Organic Letters, 2017, 19, 3815-3818.	2.4	36
134	The IPEA dilemma in CASPT2. Chemical Science, 2017, 8, 1482-1499.	3.7	194
135	The DNA nucleobase thymine in motion â€“ Intersystem crossing simulated with surface hopping. Chemical Physics, 2017, 482, 9-15.	0.9	32
136	Challenges in Simulating Light-Induced Processes in DNA. Molecules, 2017, 22, 49.	1.7	21
137	Direct observation of laser-induced O<inf>2</inf>⁺ production from CO<inf>2</inf>. , 2017, , .		0
138	Laser-Induced Oxygen Formation from Carbon Dioxide. Journal of Physics: Conference Series, 2017, 875, 032024.	0.3	0
139	Communication: GAIMSâ€"Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. Journal of Chemical Physics, 2016, 144, 101102.	1.2	93
140	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. Journal of Chemical Physics, 2016, 145, 021103.	1.2	19
141	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. Journal of Chemical Physics, 2016, 144, 074303.	1.2	46
142	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. Physical Chemistry Chemical Physics, 2016, 18, 20168-20176.	1.3	65
143	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. Journal of Physical Chemistry Letters, 2016, 7, 1978-1983.	2.1	117
144	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. Journal of the American Chemical Society, 2016, 138, 15911-15916.	6.6	69

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145	Metalâ€Free metaâ€Selective Alkyne Oxyarylation with Pyridine Nâ€Oxides: Rapid Assembly of Metyrapone Analogues. Angewandte Chemie - International Edition, 2016, 55, 15424-15428.	7.2	33
146	Metal-free intermolecular formal cycloadditions enable an orthogonal access to nitrogen heterocycles. Nature Communications, 2016, 7, 10914.	5.8	96
147	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	5.8	149
148	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. Scientific Reports, 2016, 6, 35522.	1.6	27
149	Ruthenium Carbonyl Complexes with Azole Heterocycles â€“ Synthesis, Xâ€ray Diffraction Structures, DFT Calculations, Solution Behavior, and Antiproliferative Activity. European Journal of Inorganic Chemistry, 2016, 2016, 1566-1576.	1.0	7
150	Peripheral ligands as electron storage reservoirs and their role in enhancement of photocatalytic hydrogen generation. Chemical Communications, 2016, 52, 9371-9374.	2.2	24
151	Divergent ynamide reactivity in the presence of azides â€“ an experimental and computational study. Chemical Science, 2016, 7, 6032-6040.	3.7	32
152	Chemo- and Stereoselective Transition-Metal-Free Amination of Amides with Azides. Journal of the American Chemical Society, 2016, 138, 8348-8351.	6.6	109
153	Controlling the Excited-State Dynamics of Nuclear Spin Isomers Using the Dynamic Stark Effect. Journal of Physical Chemistry A, 2016, 120, 4907-4914.	1.1	4
154	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. Journal of Chemical Theory and Computation, 2016, 12, 1207-1219.	2.3	145
155	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	2.1	89
156	A general method to describe intersystem crossing dynamics in trajectory surface hopping. International Journal of Quantum Chemistry, 2015, 115, 1215-1231.	1.0	228
157	Origin of the Regioselectivity in the Gasâ€Phase Aniline+CH₃⁺ Electrophilic Aromatic Substitution. ChemPhysChem, 2015, 16, 2366-2374.	1.0	0
158	Time-Resolved Insight into the Photosensitized Generation of Singlet Oxygen in Endoperoxides. Journal of Chemical Theory and Computation, 2015, 11, 406-414.	2.3	20
159	Enhancing Intersystem Crossing in Phenotiazinium Dyes by Intercalation into DNA. Angewandte Chemie - International Edition, 2015, 54, 4375-4378.	7.2	56
160	Unravelling the Quenching Mechanisms of a Luminescent Ru^{II} Probe for Cu^{II}. Chemistry - an Asian Journal, 2015, 10, 622-629.	1.7	10
161	Orbital entanglement and CASSCF analysis of the Ruâ€“NO bond in a Ruthenium nitrosyl complex. Physical Chemistry Chemical Physics, 2015, 17, 14383-14392.	1.3	58
162	Quenching of Charge Transfer in Nitrobenzene Induced by Vibrational Motion. Journal of Physical Chemistry Letters, 2015, 6, 3006-3011.	2.1	24

#	Article	IF	Citations
163	Separating nuclear spin isomers using a pumpâ€“dump laser scheme. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	4
164	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. Journal of the American Chemical Society, 2015, 137, 4368-4381.	6.6	72
165	Using computational chemistry to design Ru photosensitizers with directional charge transfer. Coordination Chemistry Reviews, 2015, 304-305, 146-165.	9.5	55
166	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. Journal of Physical Chemistry A, 2015, 119, 9524-9533.	1.1	69
167	Ultrafast Intersystem Crossing in SO2 and Nucleobases. Springer Proceedings in Physics, 2015, , 509-513.	0.1	1
168	Excitation of Nucleobases from a Computational Perspective II: Dynamics. Topics in Current Chemistry, 2014, 355, 99-153.	4.0	43
169	Non-adiabatic and intersystem crossing dynamics in SO₂. II. The role of triplet states in the bound state dynamics studied by surface-hopping simulations. Journal of Chemical Physics, 2014, 140, 204302.	1.2	68
170	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	1.2	33
171	Discrimination of nuclear spin isomers exploiting the excited state dynamics of a quinodimethane derivative. Journal of Chemical Physics, 2014, 141, 164323.	1.2	7
172	Molecular Dynamics Simulations of Binding Modes between Methylene Blue and DNA with Alternating GC and AT Sequences. Biochemistry, 2014, 53, 2391-2412.	1.2	42
173	Ultrafast intersystem crossing dynamics in uracil unravelled byab initiomolecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24423-24436.	1.3	95
174	Analytical gradients of complete active space self-consistent field energies using Cholesky decomposition: Geometry optimization and spin-state energetics of a ruthenium nitrosyl complex. Journal of Chemical Physics, 2014, 140, 174103.	1.2	48
175	Gas-phase electrophilic aromatic substitution mechanism with strong electrophiles explained by ab initio non-adiabatic dynamics. Physical Chemistry Chemical Physics, 2014, 16, 18686-18689.	1.3	3
176	Beyond the molecular orbital conception of electronically excited states through the quantum theory of atoms in molecules. Physical Chemistry Chemical Physics, 2014, 16, 9249-9258.	1.3	36
177	Theoretical Spectroscopy and Photodynamics of a Ruthenium Nitrosyl Complex. Inorganic Chemistry, 2014, 53, 6415-6426.	1.9	59
178	Active and silent chromophore isoforms for phytochrome Pr photoisomerization: An alternative evolutionary strategy to optimize photoreaction quantum yields. Structural Dynamics, 2014, 1, 014701.	0.9	35
179	Ultrafast Laser-Induced Processes Described by Ab Initio Molecular Dynamics. Springer Series in Chemical Physics, 2014, , 145-170.	0.2	4
180	Ultrafast Intersystem Crossing in SO2 and Nucleobases. , 2014, , .		0

#	Article	IF	Citations
181	Singlet and Triplet Excitedâ€State Dynamics Study of the Keto and Enol Tautomers of Cytosine. ChemPhysChem, 2013, 14, 2920-2931.	1.0	86
182	Electrochemistry and time dependent DFT study of a (vinylenedithio)-TTF derivative in different oxidation states. Electrochimica Acta, 2013, 100, 188-196.	2.6	5
183	Synthesis, properties and quantum chemical evaluation of solvatochromic pyridinium-phenyl-1,3-thiazol-4-olate betaine dyes. Tetrahedron, 2013, 69, 1489-1498.	1.0	12
184	N-site de-methylation in pyrimidine bases as studied by low energy electrons and ab initio calculations. Physical Chemistry Chemical Physics, 2013, 15, 11431.	1.3	23
185	Nuclear Spin Selective Torsional States: Implications of Molecular Symmetry. Zeitschrift Fur Physikalische Chemie, 2013, 227, 1021-1048.	1.4	9
186	Mechanism Elucidation of the cisâ€“trans Isomerization of an Azole Rutheniumâ€“Nitrosyl Complex and Its Osmium Counterpart. Inorganic Chemistry, 2013, 52, 6260-6272.	1.9	26
187	Ab initio and DFT analysis of the low-lying electronic states of metal dihalides: quantum chemical calculations on the neutral BrMCl (M = Cu, Ag, Au). Physical Chemistry Chemical Physics, 2013, 15, 10151.	1.3	0
188	An Assessment of RASSCF and TDDFT Energies and Gradients on an Organic Donorâ€“Acceptor Dye Assisted by Resonance Raman Spectroscopy. Journal of Chemical Theory and Computation, 2013, 9, 543-554.	2.3	38
189	A Siliconâ€Heteroaromatic System as Photosensitizer for Lightâ€Driven Hydrogen Production by Hydrogenase Mimics. European Journal of Inorganic Chemistry, 2013, 2013, 4466-4472.	1.0	36
190	A theoretical investigation of the feasibility of Tannor-Rice type control: Application to selective bond breakage in gas-phase dihalomethanes. Journal of Chemical Physics, 2012, 136, 174303.	1.2	19
191	9D nonadiabatic quantum dynamics through a four-state conical intersection: Investigating the homolysis of the Oâ€“O bond in anthracene-9,10-endoperoxide. Journal of Chemical Physics, 2012, 137, 22A524.	1.2	8
192	Real-Time Tracking of Phytochromeâ€™s Orientational Changes During Pr Photoisomerization. Journal of the American Chemical Society, 2012, 134, 1408-1411.	6.6	72
193	Structural Control of Photoinduced Dynamics in 4H-Imidazole-Ruthenium Dyes. Journal of Physical Chemistry C, 2012, 116, 25664-25676.	1.5	38
194	IR Spectrum of FHF^{â€“} and FDF^{â€“} Revisited Using a Spectral Method in Four Dimensions. Journal of Physical Chemistry A, 2012, 116, 11361-11369.	1.1	16
195	Tribute to JÃ¶rn Manz. Journal of Physical Chemistry A, 2012, 116, 11041-11042.	1.1	0
196	Control of Nuclear Dynamics with Strong Ultrashort Laser Pulses. Journal of Physical Chemistry A, 2012, 116, 11434-11440.	1.1	33
197	Mixed Quantum-Classical Dynamics in the Adiabatic Representation To Simulate Molecules Driven by Strong Laser Pulses. Journal of Physical Chemistry A, 2012, 116, 2800-2807.	1.1	42
198	Stark Control of a Chiral Fluoroethylene Derivative. Journal of Physical Chemistry A, 2012, 116, 2743-2749.	1.1	15

#	Article	IF	Citations
199	Correction to â€œSHARC â€“ Ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplingsâ€•[J. Chem. Theory Comput.2011, 7, 1253â€“1258]. Journal of Chemical Theory and Computation, 2012, 8, 374-374.	2.3	10
200	Analysis and characterization of coordination compounds by resonance Raman spectroscopy. Coordination Chemistry Reviews, 2012, 256, 1479-1508.	9.5	95
201	Femtosecond Intersystem Crossing in the DNA Nucleobase Cytosine. Journal of Physical Chemistry Letters, 2012, 3, 3090-3095.	2.1	146
202	Arylamineâ€Modified Thiazoles as Donorâ€“Acceptor Dyes: Quantum Chemical Evaluation of the Chargeâ€Transfer Process and Testing as Ligands in Ruthenium(II) Complexes. European Journal of Organic Chemistry, 2012, 2012, 5231-5247.	1.2	26
203	A Novel Ru(II) Polypyridine Black Dye Investigated by Resonance Raman Spectroscopy and TDDFT Calculations. Journal of Physical Chemistry C, 2012, 116, 19968-19977.	1.5	30
204	An ab initio mechanism for efficient population of triplet states in cytotoxic sulfur substituted DNA bases: the case of 6-thioguanine. Chemical Communications, 2012, 48, 2134.	2.2	76
205	Ultrafast charge transfer dynamics induced by low energy collisions. Application to ion-atom and ion-molecule systems. Journal of Physics: Conference Series, 2012, 388, 082054.	0.3	0
206	H-abstraction is more efficient than cisâ€“trans isomerization in (4-methylcyclohexylidene) fluoromethane. An ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 6241-6249.	1.3	4
207	RASPT2/RASSCF vs Range-Separated/Hybrid DFT Methods: Assessing the Excited States of a Ru(II)bipyridyl Complex. Journal of Chemical Theory and Computation, 2012, 8, 203-213.	2.3	53
208	Singlet oxygen generation versus Oâ€“O homolysis in phenyl-substituted anthracene endoperoxides investigated by RASPT2, CASPT2, CC2, and TD-DFT methods. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	5
209	The role of hydrogen bonds in proteinâ€“ligand interactions. DFT calculations in 1,3â€dihydrobenzimidazoleâ€2 thione derivatives with glycinamide as model HIV RT inhibitors. International Journal of Quantum Chemistry, 2012, 112, 1786-1795.	1.0	10
210	The Radiative Decay Rates Tune the Emissive Properties of Ruthenium(II) Polypyridyl Complexes: A Computational Study. Chemistry - an Asian Journal, 2012, 7, 667-671.	1.7	17
211	Ruthenium(II) Photosensitizers of Tridentate Clickâ€Derived Cyclometalating Ligands: A Joint Experimental and Computational Study. Chemistry - A European Journal, 2012, 18, 4010-4025.	1.7	61
212	A non-adiabatic wavepacket dynamical study of the low energy charge transfer process in the S3++H collision. Chemical Physics, 2012, 400, 165-170.	0.9	14
213	4-Methoxy-1,3-thiazole based donor-acceptor dyes: Characterization, X-ray structure, DFT calculations and test as sensitizers for DSSC. Dyes and Pigments, 2012, 94, 512-524.	2.0	67
214	Progress and Challenges in the Calculation of Electronic Excited States. ChemPhysChem, 2012, 13, 28-51.	1.0	344
215	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	2.2	33
216	Influence of Multiple Protonation on the Initial Excitation in a Black Dye. Journal of Physical Chemistry C, 2011, 115, 24004-24012.	1.5	28

#	Article	IF	Citations
217	SHARC: ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings. Journal of Chemical Theory and Computation, 2011, 7, 1253-1258.	2.3	424
218	Direct Observation of Temperature-Dependent Excited-State Equilibrium in Dinuclear Ruthenium Terpyridine Complexes Bearing Electron-Poor Bridging Ligands. Journal of Physical Chemistry C, 2011, 115, 12677-12688.	1.5	27
219	Spectroscopic Properties of Azobenzene-Based pH Indicator Dyes: A Quantum Chemical and Experimental Study. Journal of Chemical Theory and Computation, 2011, 7, 1062-1072.	2.3	26
220	A non-adiabatic quantum-classical dynamics study of the intramolecular excited state hydrogen transfer in ortho-nitrobenzaldehyde. Physical Chemistry Chemical Physics, 2011, 13, 14685.	1.3	17
221	A comparative analysis of the UV/Vis absorption spectra of nitrobenzaldehydes. Physical Chemistry Chemical Physics, 2011, 13, 4269.	1.3	17
222	Protonation effects on the resonance Raman properties of a novel (terpyridine)Ru(4H-imidazole) complex: an experimental and theoretical case study. Physical Chemistry Chemical Physics, 2011, 13, 15580.	1.3	54
223	Can TD-DFT predict excited states in endoperoxides?. Computational and Theoretical Chemistry, 2011, 975, 13-19.	1.1	5
224	Nonadiabatic ab initio molecular dynamics including spinâ€“orbit coupling and laser fields. Faraday Discussions, 2011, 153, 261.	1.6	59
225	Wavelength-dependent photoproduct formation of phycocyanobilin in solution â€“ Indications for competing reaction pathways. Chemical Physics Letters, 2011, 515, 163-169.	1.2	3
226	The role of Ï€Ï*f [*] states in the photochemistry of the chiral fluoroethylene derivative (4â€methylcyclohexylidene)fluoromethane. International Journal of Quantum Chemistry, 2011, 111, 3394-3404.	1.0	3
227	Revealing the Position of the Substrate in Nickel Superoxide Dismutase: A Model Study. Angewandte Chemie - International Edition, 2011, 50, 2946-2950.	7.2	22
228	A Heteroleptic Bis(tridentate) Ruthenium(II) Complex of a Clickâ€Derived Abnormal Carbene Pincer Ligand with Potential for Photosensitzer Application. Chemistry - A European Journal, 2011, 17, 5494-5498.	1.7	117
229	Pulse-shape-dependent strong-field ionization viewed with velocity-map imaging. Physical Review A, 2011, 84, .	1.0	17
230	Creation of multihole molecular wave packets via strong-field ionization. Physical Review A, 2010, 82, .	1.0	24
231	Thermochemistry and UV Spectroscopy of Alkyl Peroxynitrates. Journal of Physical Chemistry A, 2010, 114, 9537-9544.	1.1	6
232	Biologically inspired molecular machines driven by light. Optimal control of a unidirectional rotor. New Journal of Physics, 2010, 12, 075007.	1.2	22
233	Non-adiabatic photoisomerization versus photodissociation dynamics of the chiral fluoroethylene derivative (4-methylcyclohexylidene) fluoromethane. Chemical Physics, 2010, 369, 138-144.	0.9	7
234	A Timeâ€Dependent Picture of the Ultrafast Deactivation of ketoâ€Cytosine Including Threeâ€State Conical Intersections. ChemPhysChem, 2010, 11, 3617-3624.	1.0	78

#	Article	IF	Citations
235	Inside Cover: A Timeâ€Dependent Picture of the Ultrafast Deactivation of ketoâ€Cytosine Including Threeâ€State Conical Intersections (ChemPhysChem 17/2010). ChemPhysChem, 2010, 11, 3554-3554.	1.0	2
236	Structureâ€“Property Relationship of Redâ€•and Greenâ€Emitting Iridium(III) Complexes with Respect to Their Temperature and Oxygen Sensitivity. European Journal of Inorganic Chemistry, 2010, 2010, 4875-4885.	1.0	80
237	Photochemical Fate: The First Step Determines Efficiency of H₂ Formation with a Supramolecular Photocatalyst. Angewandte Chemie - International Edition, 2010, 49, 3981-3984.	7.2	162
238	Mechanistic studies on the alcoholysis and aminolysis of [(MeZn)2{Î¼-N(H)tBu}{Î¼-N(CH2Py)2}]. Journal of Organometallic Chemistry, 2010, 695, 280-290.	0.8	11
239	Excited state dynamics of a model asymmetric molecular rotor: A five-dimensional study on 2-cyclopentylidene-tetrahydrofuran. Chemical Physics, 2010, 377, 86-95.	0.9	10
240	Four-state conical intersections: The nonradiative deactivation funnel connected to Oâ€“O homolysis in benzene endoperoxide. Chemical Physics Letters, 2010, 499, 21-25.	1.2	13
241	Synthesis and Catalytic Reactivity of Bis(alkylzinc)-hydride-di(2-pyridylmethyl)amides. Organometallics, 2010, 29, 3098-3108.	1.1	43
242	Time-Dependent DFT on Phytochrome Chromophores: A Way to the Right Conformer. Journal of Physical Chemistry Letters, 2010, 1, 796-801.	2.1	29
243	A wavepacket study of the low-energy charge transfer process in the S3+ + H reaction using time-resolved electronic densities. Physical Chemistry Chemical Physics, 2010, 12, 5439.	1.3	8
244	N-Heterocyclic Donor- and Acceptor-Type Ligands Based on 2-(1H-[1,2,3]Triazol-4-yl)pyridines and Their Ruthenium(II) Complexes. Journal of Organic Chemistry, 2010, 75, 4025-4038.	1.7	60
245	On the Light-Driven Isomerization of a Model Asymmetric Molecular Rotor: Conformations and Conical Intersections of 2-Cyclopentylidene-tetrahydrofuran. Journal of Physical Chemistry A, 2010, 114, 9342-9348.	1.1	12
246	Simulation of the resonance Raman intensities of a rutheniumâ€“palladium photocatalyst by time dependent density functional theory. Physical Chemistry Chemical Physics, 2010, 12, 14812.	1.3	47
247	Photochemical behavior of (bisphosphane)(Î·2-tolane)Pt0 complexes. Part B: An insight from DFT calculations. Dalton Transactions, 2010, 39, 9505.	1.6	14
248	Photochemical behavior of (diphosphine)(Î·2-tolane)Pt0 complexes. Part A: Experimental considerations in solution and in the solid state. Dalton Transactions, 2010, 39, 9493.	1.6	15
249	Four Plus Four State Degeneracies in the Oâ^'O Photolysis of Aromatic Endoperoxides. Journal of Physical Chemistry Letters, 2010, 1, 1036-1040.	2.1	19
250	Mechanistic insight into light-driven molecular rotors: a conformational search in chiral overcrowded alkenes by a pseudo-random approach. Physical Chemistry Chemical Physics, 2010, 12, 12279.	1.3	21
251	Quantum chemical investigation of the thermal rearrangement of cis- and trans-pinane. Physical Chemistry Chemical Physics, 2010, 12, 9884.	1.3	7
252	Exploring wavepacket dynamics behind strong-field momentum-dependent photodissociation in CH2BrI+. Physical Chemistry Chemical Physics, 2010, 12, 14203.	1.3	37

#	Article	IF	Citations
253	Laser control of conical intersections: Quantum model simulations for the averaged loss-gain strategies of fast electronic deactivation in 1,1-difluoroethylene. Journal of Chemical Physics, 2009, 131, 104302.	1.2	20
254	Few-cycle laser pulses to obtain spatial separation of OHFâ˜ dissociation products. Journal of Chemical Physics, 2009, 130, 024310.	1.2	7
255	Density functional theory rationalization of the substituent effects in trifluoromethyl-pyridinol derivatives. Tetrahedron, 2009, 65, 232-239.	1.0	17
256	The role of molecular orientation and light polarization on the control of bond dissociation. Time-dependent simulations for CH₂BrCl. Journal of Modern Optics, 2009, 56, 790-798.	0.6	7
257	Phenyl-1H-[1,2,3]triazoles as New Cyclometalating Ligands for Iridium(III) Complexes. Organometallics, 2009, 28, 5478-5488.	1.1	142
258	Substituent effects on the light-induced Câ€“C and Câ€“Br bond activation in (bisphosphine)(Î·2-tolane)Pt0 complexes. A TD-DFT study. Physical Chemistry Chemical Physics, 2009, 11, 4593.	1.3	13
259	Thymine relaxation after UV irradiation: the role of tautomerization and Ï€Ïƒ* states. Physical Chemistry Chemical Physics, 2009, 11, 3927.	1.3	56
260	A CASSCF and CASPT2 study of the photochemistry of 1,1- and 1,2-difluoroethylenes. Chemical Physics, 2008, 349, 287-295.	0.9	12
261	Design of acidochromic dyes for facile preparation of pH sensor layers. Analytical and Bioanalytical Chemistry, 2008, 392, 1411-1418.	1.9	41
262	Rydberg or Valence? The Longâ€Standing Question in the UV Absorption Spectrum of 1,1â€²â€Bicyclohexylidene. ChemPhysChem, 2008, 9, 2544-2549.	1.0	11
263	Theoretical investigation of anthraceneâ€9,10â€endoperoxide vertical singlet and triplet excitation spectra. Journal of Computational Chemistry, 2008, 29, 1982-1991.	1.5	15
264	Identifying the low-lying electronic states of anthracene-9,10-endoperoxide. Chemical Physics Letters, 2008, 452, 67-71.	1.2	17
265	Control of the photodissociation of CH2BrCl using a few-cycle IR driving laser pulse and a UV control pulse. Chemical Physics Letters, 2008, 459, 39-43.	1.2	11
266	Selective carbonâ€“carbon bond cleavage of 2,2â€²-dibromotolane via photolysis of its appropriate (diphosphine)Pt0 complex in the solid state. Dalton Transactions, 2008, , 1979.	1.6	18
267	Annulated Dinuclear Metal-Free and Zn(II) Phthalocyanines: Photophysical Studies and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2008, 112, 8466-8476.	1.2	25
268	A Two-Dimensional Wavepacket Study of the Nonadiabatic Dynamics of CH2BrCl. Journal of Physical Chemistry A, 2008, 112, 5573-5581.	1.1	27
269	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	1.1	30
270	The Chromophore Structure of the Cyanobacterial Phytochrome Cph1 As Predicted by Time-Dependent Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 16253-16256.	1.2	33

#	Article	IF	Citations
271	Kinetic Model for the Thermal Rearrangement of cis- and trans-Pinane. Journal of Physical Chemistry A, 2008, 112, 5885-5892.	1.1	13
272	On the puzzling deactivation mechanism of thymine after light irradiation. , 2008, , .		3
273	Ortho-Nitrobenzaldehyde 1:1 Water Complexes. The Influence of Solute Water Interactions in the Vertical Excited Spectrum. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1263-1278.	1.4	2
274	EinfÃ¼hrung in die computergestÃ¼tzte Quantenchemie. EXamen Press, 2008, , 391-413.	0.0	0
275	Theory of ultrafast nonresonant multiphoton transitions in polyatomic molecules: Basics and application to optimal control theory. Journal of Chemical Physics, 2007, 127, 144102.	1.2	5
276	Laser Control of Wavepacket Photodissociation and Photoisomerization Dynamics in Isolated Molecules. AIP Conference Proceedings, 2007, , .	0.3	0
277	Control of concerted two bond versus single bond dissociation in CH3Co(CO)4 via an intermediate state using pump-dump laser pulses. Journal of Chemical Physics, 2007, 127, 134311.	1.2	1
278	Laserkontrolle. Nachrichten Aus Der Chemie, 2007, 55, 315-317.	0.0	0
279	Photoactivity and UV Absorption Spectroscopy of RCo(CO)4 (R = H, CH3) Organometallic Complexes. Journal of Physical Chemistry A, 2007, 111, 4737-4742.	1.1	11
280	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, 238-243.	1.1	17
281	Nuclear Magnetic Resonance and ab Initio Studies of Small Complexes Formed between Water and Pyridine Derivatives in Solid and Liquid Phases. Journal of Physical Chemistry A, 2007, 111, 6084-6093.	1.1	43
282	Structure and bonding of Ag(I)-DNA base complexes and Ag(I)-adenine-cytosine mispairs: An ab Initio study. Journal of Computational Chemistry, 2007, 28, 2299-2308.	1.5	32
283	A CASPT2 study of the excited states of adenine tautomers with silver ions. Chemical Physics Letters, 2007, 435, 136-141.	1.2	8
284	Conical intersections in the photoisomerization and photodissociation of a chiral fluoroethylene derivative ((4-methylcyclohexylidene) fluoromethane). Chemical Physics Letters, 2007, 443, 43-48.	1.2	3
285	The electronic excited states of a model organic endoperoxide: A comparison of TD-DFT and ab initio methods. Chemical Physics Letters, 2007, 446, 262-267.	1.2	10
286	Spectroscopy of Ru(II) polypyridyl complexes used as intercalators in DNA: Towards a theoretical study of the light switch effect. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 310-320.	2.0	57
287	The role of Ag(I) ions in the electronic spectroscopy of adenineâ€“cytosine mispairs. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 301-309.	2.0	9
288	Complex systems in the gas phase. , 2007, , 153-256.		1

#	Article	IF	Citations
289	Biological systems: Applications and perspectives. , 2007, , 733-828.		0
290	A theoretical anharmonic study of the infrared absorption spectra of FHFâ¯, FDFâ¯, OHFâ¯, and ODFâ¯ anions. Journal of Chemical Physics, 2006, 124, 174308.	1.2	29
291	On the Location of Conical Intersections in CH2BrCl Using MS-CASPT2 Methods. Journal of Physical Chemistry A, 2006, 110, 10251-10259.	1.1	19
292	A multi state-CASPT2 vs. TD-DFT study of the electronic excited states of RCo(CO)4 (R=H, CH3) organometallic complexes. Chemical Physics Letters, 2006, 417, 545-549.	1.2	10
293	Application of optimal control theory to ultrafast nonresonant multiphoton transitions in polyatomic molecules. Optics Communications, 2006, 264, 502-510.	1.0	8
294	A first principles approach to optimal control. Theoretical Chemistry Accounts, 2006, 116, 148-159.	0.5	7
295	Quantum chemistry based inversion of experimental pumpâ€“probe spectra: Model simulations for CpMn(CO)3. Chemical Physics, 2006, 329, 126-138.	0.9	7
296	Photochemistry of CH3Mn(CO)5: A multiconfigurationalab initio study. Journal of Computational Chemistry, 2006, 27, 1781-1786.	1.5	9
297	Auf dem Weg zur Professorin. Nachrichten Aus Der Chemie, 2005, 53, 713-713.	0.0	0
298	Neutral-to-ionic ZEKE transition dipole couplings beyond Koopmansâ€™ picture: Application to femtosecond pumpâ€“probe spectroscopy. Chemical Physics, 2005, 314, 143-158.	0.9	10
299	Optical resolution of oriented enantiomers via photodissociation: quantum model simulations for H2POSD. Physical Chemistry Chemical Physics, 2005, 7, 4096.	1.3	9
300	Quantum ignition of intramolecular rotation by means of IR+UV laser pulses. Chemical Physics Letters, 2004, 386, 248-253.	1.2	43
301	Quantum control of reactions with few-cycle infrared and ultraviolet laser pulses. Computational and Theoretical Chemistry, 2004, 709, 207-213.	1.5	0
302	Optical enantioselection in a random ensemble of unidirectionally oriented chiral olefins. Chemical Physics, 2004, 298, 55-63.	0.9	19
303	Breaking the strong and weak bonds of OHFâ¯using few-cycle IR + UV laser pulses. Physical Chemistry Chemical Physics, 2004, 6, 4071-4073.	1.3	22
304	Sequential Pump-Dump Control of Photoisomerization Competing with Photodissociation of Optical Isomers. Journal of Physical Chemistry A, 2004, 108, 6455-6463.	1.1	10
305	Quantum model simulations of symmetry breaking and control of bond selective dissociation of FHFâ¯ using IR+UV laser pulses. Journal of Chemical Physics, 2004, 120, 8002-8014.	1.2	33
306	Chiral Molecular Motors Ignited by Femtosecond Pumpâ¯Dump Laser Pulses. Journal of Physical Chemistry B, 2004, 108, 4916-4921.	1.2	39

#	Article	IF	Citations
307	Quantum Simulations for Isotope Effects of IR + UV Laser Pulses on Symmetry and Selective Hydrogen Bond Breaking. Zeitschrift Fur Physikalische Chemie, 2003, 217, 1577-1596.	1.4	9
308	Deciphering the Reaction Dynamics Underlying Optimal Control Laser Fields. Science, 2003, 299, 536-539.	6.0	388
309	Theory of ultrafast non-resonant multi-photon transitions: basics and application to CpMn(CO)3. Chemical Physics Letters, 2003, 380, 536-541.	1.2	10
310	Asymmetric laser excitation in chiral molecules: quantum simulations for a proposed experiment. Chemical Physics Letters, 2003, 372, 242-248.	1.2	29
311	Enantioselective separation of axial chiral olefins by laser pulses using coupled torsion and pyramidalization motions. Physical Chemistry Chemical Physics, 2003, 5, 3933-3942.	1.3	20
312	Ultrafast non-adiabatic laser-induced photodissociation dynamics of CpMn(CO)3. An ab initio quantum chemical and dynamical study. Physical Chemistry Chemical Physics, 2003, 5, 87-96.	1.3	24
313	Quantum control of molecular handedness in a randomly oriented racemic mixture using three polarization components of electric fields. Journal of Chemical Physics, 2002, 116, 8799-8802.	1.2	55
314	Photochemistry of CH2BrCl:Â An ab Initio and Dynamical Study. Journal of Physical Chemistry A, 2002, 106, 11150-11161.	1.1	26
315	Control of molecular handedness using pump-dump laser pulses. Journal of Chemical Physics, 2002, 116, 2433-2438.	1.2	43
316	A CASSCF/CASPT2 and TD-DFT Study of the Low-Lying Excited States of Î·5-CpMn(CO)3. Journal of Physical Chemistry A, 2001, 105, 184-189.	1.1	44
317	Isotopic effects on the control of molecular handedness of H2 POSH by ultrashort laser pulses. European Physical Journal D, 2001, 14, 185-190.	0.6	7
318	Analysis and control of laser induced fragmentation processes in CpMn(CO)3. Chemical Physics, 2001, 267, 247-260.	0.9	77
319	Spontaneous Self-Ionization in the Gas Phase: A Theoretical Prediction. ChemPhysChem, 2001, 2, 465-467.	1.0	27
320	A MS-CASPT2 study of the low-lying electronic excited states of CH2BrCl. Chemical Physics Letters, 2001, 350, 155-164.	1.2	19
321	Separation of enantiomers by ultraviolet laser pulses in H2POSH: Ï€ pulses versus adiabatic transitions. Journal of Chemical Physics, 2001, 115, 2519-2529.	1.2	48
322	From a Racemate to a Pure Enantiomer by Laser Pulses: Quantum Model Simulations for H2POSH. Angewandte Chemie - International Edition, 2000, 39, 4586-4588.	7.2	48
323	Selective preparation of enantiomers by laser pulses: From optimal control to specific pump and dump transitions. Journal of Chemical Physics, 2000, 113, 11134-11142.	1.2	25
324	Ground- and Excited-State Surfaces for the [2+2]-Photocycloaddition of Î±,Î²-Enones to Alkenes. Journal of the American Chemical Society, 2000, 122, 5866-5876.	6.6	59

#	Article	IF	Citations
325	Thermochemistry of the Reactions F+(3P,1D) + PH3in the Gas Phase. Journal of Physical Chemistry A, 2000, 104, 8075-8080.	1.1	3
326	Selective preparation of enantiomers by laser pulses: quantum model simulation for H2POSH. Chemical Physics Letters, 1999, 306, 1-8.	1.2	101
327	Density functional theory study on ethanol dimers and cyclic ethanol trimers. Journal of Chemical Physics, 1999, 111, 3855-3861.	1.2	92
328	Ultrafast photoinduced dissipative hydrogen switching dynamics in thioacetylacetone. Physical Chemistry Chemical Physics, 1999, 1, 1249-1257.	1.3	63
329	Substituent Effects on the Strength of the Intramolecular Hydrogen Bond of Thiomalonaldehyde. Journal of Organic Chemistry, 1999, 64, 2314-2321.	1.7	48
330	Proton Transfer in Dissociative Protonation Processes. Journal of Physical Chemistry A, 1998, 102, 1356-1364.	1.1	18
331	Very strong hydrogen bonds in neutral molecules: The phosphinic acid dimers. Journal of Chemical Physics, 1998, 109, 2685-2693.	1.2	100
332	High level ab initio and density functional theory studies on methanolâ€“water dimers and cyclic methanol(water)2 trimer. Journal of Chemical Physics, 1998, 109, 139-150.	1.2	126
333	High-Level ab Initio Calculations on the Intramolecular Hydrogen Bond in Thiomalonaldehyde. Journal of Physical Chemistry A, 1997, 101, 9710-9719.	1.1	95
334	High-levelab initio versus DFT calculations on (H2O2)2 and H2O2-H2O complexes as prototypes of multiple hydrogen bond systems. , 1997, 18, 1124-1135.		127
335	Title is missing!. Journal of Computational Chemistry, 1997, 18, 1124.	1.5	49
336	Cooperative effects in water trimers. The performance of density functional approaches. Computational and Theoretical Chemistry, 1996, 371, 1-10.	1.5	117
337	High-level ab initio calculations on the 1,2-dithioglyoxal/1,2-dithiete isomerism. Chemical Physics Letters, 1996, 263, 407-413.	1.2	17
338	Quantum Control of Ultrafast Laser-Driven Isomerization Reactions: Proton Transfer and Selective Preparation of Enantiomers. , 0, , 189-198.		2
339	Laser-driven Ultrafast Hydrogen Transfer Dynamics. , 0, , 79-103.		1
340	HFIP Mediates a Direct Câ€“C Coupling between Michael Acceptors and Eschenmoserâ€™s salt. Angewandte Chemie, 0, , .	1.6	2
341	Unravelling the Turnâ€On Fluorescence Mechanism of a Fluoresceinâ€Based Probe in GABA _A Receptors. Angewandte Chemie, 0, , .	1.6	4