Leticia Gonzalez

List of Publications by Year
in descending order

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341 papers	12,447 citations	26610 56 h-index	42364 92 g-index
374 all docs	374 docs citations	374 times ranked	8497 citing authors

#	Article	IF	Citations
1	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
2	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
3	Deciphering the Reaction Dynamics Underlying Optimal Control Laser Fields. Science, 2003, 299, 536-539.	6.0	388
4	Progress and Challenges in the Calculation of Electronic Excited States. ChemPhysChem, 2012, 13, 28-51.	1.0	344
5	Nonadiabatic dynamics: The SHARC approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1370.	6.2	274
6	A general method to describe intersystem crossing dynamics in trajectory surface hopping. International Journal of Quantum Chemistry, 2015, 115, 1215-1231.	1.0	228
7	The IPEA dilemma in CASPT2. Chemical Science, 2017, 8, 1482-1499.	3.7	194
8	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
9	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	5.8	149
10	Femtosecond Intersystem Crossing in the DNA Nucleobase Cytosine. Journal of Physical Chemistry Letters, 2012, 3, 3090-3095.	2.1	146
11	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. Journal of Chemical Theory and Computation, 2016, 12, 1207-1219.	2.3	145
12	Phenyl-1H-[1,2,3]triazoles as New Cyclometalating Ligands for Iridium(III) Complexes. Organometallics, 2009, 28, 5478-5488.	1.1	142
13	Machine learning enables long time scale molecular photodynamics simulations. Chemical Science, 2019, 10, 8100-8107.	3.7	140
14	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
15	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
16	Cooperative effects in water trimers. The performance of density functional approaches. Computational and Theoretical Chemistry, 1996, 371, 1-10.	1.5	117
17	A Heteroleptic Bis(tridentate) Ruthenium(II) Complex of a Clickâ€Đerived Abnormal Carbene Pincer Ligand with Potential for Photosensitzer Application. Chemistry - A European Journal, 2011, 17, 5494-5498.	1.7	117
18	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

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19	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
20	Chemo- and Stereoselective Transition-Metal-Free Amination of Amides with Azides. Journal of the American Chemical Society, 2016, 138, 8348-8351.	6.6	109
21	Quantitative wave function analysis for excited states of transition metal complexes. Coordination Chemistry Reviews, 2018, 361, 74-97.	9.5	109
22	Trajectory Surface-Hopping Dynamics Including Intersystem Crossing in [Ru(bpy)₃]²⁺. Journal of Physical Chemistry Letters, 2017, 8, 3840-3845.	2.1	108
23	Selective preparation of enantiomers by laser pulses: quantum model simulation for H2POSH. Chemical Physics Letters, 1999, 306, 1-8.	1.2	101
24	Very strong hydrogen bonds in neutral molecules: The phosphinic acid dimers. Journal of Chemical Physics, 1998, 109, 2685-2693.	1.2	100
25	Metal-free intermolecular formal cycloadditions enable an orthogonal access to nitrogen heterocycles. Nature Communications, 2016, 7, 10914.	5.8	96
26	High-Level ab Initio Calculations on the Intramolecular Hydrogen Bond in Thiomalonaldehyde. Journal of Physical Chemistry A, 1997, 101, 9710-9719.	1.1	95
27	Analysis and characterization of coordination compounds by resonance Raman spectroscopy. Coordination Chemistry Reviews, 2012, 256, 1479-1508.	9.5	95
28	Ultrafast intersystem crossing dynamics in uracil unravelled byab initiomolecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24423-24436.	1.3	95
29	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
30	Density functional theory study on ethanol dimers and cyclic ethanol trimers. Journal of Chemical Physics, 1999, 111, 3855-3861.	1.2	92
31	Molecular Photochemistry: Recent Developments in Theory. Angewandte Chemie - International Edition, 2020, 59, 16832-16846.	7.2	91
32	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	2.1	89
33	Singlet and Triplet Excitedâ€State Dynamics Study of the Keto and Enol Tautomers of Cytosine. ChemPhysChem, 2013, 14, 2920-2931.	1.0	86
34	Highly efficient surface hopping dynamics using a linear vibronic coupling model. Physical Chemistry Chemical Physics, 2019, 21, 57-69.	1.3	81
35	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
36	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

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37	A Timeâ€Dependent Picture of the Ultrafast Deactivation of ketoâ€Cytosine Including Threeâ€State Conical Intersections. ChemPhysChem, 2010, 11, 3617-3624.	1.0	78
38	Analysis and control of laser induced fragmentation processes in CpMn(CO)3. Chemical Physics, 2001, 267, 247-260.	0.9	77
39	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
40	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
41	Real-Time Tracking of Phytochromeâ€™s Orientational Changes During Pr Photoisomerization. Journal of the American Chemical Society, 2012, 134, 1408-1411.	6.6	72
42	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
43	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
44	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. Journal of the American Chemical Society, 2016, 138, 15911-15916.	6.6	69
45	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
46	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
47	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
48	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
49	Ultrafast photoinduced dissipative hydrogen switching dynamics in thioacetylacetone. Physical Chemistry Chemical Physics, 1999, 1, 1249-1257.	1.3	63
50	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
51	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
52	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
53	Nonadiabatic ab initio molecular dynamics including spinâ€“orbit coupling and laser fields. Faraday Discussions, 2011, 153, 261.	1.6	59
54	Theoretical Spectroscopy and Photodynamics of a Ruthenium Nitrosyl Complex. Inorganic Chemistry, 2014, 53, 6415-6426.	1.9	59

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55	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
56	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
57	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
58	Thymine relaxation after UV irradiation: the role of tautomerization and Ï€Ïƒ* states. Physical Chemistry Chemical Physics, 2009, 11, 3927.	1.3	56
59	Enhancing Intersystem Crossing in Phenotiazinium Dyes by Intercalation into DNA. Angewandte Chemie - International Edition, 2015, 54, 4375-4378.	7.2	56
60	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
61	Using computational chemistry to design Ru photosensitizers with directional charge transfer. Coordination Chemistry Reviews, 2015, 304-305, 146-165.	9.5	55
62	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
63	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
64	Mechanism of Ultrafast Intersystem Crossing in 2â€Nitronaphthalene. Chemistry - A European Journal, 2018, 24, 5379-5387.	1.7	50
65	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
66	Title is missing!. Journal of Computational Chemistry, 1997, 18, 1124.	1.5	49
67	Substituent Effects on the Strength of the Intramolecular Hydrogen Bond of Thiomalonaldehyde. Journal of Organic Chemistry, 1999, 64, 2314-2321.	1.7	48
68	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
69	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
70	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
71	Simulation of the resonance Raman intensities of a ruthenâ€“palladium photocatalyst by time dependent density functional theory. Physical Chemistry Chemical Physics, 2010, 12, 14812.	1.3	47
72	Computational Photophysics in the Presence of an Environment. Annual Review of Physical Chemistry, 2018, 69, 473-497.	4.8	47

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73	The Reactivity and Stability of Polyoxometalate Water Oxidation Electrocatalysts. Molecules, 2020, 25, 157.	1.7	47
74	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. Journal of Chemical Physics, 2016, 144, 074303.	1.2	46
75	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
76	Control of molecular handedness using pump-dump laser pulses. Journal of Chemical Physics, 2002, 116, 2433-2438.	1.2	43
77	Quantum ignition of intramolecular rotation by means of IR+UV laser pulses. Chemical Physics Letters, 2004, 386, 248-253.	1.2	43
78	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
79	Synthesis and Catalytic Reactivity of Bis(alkylzinc)-hydride-di(2-pyridylmethyl)amides. Organometallics, 2010, 29, 3098-3108.	1.1	43
80	Excitation of Nucleobases from a Computational Perspective II: Dynamics. Topics in Current Chemistry, 2014, 355, 99-153.	4.0	43
81	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
82	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
83	Direct Regioselective Synthesis of Tetrazolium Salts by Activation of Secondary Amides under Mild Conditions. Organic Letters, 2017, 19, 2662-2665.	2.4	42
84	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
85	Design of acidochromic dyes for facile preparation of pH sensor layers. Analytical and Bioanalytical Chemistry, 2008, 392, 1411-1418.	1.9	41
86	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
87	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
88	Chiral Molecular Motors Ignited by Femtosecond Pumpâ^'Dump Laser Pulses. Journal of Physical Chemistry B, 2004, 108, 4916-4921.	1.2	39
89	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
90	Structural Control of Photoinduced Dynamics in 4H-Imidazole-Ruthenium Dyes. Journal of Physical Chemistry C, 2012, 116, 25664-25676.	1.5	38

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91	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
92	Asymmetrische Redoxarylierung: ChiralitÃ¤stransfer von Schwefel zu Kohlenstoff durch sigmatrope Sulfoniumâ€[3,3]â€Umlagerung. Angewandte Chemie, 2017, 129, 2248-2252.	1.6	38
93	Exploring wavepacket dynamics behind strong-field momentum-dependent photodissociation in CH2BrI+. Physical Chemistry Chemical Physics, 2010, 12, 14203.	1.3	37
94	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
95	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
96	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
97	Mechanistic Pathways in Amide Activation: Flexible Synthesis of Oxazoles and Imidazoles. Organic Letters, 2017, 19, 3815-3818.	2.4	36
98	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
99	Unconventional two-step spin relaxation dynamics of [Re(CO)₃(im)(phen)]⁺ in aqueous solution. Chemical Science, 2019, 10, 10405-10411.	3.7	35
100	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
101	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
102	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	2.2	33
103	Control of Nuclear Dynamics with Strong Ultrashort Laser Pulses. Journal of Physical Chemistry A, 2012, 116, 11434-11440.	1.1	33
104	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	1.2	33
105	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
106	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
107	Interstate vibronic coupling constants between electronic excited states for complex molecules. Journal of Chemical Physics, 2018, 148, 124119.	1.2	33
108	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

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109	Divergent ynamide reactivity in the presence of azides â€“ an experimental and computational study. Chemical Science, 2016, 7, 6032-6040.	3.7	32
110	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. Journal of Chemical Physics, 2017, 147, 184109.	1.2	32
111	The DNA nucleobase thymine in motion â€“ Intersystem crossing simulated with surface hopping. Chemical Physics, 2017, 482, 9-15.	0.9	32
112	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. Scientific Reports, 2018, 8, 17273.	1.6	32
113	Surface Hopping Dynamics on Vibronic Coupling Models. Accounts of Chemical Research, 2021, 54, 3760-3771.	7.6	32
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	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	1.2	31
116	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	1.1	30
117	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
118	A redox-neutral synthesis of ketones by coupling of alkenes and amides. Nature Communications, 2019, 10, 2327.	5.8	30
119	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
120	The Quest to Simulate Excited-State Dynamics of Transition Metal Complexes. Jacs Au, 2021, 1, 1116-1140.	3.6	30
121	Asymmetric laser excitation in chiral molecules: quantum simulations for a proposed experiment. Chemical Physics Letters, 2003, 372, 242-248.	1.2	29
122	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
123	Time-Dependent DFT on Phytochrome Chromophores: A Way to the Right Conformer. Journal of Physical Chemistry Letters, 2010, 1, 796-801.	2.1	29
124	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. Journal of Chemical Theory and Computation, 2018, 14, 6139-6148.	2.3	29
125	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
126	Î±â€Functionalisation of Ketones Through Metalâ€Free Electrophilic Activation. Angewandte Chemie - International Edition, 2020, 59, 20935-20939.	7.2	29

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127	Influence of Multiple Protonation on the Initial Excitation in a Black Dye. Journal of Physical Chemistry C, 2011, 115, 24004-24012.	1.5	28
128	Unusual mechanisms in Claisen rearrangements: an ionic fragmentation leading to a meta-selective rearrangement. Chemical Science, 2018, 9, 4124-4131.	3.7	28
129	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. Frontiers in Chemistry, 2018, 6, 495.	1.8	28
130	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. Molecules, 2018, 23, 2836.	1.7	28
131	Spontaneous Self-Ionization in the Gas Phase: A Theoretical Prediction. ChemPhysChem, 2001, 2, 465-467.	1.0	27
132	A Two-Dimensional Wavepacket Study of the Nonadiabatic Dynamics of CH2BrCl. Journal of Physical Chemistry A, 2008, 112, 5573-5581.	1.1	27
133	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
134	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. Scientific Reports, 2016, 6, 35522.	1.6	27
135	Photochemistry of CH2BrCl:Â An ab Initio and Dynamical Study. Journal of Physical Chemistry A, 2002, 106, 11150-11161.	1.1	26
136	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
137	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
138	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
139	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
140	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
141	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
142	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
143	Creation of multihole molecular wave packets via strong-field ionization. Physical Review A, 2010, 82, .	1.0	24
144	Quenching of Charge Transfer in Nitrobenzene Induced by Vibrational Motion. Journal of Physical Chemistry Letters, 2015, 6, 3006-3011.	2.1	24

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145	Peripheral ligands as electron storage reservoirs and their role in enhancement of photocatalytic hydrogen generation. Chemical Communications, 2016, 52, 9371-9374.	2.2	24
146	Hydrative Aminoxylation of Ynamides: One Reaction, Two Mechanisms. Chemistry - A European Journal, 2018, 24, 2515-2519.	1.7	24
147	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
148	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
149	QM/MM Nonadiabatic Dynamics: the SHARC/COBRAMM Approach. Journal of Chemical Theory and Computation, 2021, 17, 4639-4647.	2.3	24
150	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
151	Intersystem Crossing and Triplet Dynamics in an Iron(II) N-Heterocyclic Carbene Photosensitizer. Inorganic Chemistry, 2020, 59, 14666-14678.	1.9	23
152	Early Relaxation Dynamics in the Photoswitchable Complex transâ€[RuCl(NO)(py)₄]²⁺. Chemistry - A European Journal, 2020, 26, 11522-11528.	1.7	23
153	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
154	Biologically inspired molecular machines driven by light. Optimal control of a unidirectional rotor. New Journal of Physics, 2010, 12, 075007.	1.2	22
155	Revealing the Position of the Substrate in Nickel Superoxide Dismutase: A Model Study. Angewandte Chemie - International Edition, 2011, 50, 2946-2950.	7.2	22
156	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
157	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
158	Challenges in Simulating Light-Induced Processes in DNA. Molecules, 2017, 22, 49.	1.7	21
159	Solvent Effects on Electronically Excited States: QM/Continuum Versus QM/Explicit Models. Journal of Physical Chemistry B, 2018, 122, 2975-2984.	1.2	21
160	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
161	The Role of Electronic Triplet States and Highâ€Łying Singlet States in the Deactivation Mechanism of the Parent BODIPY: An ADC(2) and CASPT2 Study. ChemPhotoChem, 2019, 3, 727-738.	1.5	21
162	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

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