Leticia Gonzalez

List of Publications by Citations

346 papers	9,708 citations	50 h-index	81 g-index
374 ext. papers	10,984 ext. citations	5.2 avg, IF	6.72 L-index

#	Paper	IF	Citations
346	Deciphering the reaction dynamics underlying optimal control laser fields. *Science*, **2003**, 299, 536-9	33.3	363
345	SHARC: ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings. *Journal of Chemical Theory and Computation*, **2011**, 7, 1253-8	6.4	329
344	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
343	Progress and challenges in the calculation of electronic excited states. *ChemPhysChem*, **2012**, 13, 28-51	3.2	300
342	A general method to describe intersystem crossing dynamics in trajectory surface hopping. *International Journal of Quantum Chemistry*, **2015**, 115, 1215-1231	2.1	178
341	Nonadiabatic dynamics: The SHARC approach. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1370	7.9	158
340	Photochemical fate: the first step determines efficiency of H2 formation with a supramolecular photocatalyst. *Angewandte Chemie - International Edition*, **2010**, 49, 3981-4	16.4	150
339	The IPEA dilemma in CASPT2. *Chemical Science*, **2017**, 8, 1482-1499	9.4	134
338	Femtosecond Intersystem Crossing in the DNA Nucleobase Cytosine. *Journal of Physical Chemistry Letters*, **2012**, 3, 3090-5	6.4	134
337	Phenyl-1H-[1,2,3]triazoles as New Cyclometalating Ligands for Iridium(III) Complexes. *Organometallics*, **2009**, 28, 5478-5488	3.8	134
336	High level ab initio and density functional theory studies on methanol□water dimers and cyclic methanol(water)2 trimer. *Journal of Chemical Physics*, **1998**, 109, 139-150	3.9	122
335	High-level ab initio versus DFT calculations on (H2O2)2 and H2O2□H2O complexes as prototypes of multiple hydrogen bond systems **1997**, 18, 1124-1135		119
334	Cooperative effects in water trimers. The performance of density functional approaches. *Computational and Theoretical Chemistry*, **1996**, 371, 1-10		117
333	The origin of efficient triplet state population in sulfur-substituted nucleobases. *Nature Communications*, **2016**, 7, 13077	17.4	110
332	A heteroleptic bis(tridentate) ruthenium(II) complex of a click-derived abnormal carbene pincer ligand with potential for photosensitzer application. *Chemistry - A European Journal*, **2011**, 17, 5494-8	4.8	108
331	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. *Journal of Chemical Theory and Computation*, **2016**, 12, 1207-19	6.4	100
330	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. *Journal of Physical Chemistry Letters*, **2016**, 7, 1978-83	6.4	97

329	Machine learning enables long time scale molecular photodynamics simulations. *Chemical Science*, **2019**, 10, 8100-8107	9.4	96
328	Very strong hydrogen bonds in neutral molecules: The phosphinic acid dimers. *Journal of Chemical Physics*, **1998**, 109, 2685-2693	3.9	92
327	Selective preparation of enantiomers by laser pulses: quantum model simulation for H2POSH. *Chemical Physics Letters*, **1999**, 306, 1-8	2.5	89
326	An Asymmetric Redox Arylation: Chirality Transfer from Sulfur to Carbon through a Sulfonium [3,3]-Sigmatropic Rearrangement. *Angewandte Chemie - International Edition*, **2017**, 56, 2212-2215	16.4	88
325	Analysis and characterization of coordination compounds by resonance Raman spectroscopy. *Coordination Chemistry Reviews*, **2012**, 256, 1479-1508	23.2	88
324	Density functional theory study on ethanol dimers and cyclic ethanol trimers. *Journal of Chemical Physics*, **1999**, 111, 3855-3861	3.9	88
323	Chemo- and Stereoselective Transition-Metal-Free Amination of Amides with Azides. *Journal of the American Chemical Society*, **2016**, 138, 8348-51	16.4	87
322	High-Level ab Initio Calculations on the Intramolecular Hydrogen Bond in Thiomalonaldehyde. *Journal of Physical Chemistry A*, **1997**, 101, 9710-9719	2.8	84
321	Quantitative wave function analysis for excited states of transition metal complexes. *Coordination Chemistry Reviews*, **2018**, 361, 74-97	23.2	81
320	Trajectory Surface-Hopping Dynamics Including Intersystem Crossing in [Ru(bpy)]. *Journal of Physical Chemistry Letters*, **2017**, 8, 3840-3845	6.4	81
319	Ultrafast intersystem crossing dynamics in uracil unravelled by ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 24423-36	3.6	80
318	Singlet and triplet excited-state dynamics study of the keto and enol tautomers of cytosine. *ChemPhysChem*, **2013**, 14, 2920-31	3.2	75
317	A time-dependent picture of the ultrafast deactivation of keto-cytosine including three-state conical intersections. *ChemPhysChem*, **2010**, 11, 3617-24	3.2	74
316	Communication: GAIMS--Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. *Journal of Chemical Physics*, **2016**, 144, 101102	3.9	74
315	Structure–Property Relationship of Red- and Green-Emitting Iridium(III) Complexes with Respect to Their Temperature and Oxygen Sensitivity. *European Journal of Inorganic Chemistry*, **2010**, 2010, 4875-4885	2.3	73
314	Metal-free intermolecular formal cycloadditions enable an orthogonal access to nitrogen heterocycles. *Nature Communications*, **2016**, 7, 10914	17.4	72
313	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 622-6	6.4	71
312	Analysis and control of laser induced fragmentation processes in CpMn(CO)3. *Chemical Physics*, **2001**, 267, 247-260	2.3	70

311	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, 2134-6	5.8	66
310	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	9.4	61
309	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	4.6	60
308	Ruthenium(II) photosensitizers of tridentate click-derived cyclometalating ligands: a joint experimental and computational study. *Chemistry - A European Journal*, **2012**, 18, 4010-25	4.8	60
307	Real-time tracking of phytochrome's orientational changes during Pr photoisomerization. *Journal of the American Chemical Society*, **2012**, 134, 1408-11	16.4	59
306	Electronic and structural elements that regulate the excited-state dynamics in purine nucleobase derivatives. *Journal of the American Chemical Society*, **2015**, 137, 4368-81	16.4	58
305	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	3.9	58
304	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, 4025-38	4.2	56
303	Highly efficient surface hopping dynamics using a linear vibronic coupling model. *Physical Chemistry Chemical Physics*, **2018**, 21, 57-69	3.6	55
302	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. *Journal of Physical Chemistry A*, **2015**, 119, 9524-33	2.8	55
301	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	4.7	55
300	Ultrafast photoinduced dissipative hydrogen switching dynamics in thioacetylacetone. *Physical Chemistry Chemical Physics*, **1999**, 1, 1249-1257	3.6	55
299	Molecular Photochemistry: Recent Developments in Theory. *Angewandte Chemie - International Edition*, **2020**, 59, 16832-16846	16.4	55
298	Nonadiabatic ab initio molecular dynamics including spin-orbit coupling and laser fields. *Faraday Discussions*, **2011**, 153, 261-73; discussion 293-319	3.6	54
297	Theoretical spectroscopy and photodynamics of a ruthenium nitrosyl complex. *Inorganic Chemistry*, **2014**, 53, 6415-26	5.1	50
296	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. *Physical Chemistry Chemical Physics*, **2016**, 18, 20168-76	3.6	50
295	Orbital entanglement and CASSCF analysis of the Ru-NO bond in a Ruthenium nitrosyl complex. *Physical Chemistry Chemical Physics*, **2015**, 17, 14383-92	3.6	49
294	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, 203-13	6.4	49

293	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, 15580-8	3.6	49
292	Using computational chemistry to design Ru photosensitizers with directional charge transfer. *Coordination Chemistry Reviews*, **2015**, 304-305, 146-165	23.2	48
291	Thymine relaxation after UV irradiation: the role of tautomerization and pi-sigma* states. *Physical Chemistry Chemical Physics*, **2009**, 11, 3927-34	3.6	48
290	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. *Journal of the American Chemical Society*, **2016**, 138, 15911-15916	16.4	48
289	Separation of enantiomers by ultraviolet laser pulses in H2POSH: □pulses versus adiabatic transitions. *Journal of Chemical Physics*, **2001**, 115, 2519-2529	3.9	46
288	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	3.9	46
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284	Ground- and Excited-State Surfaces for the [2+2]-Photocycloaddition of ⌗Enones to Alkenes. *Journal of the American Chemical Society*, **2000**, 122, 5866-5876	16.4	44
283	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. *Physical Chemistry Chemical Physics*, **2017**, 19, 19756-19766	3.6	43
282	Simulation of the resonance Raman intensities of a ruthenium-palladium photocatalyst by time dependent density functional theory. *Physical Chemistry Chemical Physics*, **2010**, 12, 14812-21	3.6	43
281	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	3.9	42
280	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, 6084-93	2.8	42
279	A Vanadium(III) Complex with Blue and NIR-II Spin-Flip Luminescence in Solution. *Journal of the American Chemical Society*, **2020**, 142, 7947-7955	16.4	41
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276	Quantum ignition of intramolecular rotation by means of IR + UV laser pulses. *Chemical Physics Letters*, **2004**, 386, 248-253	2.5	40

275	Synthesis and Catalytic Reactivity of Bis(alkylzinc)-hydride-di(2-pyridylmethyl)amides. *Organometallics*, **2010**, 29, 3098-3108	3.8	38
274	Control of molecular handedness using pump-dump laser pulses. *Journal of Chemical Physics*, **2002**, 116, 2433-2438	3.9	38
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271	Mixed quantum-classical dynamics in the adiabatic representation to simulate molecules driven by strong laser pulses. *Journal of Physical Chemistry A*, **2012**, 116, 2800-7	2.8	37
270	Design of acidochromic dyes for facile preparation of pH sensor layers. *Analytical and Bioanalytical Chemistry*, **2008**, 392, 1411-8	4.4	37
269	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. *Journal of Chemical Physics*, **2016**, 144, 074303	3.9	37
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262	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	6.4	34
261	Unified Approach to the Chemoselective Functionalization of Amides with Heteroatom Nucleophiles. *Journal of the American Chemical Society*, **2019**, 141, 18437-18443	16.4	34
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258	Chiral Molecular Motors Ignited by Femtosecond PumpDump Laser Pulses. *Journal of Physical Chemistry B*, **2004**, 108, 4916-4921	3.4	33

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255	Detailed Wave Function Analysis for Multireference Methods: Implementation in the Molcas Program Package and Applications to Tetracene. *Journal of Chemical Theory and Computation*, **2017**, 13, 5343-5353	6.4	32
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