Luis Manuel Frutos Gaite

List of Publications by Year
in descending order

68	4,129	257450 24	114465 63
papers	citations	h-index	g-index

72	72	72	4431
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
3	Tracking the excited-state time evolution of the visual pigment with multiconfigurational quantum chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7764-7769.	7.1	266
4	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. Journal of Chemical Theory and Computation, 2014, 10, 3074-3084.	5.3	161
5	The Ultrafast Photoisomerizations of Rhodopsin and Bathorhodopsin Are Modulated by Bond Length Alternation and HOOP Driven Electronic Effects. Journal of the American Chemical Society, 2011, 133, 3354-3364.	13.7	157
6	E/Z Photochemical switches: syntheses, properties and applications. RSC Advances, 2013, 3, 6241.	3.6	95
7	Organic Thermochemistry at High ab Initio Levels. 1. A G2(MP2) and G2 Study of Cyclic Saturated and Unsaturated Hydrocarbons (Including Aromatics). Journal of Organic Chemistry, 1999, 64, 9011-9014.	3.2	86
8	Organic Thermochemistry at High ab Initio Levels. 3. A G3 Study of Cyclic Saturated and Unsaturated Hydrocarbons (Including Aromatics). Journal of Organic Chemistry, 2000, 65, 4298-4302.	3.2	82
9	Cyclooctatetraene Computational Photo- and Thermal Chemistry:Â A Reactivity Model for Conjugated Hydrocarbons. Journal of the American Chemical Society, 2002, 124, 13770-13789.	13.7	75
10	Photochemistry of hydrogen-bonded aromatic pairs: Quantum dynamical calculations for the pyrroleâ€“pyridine complex. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12707-12712.	7.1	74
11	Ab Initio Based Exploration of the Potential Energy Surface for the Double Proton Transfer in the First Excited Singlet Electronic State of the 7-Azaindole Dimer. Journal of Physical Chemistry A, 2001, 105, 3887-3893.	2.5	70
12	Chiral Hydrogen Bond Environment Providing Unidirectional Rotation in Photoactive Molecular Motors. Journal of Physical Chemistry Letters, 2013, 4, 1389-1396.	4.6	59
13	Relationship between the Excited State Relaxation Paths of Rhodopsin and Isorhodopsin. Journal of the American Chemical Society, 2008, 130, 3382-3388.	13.7	58
14	Modeling, Preparation, and Characterization of a Dipole Moment Switch Driven by Z/E Photoisomerization. Journal of the American Chemical Society, 2010, 132, 9310-9319.	13.7	53
15	Directionality of Double-Bond Photoisomerization Dynamics Induced by a Single Stereogenic Center. Journal of Physical Chemistry Letters, 2015, 6, 599-604.	4.6	53
16	Synthesis, Optical Properties, and Regioselective Functionalization of 4a-Aza-10a-boraphenanthrene. Organic Letters, 2017, 19, 3458-3461.	4.6	48
17	Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. Journal of Chemical Theory and Computation, 2016, 12, 839-850.	5.3	43
18	Role of bifurcation in the bond shifting of cyclooctatetraene. Journal of Computational Chemistry, 2002, 23, 732-736.	3.3	40

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19	Monocyclopentadienyl andansa-Monocyclopentadienylalkoxo Complexes of Titanium Containing the 2,2â€˙-Methylenebis(6-tert-butyl-4-methylphenoxo) Ligand. Synthesis, Characterization, and Polymerization Catalyst Behavior. Molecular Structure of Ti(Î·5-C5H5)(Î·2-MBMP)Cl, Ti(Î·5-C5Me5)(Î·2-MBMP)Cl, and Ti(Î·5-C5H4SiMe2-Î·1-MBMP)Cl2. Organometallics, 2003, 22, 2694-2704.	2.3	38
20	Theoretical Determination of the Singlet â†' Singlet and Singlet â†' Triplet Electronic Spectra, Lowest Ionization Potentials, and Electron Affinity of Cyclooctatetraene. Journal of Physical Chemistry A, 2003, 107, 5472-5478.	2.5	36
21	A theory ofnonverticaltriplet energy transfer in terms of accurate potential energy surfaces: The transfer reaction from Ï€,Ï€* triplet donors to 1,3,5,7-cyclooctatetraene. Journal of Chemical Physics, 2004, 120, 1208-1216.	3.0	34
22	Photoinduced Electron and Proton Transfer in the Hydrogen-Bonded Pyridineâ^'Pyrrole System. Journal of Physical Chemistry B, 2007, 111, 6110-6112.	2.6	31
23	Hydantoin-Based Molecular Photoswitches. Journal of Organic Chemistry, 2015, 80, 3929-3939.	3.2	31
24	Trapping Unstable Terminal Taâ^'O Multiple Bonds of Monocyclopentadienyl Tantalum Complexes with a Lewis Acid. Organometallics, 2005, 24, 2004-2007.	2.3	27
25	The Valence Isomerization of Cyclooctatetraene to Semibullvalene. Angewandte Chemie - International Edition, 2000, 39, 2095-2097.	13.8	25
26	Triplet versus Singlet Photoreaction Mechanism in the Barrelene Di-Ï€-methane Rearrangement. Organic Letters, 2004, 6, 1229-1231.	4.6	25
27	Toward an Optomechanical Control of Photoswitches by Tuning Their Spectroscopical Properties: Structural and Dynamical Insights into Azobenzene. Journal of Chemical Theory and Computation, 2014, 10, 312-323.	5.3	24
28	Optomechanical Control of Quantum Yield in Transâ€“Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. Angewandte Chemie - International Edition, 2017, 56, 3842-3846.	13.8	24
29	How Do Methyl Groups Enhance the Triplet Chemiexcitation Yield of Dioxetane?. Journal of Physical Chemistry Letters, 2017, 8, 3790-3794.	4.6	24
30	Fluorescence Emission Anisotropy Coupled to an Electrochemical System:â€‰ Study of Exciton Dynamics in Conjugated Polymers. Journal of Physical Chemistry C, 2007, 111, 18405-18410.	3.1	23
31	Thermodynamic, Kinetic, and Mechanistic Study of Oxygen Atom Transfer from Mesityl Nitrile Oxide to Phosphines and to a Terminal Metal Phosphido Complex. Inorganic Chemistry, 2011, 50, 9620-9630.	4.0	23
32	Photoinduced Proton Transfer as a Possible Mechanism for Highly Efficient Excited-State Deactivation in Proteins. Journal of Physical Chemistry Letters, 2010, 1, 425-428.	4.6	22
33	Câ€“H Functionalization of BN-Aromatics Promoted by Addition of Organolithium Compounds to the Boron Atom. Organic Letters, 2018, 20, 4902-4906.	4.6	22
34	Organic Thermochemistry at High ab Initio Levels. 2. Meeting the Challenge:Â Standard Heats of Formation of Gaseous Norbornane, 2-Norbornene, 2,5-Norbornadiene, Cubane, and Adamantane at the G2 Level. Journal of Organic Chemistry, 1999, 64, 9015-9018.	3.2	20
35	Modulating Nitric Oxide Release by S-Nitrosothiol Photocleavage: Mechanism and Substituent Effects. Journal of Physical Chemistry A, 2012, 116, 7039-7049.	2.5	19
36	Carbon Dioxide Activation Assisted by a Bis(chlorodimethylsilyl)cyclopentadienyl Titanium Compound. Angewandte Chemie - International Edition, 2005, 44, 5828-5830.	13.8	18

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37	A biomimetic molecular switch at work: coupling photoisomerization dynamics to peptide structural rearrangement. Physical Chemistry Chemical Physics, 2016, 18, 6742-6753.	2.8	16
38	Optomechanical Control of Quantum Yield in Transâ€“Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. Angewandte Chemie, 2017, 129, 3900-3904.	2.0	15
39	Mechanical Forces Alter Conical Intersections Topology. Journal of Chemical Theory and Computation, 2015, 11, 3740-3745.	5.3	14
40	Photoreactivity Control Mediated by Molecular Force Probes in Stilbene. Journal of Physical Chemistry Letters, 2019, 10, 1063-1067.	4.6	14
41	A new algorithm for predicting triplet-triplet energy-transfer activated complex coordinate in terms of accurate potential-energy surfaces. Journal of Chemical Physics, 2005, 123, 104108.	3.0	13
42	Theoretical Study on the Mechanism and Regioselectivity of the Macromolecular Substitution Reactions of [NPCl₂]_n with Bifunctional Nucleophiles by a Combination of Quantum Mechanical and Molecular Dynamics Calculations. Macromolecules, 2009, 42, 8769-8773.	4.8	13
43	Structural Substituent Effect in the Excitation Energy of a Chromophore: Quantitative Determination and Application to S-Nitrosothiols. Journal of Chemical Theory and Computation, 2012, 8, 3293-3302.	5.3	13
44	Note on the theory of bifurcation of chemical reactions. International Journal of Quantum Chemistry, 2002, 86, 422-425.	2.0	12
45	Tuning molecular excitation energy with external forces. Computational and Theoretical Chemistry, 2014, 1040-1041, 106-111.	2.5	12
46	Study of Model Systems for Bilirubin and Bilin Chromophores: Determination and Modification of Thermal and Photochemical Properties. Journal of Organic Chemistry, 2016, 81, 6292-6302.	3.2	12
47	Trapping Unstable Terminal Mâ‹®O Multiple Bonds of Monocyclopentadienyl Niobium and Tantalum Complexes with Lewis Acids. Inorganic Chemistry, 2010, 49, 10642-10648.	4.0	11
48	Intramolecular Tripletâ‹®Triplet Energy Transfer in Oxa- and Aza-di-Ï€-methane Photosensitized Systems. Journal of Physical Chemistry A, 2005, 109, 2993-2995.	2.5	10
49	Olefin isomerisation versus hydrozirconation: a case of a stable Î²-hydrogen-containing Zr-alkyl derivative. Dalton Transactions, 2008, , 2670.	3.3	10
50	Mechanochemical Improvement of Norbornadiene-Based Molecular Solarâ€“Thermal Systems Performance. ACS Sustainable Chemistry and Engineering, 2019, 7, 19496-19504.	6.7	10
51	Unusual Approach to 3-Aryl-2-aminopyridines through a Radical Mechanism: Synthesis and Theoretical Rationale from Quantum Mechanical Calculationsâ€. Journal of Organic Chemistry, 2011, 76, 1452-1455.	3.2	9
52	Alkylmono(cyclopentadienyl)titanium Complexes Containing the 2,2â€²-Methylenebis(6-tert-butyl-4-methylphenoxido) Ligand â€“ Studies on the Nature of the Catalytic Species Present in Î±-Olefin Polymerisation Processes. European Journal of Inorganic Chemistry, 2007, 2007, 147-161.	2.0	8
53	First principles study of photostability within hydrogen-bonded amino acids. Physical Chemistry Chemical Physics, 2011, 13, 7805.	2.8	8
54	Mechanochemical Tuning of Pyrene Absorption Spectrum Using Force Probes. Journal of Chemical Theory and Computation, 2017, 13, 727-736.	5.3	8

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55	The Role of the Intersection Space in the Photochemistry of Tricyclo[3.3.0.02,6]octa-3,7-diene. Journal of Physical Chemistry A, 2007, 111, 2830-2838.	2.5	7
56	Definition and determination of the triplet-triplet energy transfer reaction coordinate. Journal of Chemical Physics, 2014, 140, 034102.	3.0	7
57	Thermal and Mechanochemical Tuning of the Porphyrin Singlet-Triplet Gap for Selective Energy Transfer Processes: A Molecular Dynamics Approach. Journal of Chemical Theory and Computation, 2021, 17, 5429-5439.	5.3	7
58	Photosensitized Retinal Isomerization in Rhodopsin Mediated by a Triplet State. ChemPhotoChem, 2019, 3, 925-932.	3.0	6
59	Regioselective Synthesis of 1,2- and 1,3-Di(silylamido)cyclopentadienyl Zirconium Complexes. Organometallics, 2010, 29, 263-268.	2.3	5
60	Photostability Mechanisms in Human Î³B-Crystallin: Role of the Tyrosine Corner Unveiled by Quantum Mechanics and Hybrid Quantum Mechanics/Molecular Mechanics Methodologies. Journal of Chemical Theory and Computation, 2012, 8, 1351-1359.	5.3	5
61	How mechanical forces can modulate the metal affinity and selectivity of metal binding sites in proteins. Metallomics, 2020, 12, 363-370.	2.4	4
62	The concept of substituent-induced force in the rationale of substituent effect. Journal of Chemical Physics, 2021, 154, 224106.	3.0	4
63	Correlated MO Study of the Low-Barrier Intramolecular Motions in Donorâ^'Acceptor Ethenes. Journal of Physical Chemistry A, 2005, 109, 10388-10395.	2.5	2
64	On the mechanism of the photocyclization of azadienes. Tetrahedron, 2012, 68, 730-736.	1.9	2
65	Molecular Switching by Electron Holes. CheM, 2018, 4, 1488-1489.	11.7	2
66	Design of Improved Molecular Solarâ€Thermal Systems by Mechanochemistry: The Case of Azobenzene. Advanced Sustainable Systems, 0, , 2200097.	5.3	2
67	The Role of Intersection Space Segments in Photochemical Reactions. AIP Conference Proceedings, 2007, , .	0.4	0
68	New Computational Approaches in the Study of Nonvertical Triplet Energy Transfer. AIP Conference Proceedings, 2007, , .	0.4	0