Luis Manuel Frutos Gaite

List of Publications by Citations

67 papers	3,184 citations	24 h-index	56 g-index
72 ext. papers	3,684 ext. citations	6.1 avg, IF	4.51 L-index

#	Paper	IF	Citations
67	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
66	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
65	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, 7764-9	11.5	239
64	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, 3354-64	16.4	139
63	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, 3074-84	6.4	132
62	E/Z Photochemical switches: syntheses, properties and applications. *RSC Advances*, **2013**, 3, 6241	3.7	81
61	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	4.2	81
60	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	4.2	75
59	Photochemistry of hydrogen-bonded aromatic pairs: Quantum dynamical calculations for the pyrrole-pyridine complex. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 12707-12	11.5	72
58	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	2.8	66
57	Cyclooctatetraene computational photo- and thermal chemistry: a reactivity model for conjugated hydrocarbons. *Journal of the American Chemical Society*, **2002**, 124, 13770-89	16.4	60
56	Relationship between the excited state relaxation paths of rhodopsin and isorhodopsin. *Journal of the American Chemical Society*, **2008**, 130, 3382-8	16.4	56
55	Chiral Hydrogen Bond Environment Providing Unidirectional Rotation in Photoactive Molecular Motors. *Journal of Physical Chemistry Letters*, **2013**, 4, 1389-96	6.4	47
54	Directionality of Double-Bond Photoisomerization Dynamics Induced by a Single Stereogenic Center. *Journal of Physical Chemistry Letters*, **2015**, 6, 599-604	6.4	46
53	Modeling, preparation, and characterization of a dipole moment switch driven by Z/E photoisomerization. *Journal of the American Chemical Society*, **2010**, 132, 9310-9	16.4	46
52	Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. *Journal of Chemical Theory and Computation*, **2016**, 12, 839-50	6.4	38
51	Role of bifurcation in the bond shifting of cyclooctatetraene. *Journal of Computational Chemistry*, **2002**, 23, 732-6	3.5	35

50	Monocyclopentadienyl and ansa-Monocyclopentadienylalkoxo Complexes of Titanium Containing the 2,2-Methylenebis(6-tert-butyl-4-methylphenoxo) Ligand. Synthesis, Characterization, and Polymerization Catalyst Behavior. Molecular Structure of Ti(η5-C5H5)(κ2-MBMP)Cl, Ti(η5-C5Me5)(κ2-MBMP)Cl, and Ti(η5-C5H4SiMe2-κ1-MBMP)Cl2. *Organometallics*, **2003**, 22, 2694-2704	3.8	33
49	Synthesis, Optical Properties, and Regioselective Functionalization of 4a-Aza-10a-boraphenanthrene. *Organic Letters*, **2017**, 19, 3458-3461	6.2	32
48	Photoinduced electron and proton transfer in the hydrogen-bonded pyridine-pyrrole system. *Journal of Physical Chemistry B*, **2007**, 111, 6110-2	3.4	30
47	Theoretical Determination of the Singlet -πSinglet and Singlet -πTriplet Electronic Spectra, Lowest Ionization Potentials, and Electron Affinity of Cyclooctatetraene. *Journal of Physical Chemistry A*, **2003**, 107, 5472-5478	2.8	30
46	A theory of nonvertical triplet energy transfer in terms of accurate potential energy surfaces: the transfer reaction from pi,pi* triplet donors to 1,3,5,7-cyclooctatetraene. *Journal of Chemical Physics* , **2004**, 120, 1208-16	3.9	28
45	Trapping Unstable Terminal Ta Multiple Bonds of Monocyclopentadienyl Tantalum Complexes with a Lewis Acid. *Organometallics*, **2005**, 24, 2004-2007	3.8	25
44	Hydantoin-based molecular photoswitches. *Journal of Organic Chemistry*, **2015**, 80, 3929-39	4.2	24
43	Fluorescence Emission Anisotropy Coupled to an Electrochemical System: Study of Exciton Dynamics in Conjugated Polymers. *Journal of Physical Chemistry C*, **2007**, 111, 18405-18410	3.8	23
42	Triplet versus singlet photoreaction mechanism in the barrelene di-pi-methane rearrangement. *Organic Letters*, **2004**, 6, 1229-31	6.2	23
41	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, 9620-30	5.1	21
40	Photoinduced Proton Transfer as a Possible Mechanism for Highly Efficient Excited-State Deactivation in Proteins. *Journal of Physical Chemistry Letters*, **2010**, 1, 425-428	6.4	19
39	The Valence Isomerization of Cyclooctatetraene to Semibullvalene. *Angewandte Chemie - International Edition*, **2000**, 39, 2095-2097	16.4	19
38	Organic Thermochemistry at High ab Initio Levels. 2. Meeting the Challenge: 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	4.2	19
37	Optomechanical Control of Quantum Yield in Trans-Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. *Angewandte Chemie - International Edition*, **2017**, 56, 3842-3846	16.4	18
36	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, 312-23	6.4	18
35	C-H Functionalization of BN-Aromatics Promoted by Addition of Organolithium Compounds to the Boron Atom. *Organic Letters*, **2018**, 20, 4902-4906	6.2	16
34	How Do Methyl Groups Enhance the Triplet Chemiexcitation Yield of Dioxetane?. *Journal of Physical Chemistry Letters*, **2017**, 8, 3790-3794	6.4	16
33	Carbon dioxide activation assisted by a bis(chlorodimethylsilyl)cyclopentadienyl titanium compound. *Angewandte Chemie - International Edition*, **2005**, 44, 5828-30	16.4	16

32	Modulating nitric oxide release by S-nitrosothiol photocleavage: mechanism and substituent effects. *Journal of Physical Chemistry A*, **2012**, 116, 7039-49	2.8	14
31	A biomimetic molecular switch at work: coupling photoisomerization dynamics to peptide structural rearrangement. *Physical Chemistry Chemical Physics*, **2016**, 18, 6742-53	3.6	12
30	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	5.5	12
29	Note on the theory of bifurcation of chemical reactions. *International Journal of Quantum Chemistry* , **2002**, 86, 422-425	2.1	12
28	Mechanical Forces Alter Conical Intersections Topology. *Journal of Chemical Theory and Computation*, **2015**, 11, 3740-5	6.4	11
27	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	3.9	11
26	Tuning molecular excitation energy with external forces. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 106-111	2	10
25	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, 3293-302	6.4	10
24	Trapping unstable terminal M-O multiple bonds of monocyclopentadienyl niobium and tantalum complexes with Lewis acids. *Inorganic Chemistry*, **2010**, 49, 10642-8	5.1	10
23	Photoreactivity Control Mediated by Molecular Force Probes in Stilbene. *Journal of Physical Chemistry Letters*, **2019**, 10, 1063-1067	6.4	8
22	Study of Model Systems for Bilirubin and Bilin Chromophores: Determination and Modification of Thermal and Photochemical Properties. *Journal of Organic Chemistry*, **2016**, 81, 6292-302	4.2	8
21	Unusual approach to 3-aryl-2-aminopyridines through a radical mechanism: synthesis and theoretical rationale from quantum mechanical calculations. *Journal of Organic Chemistry*, **2011**, 76, 1452-5	4.2	8
20	Olefin isomerisation versus hydrozirconation: a case of a stable beta-hydrogen-containing Zr-alkyl derivative. *Dalton Transactions*, **2008**, 2670-3	4.3	8
19	Intramolecular triplet-triplet energy transfer in oxa- and aza-di-pi-methane photosensitized systems. *Journal of Physical Chemistry A*, **2005**, 109, 2993-5	2.8	8
18	Mechanochemical Tuning of Pyrene Absorption Spectrum Using Force Probes. *Journal of Chemical Theory and Computation*, **2017**, 13, 727-736	6.4	6
17	First principles study of photostability within hydrogen-bonded amino acids. *Physical Chemistry Chemical Physics*, **2011**, 13, 7805-11	3.6	6
16	The role of the intersection space in the photochemistry of tricyclo[3.3.0.0(2,6)]octa-3,7-diene. *Journal of Physical Chemistry A*, **2007**, 111, 2830-8	2.8	6
15	Alkylmono(cyclopentadienyl)titanium Complexes Containing the 2,2?-Methylenebis(6-tert-butyl-4-methylphenoxido) Ligand Studies on the Nature of the Catalytic Species Present in Olefin Polymerisation Processes. *European Journal of Inorganic Chemistry*, **2007**, 2007, 147-161	2.3	6

14	Definition and determination of the triplet-triplet energy transfer reaction coordinate. *Journal of Chemical Physics*, **2014**, 140, 034102	3.9	5
13	Regioselective Synthesis of 1,2- and 1,3-Di(silylamido)cyclopentadienyl Zirconium Complexes. *Organometallics*, **2010**, 29, 263-268	3.8	5
12	Photosensitized Retinal Isomerization in Rhodopsin Mediated by a Triplet State. *ChemPhotoChem*, **2019**, 3, 925-932	3.3	4
11	Photostability Mechanisms in Human B-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, 1351-9	6.4	4
10	OpenMolcas: From Source Code to Insight		4
9	Optomechanical Control of Quantum Yield in Trans□is Ultrafast Photoisomerization of a Retinal Chromophore Model. *Angewandte Chemie*, **2017**, 129, 3900-3904	3.6	3
8	Mechanochemical Improvement of Norbornadiene-Based Molecular Solar□hermal Systems Performance. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 19496-19504	8.3	3
7	Molecular Switching by Electron Holes. *CheM*, **2018**, 4, 1488-1489	16.2	2
6	On the mechanism of the photocyclization of azadienes. *Tetrahedron*, **2012**, 68, 730-736	2.4	2
5	Correlated MO study of the low-barrier intramolecular motions in donor-acceptor ethenes. *Journal of Physical Chemistry A*, **2005**, 109, 10388-95	2.8	2
4	How mechanical forces can modulate the metal affinity and selectivity of metal binding sites in proteins. *Metallomics*, **2020**, 12, 363-370	4.5	2
3	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	6.4	2
2	The concept of substituent-induced force in the rationale of substituent effect. *Journal of Chemical Physics*, **2021**, 154, 224106	3.9	0
1	Design of Improved Molecular Solar-Thermal Systems by Mechanochemistry: The Case of Azobenzene. *Advanced Sustainable Systems*,2200097	5.9	0