# Luis Manuel Frutos Gaite

List of Publications by Year
in descending order

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Version: 2024-02-01

| 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 | The concept of substituent-induced force in the rationale of substituent effect. Journal of Chemical Physics, 2021, 154, 224106. | 3.0 | 4 |
| 2 | 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 |
| 3 | How mechanical forces can modulate the metal affinity and selectivity of metal binding sites in proteins. Metallomics, 2020, 12, 363-370. | 2.4 | 4 |
| 4 | OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964. | 5.3 | 661 |
| 5 | Photoreactivity Control Mediated by Molecular Force Probes in Stilbene. Journal of Physical Chemistry Letters, 2019, 10, 1063-1067. | 4.6 | 14 |
| 6 | Photosensitized Retinal Isomerization in Rhodopsin Mediated by a Triplet State. ChemPhotoChem, 2019, 3, 925-932. | 3.0 | 6 |
| 7 | Mechanochemical Improvement of Norbornadiene-Based Molecular Solarâ€“Thermal Systems Performance. ACS Sustainable Chemistry and Engineering, 2019, 7, 19496-19504. | 6.7 | 10 |
| 8 | 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 |
| 9 | Molecular Switching by Electron Holes. CheM, 2018, 4, 1488-1489. | 11.7 | 2 |
| 10 | Mechanochemical Tuning of Pyrene Absorption Spectrum Using Force Probes. Journal of Chemical Theory and Computation, 2017, 13, 727-736. | 5.3 | 8 |
| 11 | 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 |
| 12 | Optomechanical Control of Quantum Yield in Transâ€“Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. Angewandte Chemie, 2017, 129, 3900-3904. | 2.0 | 15 |
| 13 | Synthesis, Optical Properties, and Regioselective Functionalization of 4a-Aza-10a-boraphenanthrene. Organic Letters, 2017, 19, 3458-3461. | 4.6 | 48 |
| 14 | How Do Methyl Groups Enhance the Triplet Chemiexcitation Yield of Dioxetane?. Journal of Physical Chemistry Letters, 2017, 8, 3790-3794. | 4.6 | 24 |
| 15 | <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 |
| 16 | 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 |
| 17 | Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. Journal of Chemical Theory and Computation, 2016, 12, 839-850. | 5.3 | 43 |
| 18 | A biomimetic molecular switch at work: coupling photoisomerization dynamics to peptide structural rearrangement. Physical Chemistry Chemical Physics, 2016, 18, 6742-6753. | 2.8 | 16 |

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|---|---|---|---|
| 19 | Directionality of Double-Bond Photoisomerization Dynamics Induced by a Single Stereogenic Center. Journal of Physical Chemistry Letters, 2015, 6, 599-604. | 4.6 | 53 |
| 20 | Mechanical Forces Alter Conical Intersections Topology. Journal of Chemical Theory and Computation, 2015, 11, 3740-3745. | 5.3 | 14 |
| 21 | Hydantoin-Based Molecular Photoswitches. Journal of Organic Chemistry, 2015, 80, 3929-3939. | 3.2 | 31 |
| 22 | Definition and determination of the triplet-triplet energy transfer reaction coordinate. Journal of Chemical Physics, 2014, 140, 034102. | 3.0 | 7 |
| 23 | Tuning molecular excitation energy with external forces. Computational and Theoretical Chemistry, 2014, 1040-1041, 106-111. | 2.5 | 12 |
| 24 | 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 |
| 25 | 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 |
| 26 | E/Z Photochemical switches: syntheses, properties and applications. RSC Advances, 2013, 3, 6241. | 3.6 | 95 |
| 27 | Chiral Hydrogen Bond Environment Providing Unidirectional Rotation in Photoactive Molecular Motors. Journal of Physical Chemistry Letters, 2013, 4, 1389-1396. | 4.6 | 59 |
| 28 | Modulating Nitric Oxide Release by S-Nitrosothiol Photocleavage: Mechanism and Substituent Effects. Journal of Physical Chemistry A, 2012, 116, 7039-7049. | 2.5 | 19 |
| 29 | 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 |
| 30 | 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 |
| 31 | On the mechanism of the photocyclization of azadienes. Tetrahedron, 2012, 68, 730-736. | 1.9 | 2 |
| 32 | 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 |
| 33 | First principles study of photostability within hydrogen-bonded amino acids. Physical Chemistry Chemical Physics, 2011, 13, 7805. | 2.8 | 8 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

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| 37 | 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 |
| 38 | 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 |
| 39 | Regioselective Synthesis of 1,2- and 1,3-Di(silylamido)cyclopentadienyl Zirconium Complexes. Organometallics, 2010, 29, 263-268. | 2.3 | 5 |
| 40 | Theoretical Study on the Mechanism and Regioselectivity of the Macromolecular Substitution Reactions of [NPCl<sub>2</sub>]<sub>n</sub> with Bifunctional Nucleophiles by a Combination of Quantum Mechanical and Molecular Dynamics Calculations. Macromolecules, 2009, 42, 8769-8773. | 4.8 | 13 |
| 41 | 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 |
| 42 | Olefin isomerisation versus hydrozirconation: a case of a stable Î²-hydrogen-containing Zr-alkyl derivative. Dalton Transactions, 2008, , 2670. | 3.3 | 10 |
| 43 | Relationship between the Excited State Relaxation Paths of Rhodopsin and Isorhodopsin. Journal of the American Chemical Society, 2008, 130, 3382-3388. | 13.7 | 58 |
| 44 | 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 |
| 45 | The Role of Intersection Space Segments in Photochemical Reactions. AIP Conference Proceedings, 2007, , . | 0.4 | 0 |
| 46 | 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 |
| 47 | 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 |
| 48 | Photoinduced Electron and Proton Transfer in the Hydrogen-Bonded Pyridineâ‹¯Pyrrole System. Journal of Physical Chemistry B, 2007, 111, 6110-6112. | 2.6 | 31 |
| 49 | New Computational Approaches in the Study of Nonvertical Triplet Energy Transfer. AIP Conference Proceedings, 2007, , . | 0.4 | 0 |
| 50 | 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 |
| 51 | Carbon Dioxide Activation Assisted by a Bis(chlorodimethylsilyl)cyclopentadienyl Titanium Compound. Angewandte Chemie - International Edition, 2005, 44, 5828-5830. | 13.8 | 18 |
| 52 | 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 |
| 53 | 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 |
| 54 | Trapping Unstable Terminal Taâ‹¯O Multiple Bonds of Monocyclopentadienyl Tantalum Complexes with a Lewis Acid. Organometallics, 2005, 24, 2004-2007. | 2.3 | 27 |

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| 55 | 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 |
| 56 | Triplet versus Singlet Photoreaction Mechanism in the Barrelene Di-Ï€-methane Rearrangement. Organic Letters, 2004, 6, 1229-1231. | 4.6 | 25 |
| 57 | 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 |
| 58 | 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 |
| 59 | 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 |
| 60 | Role of bifurcation in the bond shifting of cyclooctatetraene. Journal of Computational Chemistry, 2002, 23, 732-736. | 3.3 | 40 |
| 61 | Note on the theory of bifurcation of chemical reactions. International Journal of Quantum Chemistry, 2002, 86, 422-425. | 2.0 | 12 |
| 62 | 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 |
| 63 | 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 |
| 64 | The Valence Isomerization of Cyclooctatetraene to Semibullvalene. Angewandte Chemie - International Edition, 2000, 39, 2095-2097. | 13.8 | 25 |
| 65 | 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 |
| 66 | 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 |
| 67 | 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 |
| 68 | Design of Improved Molecular Solarâ€Thermal Systems by Mechanochemistry: The Case of Azobenzene. Advanced Sustainable Systems, 0, , 2200097. | 5.3 | 2 |