# LuÃ-s Pinto da Silva

List of Publications by Year
in descending order



| 106 | 2,000 | 218592 | 315616 |
|---|---|---|---|
| papers | citations | 26 h-index | 38 g-index |

| 108 | 108 | 108 | 1481 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Synthesis of Fe- and Co-Doped TiO2 with Improved Photocatalytic Activity Under Visible Irradiation Toward Carbamazepine Degradation. Materials, 2019, 12, 3874. | 1.3 | 93 |
| 2 | Chemiluminescence and Bioluminescence as an Excitation Source in the Photodynamic Therapy of Cancer: A Critical Review. ChemPhysChem, 2016, 17, 2286-2294. | 1.0 | 79 |
| 3 | Computational Studies of the Luciferase Light-Emitting Product: Oxyluciferin. Journal of Chemical Theory and Computation, 2011, 7, 809-817. | 2.3 | 78 |
| 4 | Advances in the knowledge of light emission by firefly luciferin and oxyluciferin. Journal of Photochemistry and Photobiology B: Biology, 2012, 117, 33-39. | 1.7 | 73 |
| 5 | Firefly Chemiluminescence and Bioluminescence: Efficient Generation of Excited States. ChemPhysChem, 2012, 13, 2257-2262. | 1.0 | 67 |
| 6 | Computational Investigation of the Effect of pH on the Color of Firefly Bioluminescence by DFT. ChemPhysChem, 2011, 12, 951-960. | 1.0 | 66 |
| 7 | Kinetics of inhibition of firefly luciferase by dehydroluciferyl-coenzyme A, dehydroluciferin and l-luciferin. Photochemical and Photobiological Sciences, 2011, 10, 1039-1045. | 1.6 | 49 |
| 8 | Evaluation of Different Bottom-up Routes for the Fabrication of Carbon Dots. Nanomaterials, 2020, 10, 1316. | 1.9 | 47 |
| 9 | Comparative life cycle assessment of bottom-up synthesis routes for carbon dots derived from citric acid and urea. Journal of Cleaner Production, 2020, 254, 120080. | 4.6 | 44 |
| 10 | Comparative Study of the Photoprotolytic Reactions of <scp>d</scp>-Luciferin and Oxyluciferin. Journal of Physical Chemistry A, 2012, 116, 7452-7461. | 1.1 | 41 |
| 11 | Insight into the hybrid luminescence showed by carbon dots and molecular fluorophores in solution. Physical Chemistry Chemical Physics, 2019, 21, 20919-20926. | 1.3 | 40 |
| 12 | Evaluation of the Environmental Impact and Efficiency of N-Doping Strategies in the Synthesis of Carbon Dots. Materials, 2020, 13, 504. | 1.3 | 39 |
| 13 | Chemical Composition, Bioactive Compounds, and Antioxidant Activity of Two Wild Edible Mushrooms Armillaria mellea and Macrolepiota procera from Two Countries (Morocco and Portugal). Biomolecules, 2021, 11, 575. | 1.8 | 37 |
| 14 | Turning Spent Coffee Grounds into Sustainable Precursors for the Fabrication of Carbon Dots. Nanomaterials, 2020, 10, 1209. | 1.9 | 36 |
| 15 | Photocatalytic removal of pharmaceutical water pollutants by TiO2 â€“ Carbon dots nanocomposites: A review. Chemosphere, 2022, 301, 134731. | 4.2 | 36 |
| 16 | Glucose Sensing by Fluorescent Nanomaterials. Critical Reviews in Analytical Chemistry, 2019, 49, 542-552. | 1.8 | 34 |
| 17 | Study on the Effects of Intermolecular Interactions on Firefly Multicolor Bioluminescence. ChemPhysChem, 2011, 12, 3002-3008. | 1.0 | 33 |
| 18 | Hypochlorite fluorescence sensing by phenylboronic acid-alizarin adduct based carbon dots. Talanta, 2020, 208, 120447. | 2.9 | 31 |

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|---|---|---|---|
| 19 | Theoretical modulation of the color of light emitted by firefly oxyluciferin. Journal of Computational Chemistry, 2011, 32, 2654-2663. | 1.5 | 30 |
| 20 | TD-DFT/Molecular Mechanics Study of the Photinus pyralis Bioluminescence System. Journal of Physical Chemistry B, 2012, 116, 2008-2013. | 1.2 | 29 |
| 21 | Study of the Combination of Self-Activating Photodynamic Therapy and Chemotherapy for Cancer Treatment. Biomolecules, 2019, 9, 384. | 1.8 | 29 |
| 22 | Efficient Firefly Chemi/Bioluminescence: Evidence for Chemiexcitation Resulting from the Decomposition of a Neutral Firefly Dioxetanone Molecule. Journal of Physical Chemistry A, 2013, 117, 94-100. | 1.1 | 28 |
| 23 | Oxyluciferin Photoacidity: The Missing Element for Solving the Ketoâ€“Enol Mystery?. ChemPhysChem, 2013, 14, 3441-3446. | 1.0 | 27 |
| 24 | Chemiexcitation Induced Proton Transfer: Enolate Oxyluciferin as the Firefly Bioluminophore. Journal of Physical Chemistry B, 2015, 119, 2140-2148. | 1.2 | 27 |
| 25 | Theoretically obtained insight into the mechanism and dioxetanone species responsible for the singlet chemiexcitation of Coelenterazine. Journal of Photochemistry and Photobiology B: Biology, 2017, 174, 18-26. | 1.7 | 27 |
| 26 | Mechanistic Insight into Cypridina Bioluminescence with a Combined Experimental and Theoretical Chemiluminescent Approach. Journal of Physical Chemistry B, 2017, 121, 7862-7871. | 1.2 | 27 |
| 27 | Single-molecule chemiluminescent photosensitizer for a self-activating and tumor-selective photodynamic therapy of cancer. European Journal of Medicinal Chemistry, 2019, 183, 111683. | 2.6 | 27 |
| 28 | Interstate Crossingâ€Induced Chemiexcitation as the Reason for the Chemiluminescence of Dioxetanones. ChemPhysChem, 2013, 14, 1071-1079. | 1.0 | 26 |
| 29 | Structural, Energetic, and UVâ€“Vis Spectral Analysis of UVA Filter 4-tert-Butyl-4â€²-methoxydibenzoylmethane. Journal of Physical Chemistry A, 2014, 118, 1511-1518. | 1.1 | 26 |
| 30 | Density Functional Theory Calculation of the Absorption Properties of Brown Carbon Chromophores Generated by Catechol Heterogeneous Ozonolysis. ACS Earth and Space Chemistry, 2017, 1, 353-360. | 1.2 | 25 |
| 31 | Excited-State Proton Transfer from the Photoacid 2-Naphthol-8-sulfonate to Acetonitrile/Water Mixtures. Journal of Physical Chemistry A, 2018, 122, 6166-6175. | 1.1 | 25 |
| 32 | UV filter 2â€ethylhexyl 4â€methoxycinnamate: a structure, energetic and UVâ€“vis spectral analysis based on density functional theory. Journal of Physical Organic Chemistry, 2014, 27, 47-56. | 0.9 | 24 |
| 33 | Study of coelenterazine luminescence: Electrostatic interactions as the controlling factor for efficient chemiexcitation. Journal of Luminescence, 2018, 199, 339-347. | 1.5 | 23 |
| 34 | Comparative study of the chemiluminescence of coelenterazine, coelenterazine-e and Cypridina luciferin with an experimental and theoretical approach. Journal of Photochemistry and Photobiology B: Biology, 2019, 190, 21-31. | 1.7 | 23 |
| 35 | Comparative life cycle assessment of high-yield synthesis routes for carbon dots. NanoImpact, 2021, 23, 100332. | 2.4 | 22 |
| 36 | Interstate Crossing-Induced Chemiexcitation Mechanism as the Basis for Imidazopyrazinone Bioluminescence. ChemistrySelect, 2016, 1, 3343-3356. | 0.7 | 21 |

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|---|---|---|---|
| 37 | Theoretical modulation of singlet/triplet chemiexcitation of chemiluminescent imidazopyrazinone dioxetanone via C8-substitution. Photochemical and Photobiological Sciences, 2017, 16, 897-907. | 1.6 | 21 |
| 38 | Normal breast epithelial MCF-10A cells to evaluate the safety of carbon dots. RSC Medicinal Chemistry, 2021, 12, 245-253. | 1.7 | 21 |
| 39 | Theoretical Study of the Ring-Opening of Epoxides Catalyzed by Boronic Acids and Pyridinic Bases. Journal of Physical Chemistry C, 2017, 121, 16300-16307. | 1.5 | 20 |
| 40 | 3-Hydroxyphenylboronic Acid-Based Carbon Dot Sensors for Fructose Sensing. Journal of Fluorescence, 2019, 29, 265-270. | 1.3 | 20 |
| 41 | Life Cycle Assessment of the Sustainability of Enhancing the Photodegradation Activity of TiO2 with Metal-Doping. Materials, 2020, 13, 1487. | 1.3 | 20 |
| 42 | Target-Oriented Synthesis of Marine Coelenterazine Derivatives with Anticancer Activity by Applying the Heavy-Atom Effect. Biomedicines, 2021, 9, 1199. | 1.4 | 20 |
| 43 | Theoretical Photodynamic Study of the Photoprotolytic Cycle of Firefly Oxyluciferin. ChemPhysChem, 2013, 14, 2711-2716. | 1.0 | 18 |
| 44 | Theoretical Study of the Nontraditional Enolâ€Based Photoacidity of Firefly Oxyluciferin. ChemPhysChem, 2015, 16, 455-464. | 1.0 | 18 |
| 45 | Comparison of the Photoprotolytic Processes of Three 7-Hydroxycoumarins. Journal of Physical Chemistry B, 2016, 120, 10297-10310. | 1.2 | 18 |
| 46 | A Computational Investigation of the Equilibrium Constants for the Fluorescent and Chemiluminescent States of Coelenteramide. ChemPhysChem, 2017, 18, 117-123. | 1.0 | 18 |
| 47 | Reversed-phase HPLC/FD method for the quantitative analysis of the neurotoxin BMAA (Î²-N-methylamino-l-alanine) in cyanobacteria. Toxicon, 2012, 59, 379-384. | 0.8 | 16 |
| 48 | Combined experimental and theoretical study of the photochemistry of 4- and 3-hydroxycoumarin. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 338, 23-36. | 2.0 | 16 |
| 49 | Combined experimental and theoretical study of Coelenterazine chemiluminescence in aqueous solution. Journal of Luminescence, 2018, 194, 139-145. | 1.5 | 16 |
| 50 | Analysis of the performance of DFT functionals in the study of light emission by oxyluciferin analogs. International Journal of Quantum Chemistry, 2013, 113, 45-51. | 1.0 | 15 |
| 51 | Theoretical fingerprinting of the photophysical properties of four firefly bioluminophores. Photochemical and Photobiological Sciences, 2013, 12, 2028. | 1.6 | 15 |
| 52 | Mechanistic study of the unimolecular decomposition of 1,2â€dioxetanedione. Journal of Physical Organic Chemistry, 2013, 26, 659-663. | 0.9 | 15 |
| 53 | Quantum/molecular mechanics study of firefly bioluminescence on luciferase oxidative conformation. Chemical Physics Letters, 2014, 608, 45-49. | 1.2 | 15 |
| 54 | Mechanistic Insight into the Chemiluminescent Decomposition of Cypridina Dioxetanone and the Chemiluminescent, Fluorescent Properties of the Light Emitter of Cypridina Bioluminescence. Journal of Chemical Information and Modeling, 2019, 59, 4393-4401. | 2.5 | 15 |

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|---|---|---|---|
| 55 | Excited-State Proton Transfer of Firefly Dehydroluciferin. Journal of Physical Chemistry A, 2012, 116, 10770-10779. | 1.1 | 14 |
| 56 | Mechanistic insights into the efficient intramolecular chemiexcitation of dioxetanones from TDâ€ÐFT and multireference calculations. International Journal of Quantum Chemistry, 2019, 119, e25881. | 1.0 | 14 |
| 57 | Enhanced Excited-State Proton Transfer via a Mixed Waterâ€“Methanol Molecular Bridge of 1-Naphthol-5-Sulfonate in Methanolâ€“Water Mixtures. Journal of Physical Chemistry A, 2018, 122, 4704-4716. | 1.1 | 13 |
| 58 | Copper(II)-Doped Carbon Dots as Catalyst for Ozone Degradation of Textile Dyes. Nanomaterials, 2022, 12, 1211. | 1.9 | 13 |
| 59 | Density functional theory study of 1,2â€dioxetanone decomposition in condensed phase. Journal of Computational Chemistry, 2012, 33, 2118-2123. | 1.5 | 12 |
| 60 | Chemical composition and antioxidant and antimicrobial activities of Lactarius sanguifluus, a wild edible mushroom from northern Morocco. Euro-Mediterranean Journal for Environmental Integration, 2021, 6, 1. | 0.6 | 12 |
| 61 | Theoretical analysis of the color tuning mechanism of oxyluciferin and 5-hydroxyoxyluciferin. Computational and Theoretical Chemistry, 2012, 988, 56-62. | 1.1 | 11 |
| 62 | Theoretical study of the efficient fluorescence quenching process of the firefly luciferin. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 266, 47-54. | 2.0 | 11 |
| 63 | An Active Surface Preservation Strategy for the Rational Development of Carbon Dots as pH-Responsive Fluorescent Nanosensors. Chemosensors, 2021, 9, 191. | 1.8 | 11 |
| 64 | Modelling the absorption properties of polycyclic aromatic hydrocarbons and derivatives over three European cities by TD-DFT calculations. Science of the Total Environment, 2019, 695, 133881. | 3.9 | 10 |
| 65 | Insights into the Photodecomposition of Azidomethyl Methyl Sulfide: A S<sub>2</sub>/S<sub>1</sub> Conical Intersection on Nitrene Potential Energy Surfaces Leading to the Formation of S-Methyl-N-sulfenylmethanimine. Journal of Physical Chemistry A, 2020, 124, 1911-1921. | 1.1 | 10 |
| 66 | Dioxetanonesâ€™ peroxide bond as a charge-shifted bond: implications in the chemiluminescence process. Structural Chemistry, 2014, 25, 1075-1081. | 1.0 | 9 |
| 67 | A theoretical study of the UV absorption of 4-methylbenzylidene camphor: from the UVB to the UVA region. Photochemical and Photobiological Sciences, 2015, 14, 465-472. | 1.6 | 9 |
| 68 | Enhanced Excited-State Proton Transfer via a Mixed Methanolâ€“Water Molecular Bridge of 1-Naphthol-3,6-disulfonate in Methanolâ€“Water Mixtures. Journal of Physical Chemistry A, 2019, 123, 48-58. | 1.1 | 9 |
| 69 | Comparative theoretical study of the binding of luciferyl-adenylate and dehydroluciferyl-adenylate to firefly luciferase. Chemical Physics Letters, 2012, 543, 137-141. | 1.2 | 8 |
| 70 | Response to â€œcomment on density functional theory study of 1,2â€dioxetanone decomposition in condensed phaseâ€• Journal of Computational Chemistry, 2012, 33, 2127-2130. | 1.5 | 8 |
| 71 | Excited-State Proton Transfer of Phenol Cyanine Picolinium Photoacid. ACS Omega, 2018, 3, 2058-2073. | 1.6 | 8 |
| 72 | Development of firefly oxyluciferin derivatives as pH sensitive fluorescent Probes: A DFT/TDDFT study. Computational and Theoretical Chemistry, 2018, 1133, 18-24. | 1.1 | 8 |

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|---|---|---|---|
| 73 | Mechanistic study of the role of hydrogen bond donors in the two-component organocatalysis of the ring-opening reaction of epoxides. Molecular Catalysis, 2019, 474, 110425. | 1.0 | 8 |
| 74 | Firefly luciferin as a multifunctional chemiluminescence molecule. Photochemical and Photobiological Sciences, 2013, 12, 1615-1621. | 1.6 | 7 |
| 75 | Excited-State Proton Transfer and Formation of the Excited Tautomer of 3-Hydroxypyridine-Dipicolinium Cyanine Dye. Journal of Physical Chemistry A, 2016, 120, 6184-6199. | 1.1 | 7 |
| 76 | Development of a Coelenterazine Derivative with Enhanced Superoxide Anion-Triggered Chemiluminescence in Aqueous Solution. Chemosensors, 2022, 10, 174. | 1.8 | 7 |
| 77 | Chemiluminescence of 1,2â€dioxetanone studied by a closedâ€shell DFT approach. International Journal of Quantum Chemistry, 2013, 113, 1709-1716. | 1.0 | 6 |
| 78 | Elucidating the chemiexcitation of dioxetanones by replacing the peroxide bond with Sâ€“S, Nâ€“N and Câ€“C bonds. New Journal of Chemistry, 2021, 45, 18518-18527. | 1.4 | 6 |
| 79 | Life Cycle Assessment-Based Comparative Study between High-Yield and â€œStandardâ€•Bottom-Up Procedures for the Fabrication of Carbon Dots. Materials, 2022, 15, 3446. | 1.3 | 6 |
| 80 | Evaluation of the carbon footprint of the life cycle of wine production: A review. , 2022, 2, 100021. | | 6 |
| 81 | Theoretical study of the correlation between superoxide anion consumption and firefly luciferin chemiluminescence. Chemical Physics Letters, 2013, 577, 127-130. | 1.2 | 5 |
| 82 | Rationalizing the role of electron/charge transfer in the intramolecular chemiexcitation of dioxetanone-based chemi-/bioluminescent systems. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 429, 113904. | 2.0 | 5 |
| 83 | Theoretical Study of the Thermolysis Reaction and Chemiexcitation of Coelenterazine Dioxetanes. Journal of Physical Chemistry A, 2022, 126, 3486-3494. | 1.1 | 5 |
| 84 | Study of firefly luciferin oxidation and isomerism as possible inhibition pathways for firefly bioluminescence. Chemical Physics Letters, 2014, 592, 188-191. | 1.2 | 4 |
| 85 | Theoretical Analysis of the Binding of Potential Inhibitors to Protein Kinases MK2 and MK3. Medicinal Chemistry, 2015, 11, 573-579. | 0.7 | 4 |
| 86 | Tuning the Intramolecular Chemiexcitation of Neutral Dioxetanones by Interaction with Ionic Species. Molecules, 2022, 27, 3861. | 1.7 | 4 |
| 87 | UV-Based Advanced Oxidation Processes of Remazol Brilliant Blue R Dye Catalyzed by Carbon Dots. Nanomaterials, 2022, 12, 2116. | 1.9 | 4 |
| 88 | Gas-phase molecular structure and energetics of UVB filter 4-methylbenzylidene camphor: A computational study. Computational and Theoretical Chemistry, 2014, 1033, 67-73. | 1.1 | 3 |
| 89 | Excited-State Proton Transfer to H<sub>2</sub>O in Mixtures of CH<sub>3</sub>CNâ€“H<sub>2</sub>O of a Superphotoacid, Chlorobenzoate Phenol Cyanine Picolinium (CBCyP). Journal of Physical Chemistry A, 2018, 122, 8126-8135. | 1.1 | 3 |
| 90 | A sustainable strategy for the assembly of GlypromateÂ® and its structurally-related analogues by tandem sequential peptide coupling. Green Chemistry, 2020, 22, 3584-3596. | 4.6 | 3 |

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| 91 | A Theoretical Analysis of the Potential Role of Ï€â€“Ï€ Stacking Interactions in the Photoprotolytic Cycle of Firefly Luciferin. ChemPhysChem, 2014, 15, 3761-3767. | 1.0 | 2 |
| 92 | Mechanistic insights for the transprotection of tertiary amines with Boc<sub>2</sub>O via charged carbamates: access to both enantiomers of 2-azanorbornane-3-exo-carboxylic acids. Organic Chemistry Frontiers, 2019, 6, 3540-3554. | 2.3 | 2 |
| 93 | Molecular vibration assisted triplet-triplet annihilation nir-upconversion luminescence of fluorescein. Optical Materials, 2019, 96, 109286. | 1.7 | 2 |
| 94 | Theoretical study of the effect of resonance on Ï€â€“Ï€ stacked firefly oxyluciferin dimers. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 278, 9-13. | 2.0 | 1 |
| 95 | A computational study of the structure, aromaticity and enthalpy of formation of UVA filter 4-tert-butyl-4â€²-methoxydibenzoylmethane. Computational and Theoretical Chemistry, 2014, 1038, 6-16. | 1.1 | 1 |
| 96 | Modelling the absorption spectra of polycyclic aromatic hydrocarbons over Seoul, South Korea. Environmental Technology and Innovation, 2020, 17, 100536. | 3.0 | 1 |
| 97 | TD-DFT Monitoring of the Absorption Spectra of Polycyclic Aromatic Hydrocarbons over the Basque Country, Spain. Sustainable Chemistry, 2021, 2, 599-609. | 2.2 | 1 |
| 98 | Isolation and structural characterization of stable carbamicâ€“carbonic anhydrides: an experimental and computational study. Organic Chemistry Frontiers, 2022, 9, 2154-2163. | 2.3 | 1 |
| 99 | Theoretical study of the superoxide anion assisted firefly oxyluciferin formation. Chemical Physics Letters, 2013, 590, 180-182. | 1.2 | 0 |
| 100 | Comparative theoretical study of the binding of potential cancer-treatment drugs to Checkpoint kinase 1. Chemical Physics Letters, 2014, 591, 273-276. | 1.2 | 0 |
| 101 | Structural and electronic characterization of a Fridericia heliota luciferin-related derivative, based on quantum chemistry. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 288, 46-54. | 2.0 | 0 |
| 102 | Theoretical Analysis of the Effect Provoked by Bromine-Addition on the Thermolysis and Chemiexcitation of a Model Dioxetanone. Journal of Chemistry, 2017, 2017, 1-8. | 0.9 | 0 |
| 103 | Editorial Materials: Special Issue on Advances in Luminescent Engineered Nanomaterials. Materials, 2021, 14, 3121. | 1.3 | 0 |
| 104 | Theoretical Modelling of Potential Chk1 Inhibitors. Letters in Drug Design and Discovery, 2014, 12, 60-65. | 0.4 | 0 |
| 105 | Carbon Dots as a Fluorescence pH Nanosensor by Application of an Active Surface Preservation Strategy. Chemistry Proceedings, 2021, 5, . | 0.1 | 0 |
| 106 | Validation of Spent Coffee Grounds as Precursors for the Development of Sustainable Carbon Dot-Based for Fe3+ Optical Sensing. , 2021, 5, . | | 0 |