LuÃ-s Pinto da Silva

List of Publications by Year
in descending order

106 papers	2,000 citations	218592 26 h-index	315616 38 g-index
108 all docs	108 docs citations	108 times ranked	1481 citing authors

#	Article	IF	Citations
1	Isolation and structural characterization of stable carbamicâ€“carbonic anhydrides: an experimental and computational study. Organic Chemistry Frontiers, 2022, 9, 2154-2163.	2.3	1
2	Copper(II)-Doped Carbon Dots as Catalyst for Ozone Degradation of Textile Dyes. Nanomaterials, 2022, 12, 1211.	1.9	13
3	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
4	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
5	Development of a Coelenterazine Derivative with Enhanced Superoxide Anion-Triggered Chemiluminescence in Aqueous Solution. Chemosensors, 2022, 10, 174.	1.8	7
6	Photocatalytic removal of pharmaceutical water pollutants by TiO2 â€“ Carbon dots nanocomposites: A review. Chemosphere, 2022, 301, 134731.	4.2	36
7	Theoretical Study of the Thermolysis Reaction and Chemiexcitation of Coelenterazine Dioxetanes. Journal of Physical Chemistry A, 2022, 126, 3486-3494.	1.1	5
8	Tuning the Intramolecular Chemiexcitation of Neutral Dioxetanones by Interaction with Ionic Species. Molecules, 2022, 27, 3861.	1.7	4
9	UV-Based Advanced Oxidation Processes of Remazol Brilliant Blue R Dye Catalyzed by Carbon Dots. Nanomaterials, 2022, 12, 2116.	1.9	4
10	Evaluation of the carbon footprint of the life cycle of wine production: A review. , 2022, 2, 100021.		6
11	Normal breast epithelial MCF-10A cells to evaluate the safety of carbon dots. RSC Medicinal Chemistry, 2021, 12, 245-253.	1.7	21
12	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
13	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
14	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
15	Editorial Materials: Special Issue on Advances in Luminescent Engineered Nanomaterials. Materials, 2021, 14, 3121.	1.3	0
16	Comparative life cycle assessment of high-yield synthesis routes for carbon dots. NanoImpact, 2021, 23, 100332.	2.4	22
17	An Active Surface Preservation Strategy for the Rational Development of Carbon Dots as pH-Responsive Fluorescent Nanosensors. Chemosensors, 2021, 9, 191.	1.8	11
18	Target-Oriented Synthesis of Marine Coelenterazine Derivatives with Anticancer Activity by Applying the Heavy-Atom Effect. Biomedicines, 2021, 9, 1199.	1.4	20

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19	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
20	Carbon Dots as a Fluorescence pH Nanosensor by Application of an Active Surface Preservation Strategy. Chemistry Proceedings, 2021, 5, .	0.1	0
21	Validation of Spent Coffee Grounds as Precursors for the Development of Sustainable Carbon Dot-Based for Fe3+ Optical Sensing. , 2021, 5, .		0
22	Hypochlorite fluorescence sensing by phenylboronic acid-alizarin adduct based carbon dots. Talanta, 2020, 208, 120447.	2.9	31
23	Modelling the absorption spectra of polycyclic aromatic hydrocarbons over Seoul, South Korea. Environmental Technology and Innovation, 2020, 17, 100536.	3.0	1
24	Turning Spent Coffee Grounds into Sustainable Precursors for the Fabrication of Carbon Dots. Nanomaterials, 2020, 10, 1209.	1.9	36
25	Life Cycle Assessment of the Sustainability of Enhancing the Photodegradation Activity of TiO2 with Metal-Doping. Materials, 2020, 13, 1487.	1.3	20
26	Evaluation of Different Bottom-up Routes for the Fabrication of Carbon Dots. Nanomaterials, 2020, 10, 1316.	1.9	47
27	Insights into the Photodecomposition of Azidomethyl Methyl Sulfide: A S₂/S₁ Conical Intersection on Nitrene Potential Energy Surfaces Leading to the Formation of <i>S</i>-Methyl-<i>N</i>-sulfenylmethanimine. Journal of Physical Chemistry A, 2020, 124, 1911-1921.	1.1	10
28	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
29	Evaluation of the Environmental Impact and Efficiency of N-Doping Strategies in the Synthesis of Carbon Dots. Materials, 2020, 13, 504.	1.3	39
30	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
31	Mechanistic Insight into the Chemiluminescent Decomposition of <i>Cypridina</i> Dioxetanone and the Chemiluminescent, Fluorescent Properties of the Light Emitter of <i>Cypridina</i> Bioluminescence. Journal of Chemical Information and Modeling, 2019, 59, 4393-4401.	2.5	15
32	Study of the Combination of Self-Activating Photodynamic Therapy and Chemotherapy for Cancer Treatment. Biomolecules, 2019, 9, 384.	1.8	29
33	Mechanistic insights for the transprotection of tertiary amines with Boc₂O <i>via</i> charged carbamates: access to both enantiomers of 2-azanorbornane-3-<i>exo</i>-carboxylic acids. Organic Chemistry Frontiers, 2019, 6, 3540-3554.	2.3	2
34	Molecular vibration assisted triplet-triplet annihilation nir-upconversion luminescence of fluorescein. Optical Materials, 2019, 96, 109286.	1.7	2
35	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
36	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

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37	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
38	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
39	Glucose Sensing by Fluorescent Nanomaterials. Critical Reviews in Analytical Chemistry, 2019, 49, 542-552.	1.8	34
40	Synthesis of Fe- and Co-Doped TiO2 with Improved Photocatalytic Activity Under Visible Irradiation Toward Carbamazepine Degradation. Materials, 2019, 12, 3874.	1.3	93
41	Mechanistic insights into the efficient intramolecular chemiexcitation of dioxetanones from TDâ€ĐFT and multireference calculations. International Journal of Quantum Chemistry, 2019, 119, e25881.	1.0	14
42	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
43	3-Hydroxyphenylboronic Acid-Based Carbon Dot Sensors for Fructose Sensing. Journal of Fluorescence, 2019, 29, 265-270.	1.3	20
44	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
45	Excited-State Proton Transfer of Phenol Cyanine Picolinium Photoacid. ACS Omega, 2018, 3, 2058-2073.	1.6	8
46	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
47	Study of coelenterazine luminescence: Electrostatic interactions as the controlling factor for efficient chemiexcitation. Journal of Luminescence, 2018, 199, 339-347.	1.5	23
48	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
49	Combined experimental and theoretical study of Coelenterazine chemiluminescence in aqueous solution. Journal of Luminescence, 2018, 194, 139-145.	1.5	16
50	Excited-State Proton Transfer to H₂O in Mixtures of CH₃CNâ€“H₂O of a Superphotoacid, Chlorobenzoate Phenol Cyanine Picolinium (CBCyP). Journal of Physical Chemistry A, 2018, 122, 8126-8135.	1.1	3
51	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
52	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
53	Theoretical modulation of singlet/triplet chemiexcitation of chemiluminescent imidazopyrazinone dioxetanone via C8-substitution. Photochemical and Photobiological Sciences, 2017, 16, 897-907.	1.6	21
54	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

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55	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
56	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
57	Mechanistic Insight into <i>Cypridina</i> Bioluminescence with a Combined Experimental and Theoretical Chemiluminescent Approach. Journal of Physical Chemistry B, 2017, 121, 7862-7871.	1.2	27
58	A Computational Investigation of the Equilibrium Constants for the Fluorescent and Chemiluminescent States of Coelenteramide. ChemPhysChem, 2017, 18, 117-123.	1.0	18
59	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
60	Chemiluminescence and Bioluminescence as an Excitation Source in the Photodynamic Therapy of Cancer: A Critical Review. ChemPhysChem, 2016, 17, 2286-2294.	1.0	79
61	Comparison of the Photoprotolytic Processes of Three 7-Hydroxycoumarins. Journal of Physical Chemistry B, 2016, 120, 10297-10310.	1.2	18
62	Interstate Crossing-Induced Chemiexcitation Mechanism as the Basis for Imidazopyrazinone Bioluminescence. ChemistrySelect, 2016, 1, 3343-3356.	0.7	21
63	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
64	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
65	Theoretical Study of the Nontraditional Enolâ€Based Photoacidity of Firefly Oxyluciferin. ChemPhysChem, 2015, 16, 455-464.	1.0	18
66	Chemiexcitation Induced Proton Transfer: Enolate Oxyluciferin as the Firefly Bioluminophore. Journal of Physical Chemistry B, 2015, 119, 2140-2148.	1.2	27
67	Theoretical Analysis of the Binding of Potential Inhibitors to Protein Kinases MK2 and MK3. Medicinal Chemistry, 2015, 11, 573-579.	0.7	4
68	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
69	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
70	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
71	Dioxetanonesâ€™ peroxide bond as a charge-shifted bond: implications in the chemiluminescence process. Structural Chemistry, 2014, 25, 1075-1081.	1.0	9
72	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

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73	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
74	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
75	Structural, Energetic, and UVâ€“Vis Spectral Analysis of UVA Filter 4-<i>tert</i>-Butyl-4â€²-methoxydibenzoylmethane. Journal of Physical Chemistry A, 2014, 118, 1511-1518.	1.1	26
76	Study of firefly luciferin oxidation and isomerism as possible inhibition pathways for firefly bioluminescence. Chemical Physics Letters, 2014, 592, 188-191.	1.2	4
77	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
78	Quantum/molecular mechanics study of firefly bioluminescence on luciferase oxidative conformation. Chemical Physics Letters, 2014, 608, 45-49.	1.2	15
79	Theoretical Modelling of Potential Chk1 Inhibitors. Letters in Drug Design and Discovery, 2014, 12, 60-65.	0.4	0
80	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
81	Theoretical Photodynamic Study of the Photoprotolytic Cycle of Firefly Oxyluciferin. ChemPhysChem, 2013, 14, 2711-2716.	1.0	18
82	Oxyluciferin Photoacidity: The Missing Element for Solving the Ketoâ€“Enol Mystery?. ChemPhysChem, 2013, 14, 3441-3446.	1.0	27
83	Theoretical study of the superoxide anion assisted firefly oxyluciferin formation. Chemical Physics Letters, 2013, 590, 180-182.	1.2	0
84	Theoretical fingerprinting of the photophysical properties of four firefly bioluminophores. Photochemical and Photobiological Sciences, 2013, 12, 2028.	1.6	15
85	Interstate Crossingâ€Induced Chemiexcitation as the Reason for the Chemiluminescence of Dioxetanones. ChemPhysChem, 2013, 14, 1071-1079.	1.0	26
86	Theoretical study of the correlation between superoxide anion consumption and firefly luciferin chemiluminescence. Chemical Physics Letters, 2013, 577, 127-130.	1.2	5
87	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
88	Chemiluminescence of 1,2â€dioxetanone studied by a closedâ€shell DFT approach. International Journal of Quantum Chemistry, 2013, 113, 1709-1716.	1.0	6
89	Firefly luciferin as a multifunctional chemiluminescence molecule. Photochemical and Photobiological Sciences, 2013, 12, 1615-1621.	1.6	7
90	Mechanistic study of the unimolecular decomposition of 1,2â€dioxetanedione. Journal of Physical Organic Chemistry, 2013, 26, 659-663.	0.9	15

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91	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
92	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
93	Theoretical analysis of the color tuning mechanism of oxyluciferin and 5-hydroxyoxyluciferin. Computational and Theoretical Chemistry, 2012, 988, 56-62.	1.1	11
94	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
95	Excited-State Proton Transfer of Firefly Dehydroluciferin. Journal of Physical Chemistry A, 2012, 116, 10770-10779.	1.1	14
96	TD-DFT/Molecular Mechanics Study of the Photinus pyralis Bioluminescence System. Journal of Physical Chemistry B, 2012, 116, 2008-2013.	1.2	29
97	Density functional theory study of 1,2â€dioxetanone decomposition in condensed phase. Journal of Computational Chemistry, 2012, 33, 2118-2123.	1.5	12
98	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
99	Firefly Chemiluminescence and Bioluminescence: Efficient Generation of Excited States. ChemPhysChem, 2012, 13, 2257-2262.	1.0	67
100	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
101	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
102	Computational Studies of the Luciferase Light-Emitting Product: Oxyluciferin. Journal of Chemical Theory and Computation, 2011, 7, 809-817.	2.3	78
103	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
104	Computational Investigation of the Effect of pH on the Color of Firefly Bioluminescence by DFT. ChemPhysChem, 2011, 12, 951-960.	1.0	66
105	Study on the Effects of Intermolecular Interactions on Firefly Multicolor Bioluminescence. ChemPhysChem, 2011, 12, 3002-3008.	1.0	33
106	Theoretical modulation of the color of light emitted by firefly oxyluciferin. Journal of Computational Chemistry, 2011, 32, 2654-2663.	1.5	30