

Leonardo Evaristo de Sousa

List of Publications by Year in descending order

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Version: 2024-02-01

28
papers

252
citations

933447

10
h-index

1058476

14
g-index

30
all docs

30
docs citations

30
times ranked

263
citing authors

#	ARTICLE	IF	CITATIONS
1	Revealing the internal heavy chalcogen atom effect on the photophysics of the dibenzo[<i>a,j</i>]phenazine-cored donor-acceptor-donor triad. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13942-13953.	5.5	29
2	Unified Framework for Photophysical Rate Calculations in TADF Molecules. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5816-5824.	5.3	19
3	The regioisomeric effect on the excited-state fate leading to room-temperature phosphorescence or thermally activated delayed fluorescence in a dibenzophenazine-cored donor-acceptor-donor system. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4905-4913.	5.5	18
4	Ultrafast direct generation of quasiparticles in graphene nanoribbons. <i>Carbon</i> , 2020, 158, 553-558.	10.3	15
5	Kinetic Monte Carlo model for the COVID-19 epidemic: Impact of mobility restriction on a COVID-19 outbreak. <i>Physical Review E</i> , 2020, 102, 032133.	2.1	15
6	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. <i>Scientific Reports</i> , 2020, 10, 8014.	3.3	15
7	Fast predictions of exciton diffusion length in organic materials. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4066-4071.	5.5	13
8	Modeling the Emission Spectra of Organic Molecules: A Competition between Franck-Condon and Nuclear Ensemble Methods. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5380-5388.	2.5	11
9	On the Physical Origins of Charge Separation at Donor-Acceptor Interfaces in Organic Solar Cells: Energy Bending versus Energy Disorder. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900230.	2.8	11
10	Dual-photofunctional organogermanium compound based on donor-acceptor-donor architecture. <i>Chemical Communications</i> , 2022, 58, 5889-5892.	4.1	11
11	Smooth gap tuning strategy for cove-type graphene nanoribbons. <i>RSC Advances</i> , 2020, 10, 26937-26943.	3.6	10
12	Exciton Diffusion in Organic Nanofibers: A Monte Carlo Study on the Effects of Temperature and Dimensionality. <i>Scientific Reports</i> , 2018, 8, 14066.	3.3	9
13	Modeling temperature dependent singlet exciton dynamics in multilayered organic nanofibers. <i>Journal of Chemical Physics</i> , 2018, 148, 204101.	3.0	8
14	Role of Exciton Density in Organic Materials: Diffusion Length, Lifetime, and Quantum Efficiency. <i>Chemistry of Materials</i> , 2019, 31, 6818-6823.	6.7	8
15	A New Entry to Purely Organic Thermally Activated Delayed Fluorescence Emitters Based on Pyrido[2,3- <i>b</i>]pyrazine-Dihydrophenazasilines Donor-Acceptor Dyad. <i>Asian Journal of Organic Chemistry</i> , 2022, 11, .	2.7	7
16	Triplet-to-singlet exciton transfer in hyperfluorescent OLED materials. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4914-4922.	5.5	7
17	Biexciton cascade emission in multilayered organic nanofibers. <i>Applied Physics Letters</i> , 2018, 112, 143301.	3.3	6
18	Concentration effects on the thermally-activated transport of polarons in conducting polymers. <i>Chemical Physics Letters</i> , 2019, 716, 162-166.	2.6	6

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19	Effective Mass of Quasiparticles in Armchair Graphene Nanoribbons. <i>Scientific Reports</i> , 2019, 9, 17990.	3.3	5
20	Charge localization and hopping in a topologically engineered graphene nanoribbon. <i>Scientific Reports</i> , 2021, 11, 5142.	3.3	5
21	Activation Energies and Diffusion Coefficients of Polarons and Bipolarons in Organic Conductors. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5925-5930.	2.5	4
22	Assessing the effects of increasing conjugation length on exciton diffusion: from small molecules to the polymeric limit. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15635-15644.	2.8	4
23	A Genetic Algorithm Approach to Design Principles for Organic Photovoltaic Materials. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000042.	2.8	3
24	A joint theoretical and experimental characterization of two acene-thiophene derivatives. <i>Journal of Molecular Modeling</i> , 2017, 23, 52.	1.8	2
25	Choice of Solubilizing Group Is Determinant for Exciton Diffusion Length in Organic Crystals. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5522-5527.	3.1	2
26	Comparative study of thermally activated delayed fluorescent properties of donor-acceptor and donor-acceptor-donor architectures based on phenoxazine and dibenzo[<i>a,j</i>]phenazine. <i>Beilstein Journal of Organic Chemistry</i> , 2022, 18, 459-468.	2.2	2
27	Optical properties of P3HT and N2200 polymers: a performance study of an optimally tuned DFT functional. <i>Journal of Molecular Modeling</i> , 2018, 24, 32.	1.8	1
28	Dynamical exciton decay in organic materials: the role of bimolecular recombination. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1711-1716.	2.8	1