

Steven A Lopez

List of Publications by Year in descending order

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Version: 2024-02-01

44
papers

1,290
citations

471509

17
h-index

361022

35
g-index

63
all docs

63
docs citations

63
times ranked

1899
citing authors

#	ARTICLE	IF	CITATIONS
1	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. <i>Joule</i> , 2017, 1, 857-870.	24.0	157
2	Isomeric Cyclopropenes Exhibit Unique Bioorthogonal Reactivities. <i>Journal of the American Chemical Society</i> , 2013, 135, 13680-13683.	13.7	134
3	Control and Design of Mutual Orthogonality in Bioorthogonal Cycloadditions. <i>Journal of the American Chemical Society</i> , 2012, 134, 17904-17907.	13.7	132
4	1,3-Dipolar Cycloaddition Reactivities of Perfluorinated Aryl Azides with Enamines and Strained Dipolarophiles. <i>Journal of the American Chemical Society</i> , 2015, 137, 2958-2966.	13.7	91
5	The Harvard organic photovoltaic dataset. <i>Scientific Data</i> , 2016, 3, 160086.	5.3	85
6	Alkene Distortion Energies and Torsional Effects Control Reactivities, and Stereoselectivities of Azide Cycloadditions to Norbornene and Substituted Norbornenes. <i>Journal of Organic Chemistry</i> , 2013, 78, 1778-1783.	3.2	75
7	Mechanochemical synthesis of an elusive fluorinated polyacetylene. <i>Nature Chemistry</i> , 2021, 13, 41-46.	13.6	64
8	Mechanisms and Transition States of 1,3-Dipolar Cycloadditions of Phenyl Azide with Enamines: A Computational Analysis. <i>Journal of Organic Chemistry</i> , 2013, 78, 1576-1582.	3.2	40
9	Automatic discovery of photoisomerization mechanisms with nanosecond machine learning photodynamics simulations. <i>Chemical Science</i> , 2021, 12, 5302-5314.	7.4	38
10	A Study of the Degree of Fluorination in Regioregular Poly(3-hexylthiophene). <i>Macromolecules</i> , 2017, 50, 162-174.	4.8	30
11	Torsional Barriers to Rotation and Planarization in Heterocyclic Oligomers of Value in Organic Electronics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5624-5638.	5.3	30
12	Quantitative prediction of morphology and electron transport in crystal and disordered organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2016, 4, 11238-11243.	5.5	26
13	Photophysical Tuning of Shortwave Infrared Flavylum Heptamethine Dyes via Substituent Placement. <i>Organic Letters</i> , 2020, 22, 6150-6154.	4.6	24
14	Machine-Learning Photodynamics Simulations Uncover the Role of Substituent Effects on the Photochemical Formation of Cubanes. <i>Journal of the American Chemical Society</i> , 2021, 143, 20166-20175.	13.7	24
15	Cyclic Thiosulfonates and Cyclic Disulfides Selectively Cross-Link Thiols While Avoiding Modification of Lone Thiols. <i>Journal of the American Chemical Society</i> , 2018, 140, 7377-7380.	13.7	23
16	Mono-, Di-, and Trifluoroalkyl Substituent Effects on the Torquoselectivities of Cyclobutene and Oxetene Electrocyclic Ring Openings. <i>Journal of Organic Chemistry</i> , 2015, 80, 11768-11772.	3.2	19
17	Stereospecific Synthesis of Substituted Aziridines by a Crystal-to-Crystal Photodenitrogenation of P^{III} -1,2,3-Triazolines. <i>Organic Letters</i> , 2015, 17, 4568-4571.	4.6	19
18	Virtual Excited State Reference for the Discovery of Electronic Materials Database: An Open-Access Resource for Ground and Excited State Properties of Organic Molecules. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6835-6841.	4.6	19

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19	Oxidation of rubrene, and implications for device stability. <i>Journal of Materials Chemistry C</i> , 2018, 6, 3757-3761.	5.5	17
20	Silicon incorporation in polymethine dyes. <i>Chemical Communications</i> , 2020, 56, 6110-6113.	4.1	17
21	“How Do We Do This at a Distance?” A Descriptive Study of Remote Undergraduate Research Programs during COVID-19. <i>CBE Life Sciences Education</i> , 2022, 21, ar1.	2.3	17
22	Substituent Effects on Rates and Torquoselectivities of Electrocyclic Ring-Openings of <i>N</i> -Substituted 2-Azetines. <i>Journal of Organic Chemistry</i> , 2014, 79, 6189-6195.	3.2	15
23	Role of the Perfluoro Effect in the Selective Photochemical Isomerization of Hexafluorobenzene. <i>Journal of the American Chemical Society</i> , 2021, 143, 7002-7012.	13.7	15
24	Molecular Recognition and Band Alignment in 3D Covalent Organic Frameworks for Cocrystalline Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9126-9133.	3.1	14
25	Theoretical Analysis of the Retro-Diels-Alder Reactivity of Oxanorbornadiene Thiol and Amine Adducts. <i>Organic Letters</i> , 2017, 19, 4504-4507.	4.6	13
26	The effect of hexyl side chains on molecular conformations, crystal packing, and charge transport of oligothiophenes. <i>Journal of Materials Chemistry C</i> , 2017, 5, 582-588.	5.5	13
27	A Sustainable Route To Synthesize the Xanthommatin Biochrome via an Electro-catalyzed Oxidation of Tryptophan Metabolites. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 8979-8985.	6.7	13
28	Coronene derivatives for transparent organic photovoltaics through inverse materials design. <i>Journal of Materials Chemistry C</i> , 2021, 9, 1310-1317.	5.5	12
29	A Look Inside the Black Box of Machine Learning Photodynamics Simulations. <i>Accounts of Chemical Research</i> , 2022, 55, 1972-1984.	15.6	12
30	Multimode selective detection of mercury by chiroptical fluorescent sensors based on methionine/cysteine. <i>Chirality</i> , 2011, 23, 916-920.	2.6	11
31	How Torsional Effects Cause Attack at Sterically Crowded Concave Faces of Bicyclic Alkenes. <i>Journal of Organic Chemistry</i> , 2014, 79, 8304-8312.	3.2	11
32	Nanosecond laser flash photolysis of a 6-nitroindolinospiropyran in solution and in nanocrystalline suspension under single excitation conditions. <i>Photochemical and Photobiological Sciences</i> , 2018, 17, 741-749.	2.9	10
33	Nucleophilic substitution reactions of cyclic thiosulfonates are accelerated by hyperconjugative interactions. <i>Chemical Science</i> , 2019, 10, 5568-5575.	7.4	10
34	Efficient Discovery of Visible Light-Activated Azoarene Photoswitches with Long Half-Lives Using Active Search. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5524-5534.	5.4	9
35	Multiconfigurational Calculations and Nonadiabatic Molecular Dynamics Explain Tricyclooctadiene Photochemical Chemoselectivity. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7623-7632.	2.5	8
36	Benchmarking of Density Functionals for <i>Z</i> -Azoarene Half-Lives via Automated Transition State Search. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6474-6485.	2.5	8

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37	Cross-conjugation controls the stabilities and photophysical properties of heteroazoarene photoswitches. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 5989-5998.	2.8	7
38	Excited-State Distortions Promote the Photochemical 4π-Electrocyclizations of Fluorobenzenes via Machine Learning Accelerated Photodynamics Simulations. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	6
39	A Theoretical Stereoselectivity Model of Photochemical Denitrogenations of Diazoalkanes Toward Strained 1,3-Dihalogenated Bicyclobutanes. <i>Journal of Organic Chemistry</i> , 2021, 86, 4061-4070.	3.2	5
40	Mechanistic insights into the pressure-induced polymerization of aryl/perfluoroaryl co-crystals. <i>Polymer Chemistry</i> , 2022, 13, 1359-1368.	3.9	5
41	Knowledge Graph-Empowered Materials Discovery. , 2021, , .		4
42	Understanding dispersive charge-transport in crystalline organic-semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 231-236.	2.8	3
43	Multiconfigurational dynamics explain photochemical reactivity and torquoselectivity towards fluorinated polyacetylenes. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10880-10888.	5.5	2
44	A Green Chemistry Approach toward the Stereospecific Synthesis of Densely Functionalized Cyclopropanes via the Solid-State Photodenitrogenation of Crystalline 1-Pyrazolines. <i>Journal of Organic Chemistry</i> , 2022, 87, 2277-2288.	3.2	1