

Adalgisa Sinicropi

List of Publications by Year in descending order

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86
papers

2,227
citations

201385

27
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253896

43
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89
all docs

89
docs citations

89
times ranked

2568
citing authors

#	ARTICLE	IF	CITATIONS
1	Properties of the Emitting State of the Green Fluorescent Protein Resolved at the CASPT2//CASCF/CHARMM Level. <i>Journal of the American Chemical Society</i> , 2005, 127, 11534-11535.	6.6	142
2	Computational Photochemistry. <i>Theoretical and Computational Chemistry</i> , 2005, , 1-33.	0.2	103
3	Bathochromic Shift in Green Fluorescent Protein: A Puzzle for QM/MM Approaches. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 112-124.	2.3	94
4	An artificial molecular switch that mimics the visual pigment and completes its photocycle in picoseconds. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 17642-17647.	3.3	89
5	Catalytic surface radical in dye-decolorizing peroxidase: a computational, spectroscopic and site-directed mutagenesis study. <i>Biochemical Journal</i> , 2015, 466, 253-262.	1.7	84
6	Excited State Geometries and Vertical Emission Energies of Solvated Dyes for DSSC: A PCM/TD-DFT Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3925-3933.	2.3	80
7	Integration of two-dimensional materials-based perovskite solar panels into a stand-alone solar farm. <i>Nature Energy</i> , 2022, 7, 597-607.	19.8	66
8	Chromophoreâ€“Protein Coupling beyond Nonpolarizable Models: Understanding Absorption in Green Fluorescent Protein. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4825-4839.	2.3	65
9	Organic dyes with intense light absorption especially suitable for application in thin-layer dye-sensitized solar cells. <i>Chemical Communications</i> , 2014, 50, 13952-13955.	2.2	64
10	Prospective life cycle assessment of third-generation photovoltaics at the pre-industrial scale: A long-term scenario approach. <i>Renewable and Sustainable Energy Reviews</i> , 2020, 121, 109703.	8.2	63
11	Structure of the intersection space associated with Z/E photoisomerization of retinal in rhodopsin proteins. <i>Faraday Discussions</i> , 2004, 127, 179-191.	1.6	60
12	Quantum Chemical Modeling and Preparation of a Biomimetic Photochemical Switch. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 414-420.	7.2	60
13	Modeling, Preparation, and Characterization of a Dipole Moment Switch Driven by $Z \rightarrow E$ Photoisomerization. <i>Journal of the American Chemical Society</i> , 2010, 132, 9310-9319.	6.6	53
14	Organic Chromophores Based on a Fused Bisâ€“Thiazole Core and Their Application in Dyeâ€“Sensitized Solar Cells. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 1916-1928.	1.2	48
15	Environmental Profile of the Manufacturing Process of Perovskite Photovoltaics: Harmonization of Life Cycle Assessment Studies. <i>Energies</i> , 2019, 12, 3746.	1.6	45
16	Characterization of the conical intersection of the visual pigment rhodopsin at the CASPT2//CASCF/AMBER level of theory. <i>Molecular Physics</i> , 2006, 104, 983-991.	0.8	43
17	Thiazolo[5,4-d]thiazole-based organic sensitizers with strong visible light absorption for transparent, efficient and stable dye-sensitized solar cells. <i>RSC Advances</i> , 2015, 5, 32657-32668.	1.7	42
18	Thiazolo[5,4-d]thiazole-based organic sensitizers with improved spectral properties for application in greenhouse-integrated dye-sensitized solar cells. <i>Sustainable Energy and Fuels</i> , 2020, 4, 2309-2321.	2.5	42

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19	Conical Intersections in Charge-Transfer Induced Quenching. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4582-4586.	7.2	39
20	Computational Study on the Origin of the Stereoselectivity for the Photochemical Denitrogenation of Diazabicycloheptene. <i>Journal of the American Chemical Society</i> , 2003, 125, 10947-10959.	6.6	39
21	Mechanism of the Norrish-Yang Photocyclization Reaction of an Alanine Derivative in the Singlet State: Origin of the Chiral-Memory Effect. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2390-2393.	7.2	37
22	Excited state quenching via unsuccessful chemical reactions. <i>Photochemical and Photobiological Sciences</i> , 2002, 1, 537-546.	1.6	36
23	Characterization of radical intermediates in laccase-mediator systems. A multifrequency EPR, ENDOR and DFT/PCM investigation. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7284.	1.3	36
24	Fluorescence Quenching by Sequential Hydrogen, Electron, and Proton Transfer in the Proximity of a Conical Intersection. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 4185-4189.	7.2	35
25	EPR parameters of amino acid radicals in <i>P. eryngii</i> versatile peroxidase and its W164Y variant computed at the QM/MM level. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5078.	1.3	30
26	Combining Dithienosilole-Based Organic Dyes with a Brookite/Platinum Photocatalyst toward Enhanced Visible-Light-Driven Hydrogen Production. <i>ACS Applied Energy Materials</i> , 2019, 2, 5600-5612.	2.5	30
27	A organic dyes with tailored green light absorption for potential application in greenhouse-integrated dye-sensitized solar cells. <i>Sustainable Energy and Fuels</i> , 2021, 5, 1171-1183.	2.5	28
28	A comparison of carboxypyridine isomers as sensitizers for dye-sensitized solar cells: assessment of device efficiency and stability. <i>Tetrahedron</i> , 2014, 70, 6285-6295.	1.0	27
29	Effects of the Protein Environment on the Spectral Properties of Tryptophan Radicals in <i>Pseudomonas aeruginosa</i> Azurin. <i>Journal of the American Chemical Society</i> , 2013, 135, 4822-4833.	6.6	26
30	Photoisomerization acceleration in retinal protonated Schiff-base models. <i>Photochemical and Photobiological Sciences</i> , 2003, 2, 1250.	1.6	25
31	Formation of a tyrosine adduct involved in lignin degradation by <i>Trametes versicolor</i> lignin peroxidase: a novel peroxidase activation mechanism. <i>Biochemical Journal</i> , 2013, 452, 575-584.	1.7	25
32	Environmental and economic optima of solar home systems design: A combined LCA and LCC approach. <i>Science of the Total Environment</i> , 2020, 744, 140569.	3.9	25
33	Modeling the Fluorescence of Protein-Embedded Tryptophans with ab Initio Multiconfigurational Quantum Chemistry: The Limiting Cases of Parvalbumin and Monellin. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16082-16090.	1.2	24
34	Spectroscopic and computational characterization of laccases and their substrate radical intermediates. <i>Cellular and Molecular Life Sciences</i> , 2015, 72, 885-896.	2.4	24
35	Environmental analysis of a nano-grid: A Life Cycle Assessment. <i>Science of the Total Environment</i> , 2020, 700, 134814.	3.9	24
36	Life Cycle Assessment of Classic and Innovative Batteries for Solar Home Systems in Europe. <i>Energies</i> , 2020, 13, 3454.	1.6	23

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37	Tuning the Properties of Benzothiadiazole Dyes for Efficient Visible Light-Driven Photocatalytic H ₂ Production under Different Conditions. ACS Applied Energy Materials, 2020, 3, 8912-8928.	2.5	20
38	Copper-induced structural propensities of the amyloidogenic region of human prion protein. Journal of Biological Inorganic Chemistry, 2014, 19, 635-645.	1.1	19
39	DEVELOPMENT OF DYE SENSITIZED SOLAR CELLS: A LIFE CYCLE PERSPECTIVE FOR THE ENVIRONMENTAL AND MARKET POTENTIAL ASSESSMENT OF A RENEWABLE ENERGY TECHNOLOGY. International Journal of Heat and Technology, 2013, 31, 143-148.	0.3	18
40	The nature of tryptophan radicals involved in the long-range electron transfer of lignin peroxidase and lignin peroxidase-like systems: Insights from quantum mechanical/molecular mechanics simulations. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1476-1483.	1.5	17
41	Environmental impact analysis applied to solar pasteurization systems. Journal of Cleaner Production, 2019, 212, 1368-1380.	4.6	17
42	Combined LCA and Green Metrics Approach for the Sustainability Assessment of an Organic Dye Synthesis on Lab Scale. Frontiers in Chemistry, 2020, 8, 214.	1.8	17
43	Benzo[1,2-d:4,5-d']bisthiazole fluorophores for luminescent solar concentrators: synthesis, optical properties and effect of the polymer matrix on the device performances. Dyes and Pigments, 2021, 188, 109207.	2.0	17
44	Redox-Active Sites in <i>Auricularia auricula-judae</i> Dye-Decolorizing Peroxidase and Several Directed Variants: A Multifrequency EPR Study. Journal of Physical Chemistry B, 2015, 119, 13583-13592.	1.2	16
45	Luminescent solar concentrators with outstanding optical properties by employment of D ⁺ A ⁻ D quinoxaline fluorophores. Journal of Materials Chemistry C, 2021, 9, 15608-15621.	2.7	16
46	Synthesis and Investigation of Solar Cell Photosensitizers Having a Fluorazone Backbone. European Journal of Organic Chemistry, 2017, 2017, 1843-1854.	1.2	15
47	Donor-Acceptor-Donor Thienopyrazine-Based Dyes as NIR-Emitting AIEgens. European Journal of Organic Chemistry, 2021, 2021, 2655-2664.	1.2	15
48	Tyrosine or Tryptophan? Modifying a Metalloradical Catalytic Site by Removal of the Cys-Tyr Cross-Link in the Galactose 6-Oxidase Homologue GlxA. Angewandte Chemie - International Edition, 2017, 56, 6502-6506.	7.2	14
49	LCA driven solar compensation mechanism for Renewable Energy Communities: the Italian case. Energy, 2021, 235, 121374.	4.5	13
50	The <i>cis</i> / <i>trans</i> isomerization of Cu(II)-bis(glycinato) complex in solution: a computer aided multifrequency EPR and DFT/PCM calculation study. Magnetic Resonance in Chemistry, 2007, 45, 846-849.	1.1	12
51	A novel biomimetic photochemical switch at work: design of a photomodulable peptide. Photochemical and Photobiological Sciences, 2009, 8, 1639-1649.	1.6	12
52	In Silico Spectroscopy of Tryptophan and Tyrosine Radicals Involved in the Long-Range Electron Transfer of Cytochrome c Peroxidase. Journal of Physical Chemistry B, 2014, 118, 9525-9537.	1.2	12
53	Fibrils of I \pm -Synuclein Abolish the Affinity of Cu ²⁺ -Binding Site to His50 and Induce Hopping of Cu ²⁺ Ions in the Termini. Inorganic Chemistry, 2019, 58, 10920-10927.	1.9	12
54	An unusual thiazolo[5,4-d]thiazole sensitizer for dye-sensitized solar cells. Tetrahedron Letters, 2013, 54, 3944-3948.	0.7	11

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55	Photoinduced excitation and charge transfer processes of organic dyes with siloxane anchoring groups: a combined spectroscopic and computational study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15310-15323.	1.3	11
56	Synthesis and Characterization of New Organic Dyes Containing the Indigo Core. <i>Molecules</i> , 2020, 25, 3377.	1.7	11
57	Toward a computational photobiology. <i>Pure and Applied Chemistry</i> , 2005, 77, 977-993.	0.9	10
58	Insights into the homocoupling reaction of 4-methylamino benzoic acid mediated by <i>Trametes versicolor</i> laccase. <i>Molecular BioSystems</i> , 2011, 7, 2967.	2.9	10
59	DFT and TDDFT investigation of four triphenylamine/phenothiazine-based molecules as potential novel organic hole transport materials for perovskite solar cells. <i>Materials Chemistry and Physics</i> , 2022, 278, 125603.	2.0	10
60	Closing the loop for perovskite solar modules. <i>Nature Sustainability</i> , 2021, 4, 754-755.	11.5	9
61	Evidence for a radical mechanism in biocatalytic degradation of synthetic dyes by fungal laccases mediated by violuric acid. <i>Biocatalysis and Biotransformation</i> , 2007, 25, 269-275.	1.1	8
62	Identification and structural characterization of a transient radical species in the uricase reaction mechanism. <i>Applied Magnetic Resonance</i> , 2007, 31, 471-482.	0.6	8
63	New Blue Donor-Acceptor Pechmann Dyes: Synthesis, Spectroscopic, Electrochemical, and Computational Studies. <i>ACS Omega</i> , 2019, 4, 7614-7627.	1.6	8
64	The critical issue of using lead for sustainable massive production of perovskite solar cells: a review of relevant literature. <i>Open Research Europe</i> , 0, 1, 44.	2.0	7
65	Tyrosyl Radical in the W164Y Mutant of <i>P. eryngii</i> Versatile Peroxidase: an EPR and DFT/PCM Study. <i>Applied Magnetic Resonance</i> , 2010, 37, 279-288.	0.6	6
66	Recent applications of a QM/MM scheme at the CASPT2//CASSCF/AMBER (or CHARMM) level of theory in photochemistry and photobiology. <i>Journal of Physics: Conference Series</i> , 2008, 101, 012001.	0.3	5
67	Structural studies in solution and in the solid state on the zinc chelate of 2-hydroxy-(4-methylthio)butanoic acid, an effective mineral supplement in animal feeding. <i>Inorganica Chimica Acta</i> , 2009, 362, 1115-1121.	1.2	5
68	Two New Dyes with Carboxypyridinium Regioisomers as Anchoring Groups for Dye-Sensitized Solar Cells. <i>Synlett</i> , 2015, 26, 2389-2394.	1.0	5
69	Design, synthesis, structure, and photophysical features of highly emissive cinnamic derivatives. <i>New Journal of Chemistry</i> , 2020, 44, 13644-13653.	1.4	5
70	The β -hairpin from the <i>Thermus thermophilus</i> HB27 laccase works as a pH-dependent switch to regulate laccase activity. <i>Journal of Structural Biology</i> , 2021, 213, 107740.	1.3	5
71	LCA as a Support Tool for the Evaluation of Industrial Scale-Up. , 2020, , 125-143.		5
72	Tyrosine or Tryptophan? Modifying a Metalloradical Catalytic Site by Removal of the Cys-Tyr Cross-Link in the Galactose 6-Oxidase Homologue GlxA. <i>Angewandte Chemie</i> , 2017, 129, 6602-6606.	1.6	4

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73	Life Cycle Inventory datasets for nano-grid configurations. <i>Data in Brief</i> , 2020, 28, 104895.	0.5	4
74	Exergo-Economic and Environmental Analysis of a Solar Integrated Thermo-Electric Storage. <i>Energies</i> , 2020, 13, 3484.	1.6	4
75	In silico investigation of catechol-based sensitizers for type II dye sensitized solar cells (DSSCs). <i>Inorganica Chimica Acta</i> , 2021, 518, 120233.	1.2	4
76	Electronic structure and interfacial features of triphenylamine- and phenothiazine-based hole transport materials for methylammonium lead iodide perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14993-15002.	1.3	4
77	Prediction of hydrogen-bonding networks around tyrosyl radical in <i>P. eryngii</i> versatile peroxidase W164Y variants: a QM/MM MD study. <i>Molecular Simulation</i> , 2014, 40, 485-490.	0.9	3
78	Tailoring the Optical Properties of Organic D- π -A Photosensitizers: Effect of Sulfur Introduction in the Acceptor Group. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 812-825.	1.2	3
79	Synthesis of Silatrane-Containing Organic Sensitizers as Precursors for the Silyloxy Anchoring Group in Dye-Sensitized Solar Cells. <i>Synthesis</i> , 2017, 49, 3975-3984.	1.2	2
80	DFT modeling of structures and redox potentials of wild-type, Nickel-substituted and mutated (N47S/M121L, HPAz) Azurin. <i>Inorganica Chimica Acta</i> , 2018, 470, 360-364.	1.2	2
81	Life Cycle Inventories datasets for future European electricity mix scenarios. <i>Data in Brief</i> , 2020, 30, 105499.	0.5	2
82	Computational Investigation of Photochemical Reaction Mechanisms. <i>Molecular and Supramolecular Photochemistry</i> , 2005, , 31-110.	0.1	2
83	Stable $\text{Methylammonium}^{\oplus}$ Perovskite Solar Cells and Mini-Modules with Phenothiazine Dimers as Hole-Transporting Materials. <i>Energy and Environmental Materials</i> , 2023, 6, .	7.3	2
84	Toward accurate computations in photobiology. , 2005, , 269-289.		1
85	Ground-State Redox Potentials Calculations of D- π -A and D-A- π -A Organic Dyes for DSSC and Visible-Light-Driven Hydrogen Production. <i>Energies</i> , 2020, 13, 2032.	1.6	1
86	The critical issue of using lead for sustainable massive production of perovskite solar cells: a review of relevant literature. <i>Open Research Europe</i> , 0, 1, 44.	2.0	1