

# Adalgisa Sinicropi

## List of Publications by Year in descending order

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86  
papers

2,227  
citations

201385

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89  
docs citations

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2568  
citing authors

| #  | ARTICLE  | IF   | CITATIONS |
|----|--|------|-----------|
| 1  | Stable <sc>Methylammonium</sc> Free Perovskite Solar Cells and <sc>Mini</sc> Modules with Phenothiazine Dimers as Hole Transporting Materials. <i>Energy and Environmental Materials</i> , 2023, 6, .  | 7.3  | 2         |
| 2  | 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        |
| 3  | 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         |
| 4  | 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        |
| 5  | 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         |
| 6  | 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. <i>Dyes and Pigments</i> , 2021, 188, 109207.                    | 2.0  | 17        |
| 7  | Donor-Acceptor Donor Thienopyrazine-Based Dyes as NIR-Emitting AIEgens. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 2655-2664.  | 1.2  | 15        |
| 8  | Closing the loop for perovskite solar modules. <i>Nature Sustainability</i> , 2021, 4, 754-755.  | 11.5 | 9         |
| 9  | The $\beta$ -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         |
| 10 | LCA driven solar compensation mechanism for Renewable Energy Communities: the Italian case. <i>Energy</i> , 2021, 235, 121374.   | 4.5  | 13        |
| 11 | 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        |
| 12 | Luminescent solar concentrators with outstanding optical properties by employment of D quinoxaline fluorophores. <i>Journal of Materials Chemistry C</i> , 2021, 9, 15608-15621.   | 2.7  | 16        |
| 13 | Environmental analysis of a nano-grid: A Life Cycle Assessment. <i>Science of the Total Environment</i> , 2020, 700, 134814.   | 3.9  | 24        |
| 14 | 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        |
| 15 | Life Cycle Inventory datasets for nano-grid configurations. <i>Data in Brief</i> , 2020, 28, 104895.   | 0.5  | 4         |
| 16 | Design, synthesis, structure, and photophysical features of highly emissive cinnamic derivatives. <i>New Journal of Chemistry</i> , 2020, 44, 13644-13653.   | 1.4  | 5         |
| 17 | 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        |
| 18 | Synthesis and Characterization of New Organic Dyes Containing the Indigo Core. <i>Molecules</i> , 2020, 25, 3377.  | 1.7  | 11        |

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|----|---|-----|-----------|
| 19 | Life Cycle Assessment of Classic and Innovative Batteries for Solar Home Systems in Europe. <i>Energies</i> , 2020, 13, 3454.   | 1.6 | 23        |
| 20 | Exergo-Economic and Environmental Analysis of a Solar Integrated Thermo-Electric Storage. <i>Energies</i> , 2020, 13, 3484.   | 1.6 | 4         |
| 21 | Tuning the Properties of Benzothiadiazole Dyes for Efficient Visible Light-Driven Photocatalytic H <sub>2</sub> Production under Different Conditions. <i>ACS Applied Energy Materials</i> , 2020, 3, 8912-8928.            | 2.5 | 20        |
| 22 | Ground-State Redox Potentials Calculations of D- $\pi$ -A and D-A- $\pi$ -A Organic Dyes for DSSC and Visible-Light-Driven Hydrogen Production. <i>Energies</i> , 2020, 13, 2032.   | 1.6 | 1         |
| 23 | Life Cycle Inventories datasets for future European electricity mix scenarios. <i>Data in Brief</i> , 2020, 30, 105499.   | 0.5 | 2         |
| 24 | Thiazolo[5,4- <i>d</i> ]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        |
| 25 | Combined LCA and Green Metrics Approach for the Sustainability Assessment of an Organic Dye Synthesis on Lab Scale. <i>Frontiers in Chemistry</i> , 2020, 8, 214.   | 1.8 | 17        |
| 26 | LCA as a Support Tool for the Evaluation of Industrial Scale-Up. , 2020, , 125-143.   |     | 5         |
| 27 | Fibrils of $\beta$ -Synuclein Abolish the Affinity of Cu <sup>2+</sup> -Binding Site to His50 and Induce Hopping of Cu <sup>2+</sup> Ions in the Termini. <i>Inorganic Chemistry</i> , 2019, 58, 10920-10927.               | 1.9 | 12        |
| 28 | 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        |
| 29 | New Blue Donor-Acceptor Pechmann Dyes: Synthesis, Spectroscopic, Electrochemical, and Computational Studies. <i>ACS Omega</i> , 2019, 4, 7614-7627.   | 1.6 | 8         |
| 30 | Environmental Profile of the Manufacturing Process of Perovskite Photovoltaics: Harmonization of Life Cycle Assessment Studies. <i>Energies</i> , 2019, 12, 3746.   | 1.6 | 45        |
| 31 | Tailoring the Optical Properties of Organic D- $\pi$ -A Photosensitizers: Effect of Sulfur Introduction in the Acceptor Group. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 812-825.                          | 1.2 | 3         |
| 32 | Environmental impact analysis applied to solar pasteurization systems. <i>Journal of Cleaner Production</i> , 2019, 212, 1368-1380.   | 4.6 | 17        |
| 33 | 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         |
| 34 | Synthesis and Investigation of Solar-Cell Photosensitizers Having a Fluorazone Backbone. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 1843-1854.  | 1.2 | 15        |
| 35 | 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 - International Edition</i> , 2017, 56, 6502-6506.   | 7.2 | 14        |
| 36 | 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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|----|---|-----|-----------|
| 37 | 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        |
| 38 | 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         |
| 39 | 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        |
| 40 | Two New Dyes with Carboxypyridinium Regioisomers as Anchoring Groups for Dye-Sensitized Solar Cells. <i>Synlett</i> , 2015, 26, 2389-2394.  | 1.0 | 5         |
| 41 | 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        |
| 42 | Redox-Active Sites in <i>Auricularia auricula-judae</i> Dye-Decolorizing Peroxidase and Several Directed Variants: A Multifrequency EPR Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13583-13592.             | 1.2 | 16        |
| 43 | 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        |
| 44 | Chromophore-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        |
| 45 | 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         |
| 46 | In Silico Spectroscopy of Tryptophan and Tyrosine Radicals Involved in the Long-Range Electron Transfer of Cytochrome c Peroxidase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9525-9537.                          | 1.2 | 12        |
| 47 | 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        |
| 48 | Copper-induced structural propensities of the amyloidogenic region of human prion protein. <i>Journal of Biological Inorganic Chemistry</i> , 2014, 19, 635-645.  | 1.1 | 19        |
| 49 | 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        |
| 50 | 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        |
| 51 | 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        |
| 52 | Organic Chromophores Based on a Fused Bis-Thiazole Core and Their Application in Dye-Sensitized Solar Cells. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 1916-1928.  | 1.2 | 48        |
| 53 | An unusual thiazolo[5,4-d]thiazole sensitizer for dye-sensitized solar cells. <i>Tetrahedron Letters</i> , 2013, 54, 3944-3948.   | 0.7 | 11        |
| 54 | Formation of a tyrosine adduct involved in lignin degradation by <i>Trametes cervina</i> lignin peroxidase: a novel peroxidase activation mechanism. <i>Biochemical Journal</i> , 2013, 452, 575-584.                       | 1.7 | 25        |

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|----|--|-----|-----------|
| 55 | DEVELOPMENT OF DYE SENSITIZED SOLAR CELLS: A LIFE CYCLE PERSPECTIVE FOR THE ENVIRONMENTAL AND MARKET POTENTIAL ASSESSMENT OF A RENEWABLE ENERGY TECHNOLOGY. <i>International Journal of Heat and Technology</i> , 2013, 31, 143-148.   | 0.3 | 18        |
| 56 | 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        |
| 57 | 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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1476-1483. | 1.5 | 17        |
| 58 | 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        |
| 59 | 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        |
| 60 | 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         |
| 61 | Modeling, Preparation, and Characterization of a Dipole Moment Switch Driven by <i>Z</i> / <i>E</i> Photoisomerization. <i>Journal of the American Chemical Society</i> , 2010, 132, 9310-9319.  | 6.6 | 53        |
| 62 | 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         |
| 63 | Modeling the Fluorescence of Protein-Embedded Tryptophans with <i>ab Initio</i> Multiconfigurational Quantum Chemistry: The Limiting Cases of Parvalbumin and Monellin. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16082-16090.   | 1.2 | 24        |
| 64 | A novel biomimetic photochemical switch at work: design of a photomodulable peptide. <i>Photochemical and Photobiological Sciences</i> , 2009, 8, 1639-1649.   | 1.6 | 12        |
| 65 | 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        |
| 66 | 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        |
| 67 | 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         |
| 68 | 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         |
| 69 | Quantum Chemical Modeling and Preparation of a Biomimetic Photochemical Switch. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 414-420.  | 7.2 | 60        |
| 70 | 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. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 846-849.   | 1.1 | 12        |
| 71 | 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         |
| 72 | Characterization of the conical intersection of the visual pigment rhodopsin at the CASPT2//CASSCF/AMBER level of theory. <i>Molecular Physics</i> , 2006, 104, 983-991.   | 0.8 | 43        |

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| 73 | 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        |
| 74 | Computational Photochemistry. <i>Theoretical and Computational Chemistry</i> , 2005, , 1-33.   | 0.2 | 103       |
| 75 | Toward a computational photobiology. <i>Pure and Applied Chemistry</i> , 2005, 77, 977-993.  | 0.9 | 10        |
| 76 | Properties of the Emitting State of the Green Fluorescent Protein Resolved at the CASPT2//CASSCF/CHARMM Level. <i>Journal of the American Chemical Society</i> , 2005, 127, 11534-11535.                           | 6.6 | 142       |
| 77 | Toward accurate computations in photobiology. , 2005, , 269-289.   |     | 1         |
| 78 | Computational Investigation of Photochemical Reaction Mechanisms. <i>Molecular and Supramolecular Photochemistry</i> , 2005, , 31-110.   | 0.1 | 2         |
| 79 | 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        |
| 80 | 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        |
| 81 | Photoisomerization acceleration in retinal protonated Schiff-base models. <i>Photochemical and Photobiological Sciences</i> , 2003, 2, 1250.   | 1.6 | 25        |
| 82 | Excited state quenching via "unsuccessful" chemical reactions. <i>Photochemical and Photobiological Sciences</i> , 2002, 1, 537-546.   | 1.6 | 36        |
| 83 | 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        |
| 84 | Conical Intersections in Charge-Transfer Induced Quenching. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4582-4586.  | 7.2 | 39        |
| 85 | 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         |
| 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         |