Cleber Fn Marchiori

List of Publications by Year
in descending order

43 papers	888 citations	516710 16 h-index	477307 29 g-index
43 all docs	43 docs citations	43 times ranked	1189 citing authors

#	Article	IF	Citations
1	On the energy gap determination of organic optoelectronic materials: the case of porphyrin derivatives. Materials Advances, 2022, 3, 1791-1803.	5.4	21
2	Exploring metastable phases during lithiation of organic battery electrode materials. ChemSusChem, 2022, , .	6.8	4
3	Tuning the photocatalytic properties of porphyrins for hydrogen evolution reaction: An in-silico design strategy. Journal of Power Sources Advances, 2022, 15, 100090.	5.1	4
4	A new CBD-CC-E spectral similarity scale for optimizing computer-simulated UVâ€“vis spectra. Computational and Theoretical Chemistry, 2021, 1197, 113116.	2.5	0
5	Assessing the Donorâ€“Acceptor Nature and the Electrochemical Stability of a Fluoreneâ€“Diketopyrrolopyrroleâ€“Thiophene-Based Copolymer. ACS Applied Polymer Materials, 2021, 3, 4223-4233.	4.4	8
6	Structureâ€“property relationships in organic battery anode materials: exploring redox reactions in crystalline Na- and Li-benzene diacrylate using combined crystallography and density functional theory calculations. Materials Advances, 2021, 2, 1024-1034.	5.4	7
7	Small Organic Molecule Based on Benzothiadiazole for Electrocatalytic Hydrogen Production. Journal of the American Chemical Society, 2021, 143, 21229-21233.	13.7	25
8	Understanding the Electrochemical Stability Window of Polymer Electrolytes in Solid-State Batteries from Atomic-Scale Modeling: The Role of Li-Ion Salts. Chemistry of Materials, 2020, 32, 7237-7246.	6.7	101
9	Understanding the effect of solvent additive in polymeric thin film: turning a bilayer into a bulk heterojunction-like photovoltaic device. Journal Physics D: Applied Physics, 2020, 53, 365101.	2.8	2
10	Thermoplastic polyurethane â€“ Ti3C2(Tx) MXene nanocomposite: The influence of functional groups upon the matrixâ€“reinforcement interaction. Applied Surface Science, 2020, 528, 146526.	6.1	24
11	Tuning the Electrochemical Properties of Organic Battery Cathode Materials: Insights from Evolutionary Algorithm DFT Calculations. ChemSusChem, 2020, 13, 2402-2409.	6.8	15
12	Comparing C60 and C70 as acceptor in organic solar cells: Influence of the electronic structure and aggregation size on the photovoltaic characteristics. Thin Solid Films, 2020, 697, 137827.	1.8	28
13	Ï€â€Conjugation Enables Ultraâ€High Rate Capabilities and Cycling Stabilities in Phenothiazine Copolymers as Cathodeâ€Active Battery Materials. Advanced Functional Materials, 2019, 29, 1906436.	14.9	88
14	Molecular origin of efficient hole transfer from non-fullerene acceptors: insights from first-principles calculations. Journal of Materials Chemistry C, 2019, 7, 12180-12193.	5.5	28
15	Tailoring the Electron-Rich Moiety in Benzothiadiazole-Based Polymers for an Efficient Photocatalytic Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2019, 123, 25531-25542.	3.1	16
16	Predicting Structure and Electrochemistry of Dilithium Thiophene-2,5-Dicarboxylate Electrodes by Density Functional Theory and Evolutionary Algorithms. Journal of Physical Chemistry C, 2019, 123, 4691-4700.	3.1	10
17	Assessing structure and stability of polymer/lithium-metal interfaces from first-principles calculations. Journal of Materials Chemistry A, 2019, 7, 8394-8404.	10.3	77
18	Light-Emitting Porphyrin Derivative Obtained from a Subproduct of the Cashew Nut Shell Liquid: A Promising Material for OLED Applications. Materials, 2019, 12, 1063.	2.9	12

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19	Symmetric Small-Molecules with Acceptorâ€“Donorâ€“Acceptor Architecture for Efficient Visible-Light Driven Hydrogen Production: Optical and Thermodynamic Aspects. Journal of Physical Chemistry C, 2019, 123, 30799-30808.	3.1	10
20	Insights into the Li-Metal/Organic Carbonate Interfacial Chemistry by Combined First-Principles Theory and X-ray Photoelectron Spectroscopy. Journal of Physical Chemistry C, 2019, 123, 347-355.	3.1	10
21	Nonradiative Energy Transfer between Porphyrin and Copolymer in Films Processed by Organic Solvent and Water-Dispersible Nanoparticles with Photovoltaic Applications. Journal of Physical Chemistry C, 2018, 122, 5796-5804.	3.1	10
22	High hole-mobility of rrP3HT in organic field-effect transistors using low-polarity polyurethane gate dielectric. Organic Electronics, 2018, 58, 33-37.	2.6	15
23	On the Design of Donorâ€“Acceptor Conjugated Polymers for Photocatalytic Hydrogen Evolution Reaction: First-Principles Theory-Based Assessment. Journal of Physical Chemistry C, 2018, 122, 26876-26888.	3.1	41
24	Electronic and structural properties of fluoreneâ€“thiophene copolymers as function of the composition ratio between the moieties: a theoretical study. Physical Chemistry Chemical Physics, 2018, 20, 20447-20458.	2.8	6
25	Additive Driven Increase in Donorâ€“Acceptor Copolymer Coupling Studied by X-ray Resonant Photoemission. Journal of Physical Chemistry C, 2017, 121, 25187-25194.	3.1	9
26	Conformational Change on a Bithiophene-Based Copolymer Induced by Additive Treatment: Application in Organic Photovoltaics. Journal of Physical Chemistry C, 2017, 121, 16035-16044.	3.1	18
27	Thermally induced anchoring of fullerene in copolymers with Si-bridging atom: Spectroscopic evidences. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 171, 376-382.	3.9	6
28	Electronic and structural properties in thermally annealed PSiF-DBT:PC71BM blends for organic photovoltaics. Thin Solid Films, 2016, 615, 165-170.	1.8	11
29	Femtosecond Electron Delocalization in Polymer:Fullerene Blend Films. Journal of Physics: Conference Series, 2015, 635, 122003.	0.4	1
30	Annealing effect on donor-acceptor interface and its impact on the performance of organic photovoltaic devices based on PSiF-DBT copolymer and C60. Applied Physics Letters, 2015, 106, 133301.	3.3	12
31	Electronic structure, molecular orientation, charge transfer dynamics and solar cells performance in donor/acceptor copolymers and fullerene: Experimental and theoretical approaches. Journal of Applied Physics, 2014, 115, 134901.	2.5	36
32	Charge Transfer Dynamics and Molecular Orientation Probed by Core Electron Spectroscopies on thermal-annealed Polysilafluorene Derivative: Experimental and Theoretical Approaches. Journal of Physical Chemistry C, 2014, 118, 23863-23873.	3.1	30
33	Density functional theory study of the dipole across the P3HTâ€‰:â€‰PCBM complex: the role of polarization and charge transfer. Journal Physics D: Applied Physics, 2014, 47, 215104.	2.8	29
34	Effect of the Temperature of Annealing on the Performance of Fluorene and Bithiophene Copolymer in Bilayer Solar Cells. Materials Research Society Symposia Proceedings, 2012, 1390, 100.	0.1	2
35	Hybrid vertical transistor based on controlled lateral channel overflow. Journal of Applied Physics, 2012, 112, 074509.	2.5	3
36	Performance of fluorene and terthiophene copolymer in bilayer photovoltaic devices: The role of the polymer conformations. Organic Electronics, 2012, 13, 2716-2726.	2.6	15

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37	The role of the double peaked absorption spectrum in the efficiency of solar cells based on donorâ€“acceptorâ€“donor copolymers. Solar Energy Materials and Solar Cells, 2011, 95, 2287-2294.	6.2	33
38	Hole mobility effect in the efficiency of bilayer heterojunction polymer/C60 photovoltaic cells. Applied Physics Letters, 2011, 98, 253501.	3.3	23
39	Dipole assisted exciton dissociation at conjugated polymer/fullerene photovoltaic interfaces: A molecular study using density functional theory calculations. Synthetic Metals, 2010, 160, 643-650.	3.9	98
40	Photo-oxidation of a non-fullerene acceptor polymer. , 0, , .		0
41	Fundamentals of charge transfer processes in non-fullerene-based photovoltaics: Insights from atomic scale modelling. , 0, , .		0
42	Donor-acceptor polymer complex formation in solution behind highly efficient all-polymer solar cells ?. , 0, , .		0
43	Thermodynamics aspects of charge transfer processes in organic photovoltaics materials: Insights from atomic scale modelling. , 0, , .		0