Gjergji Sini

List of Publications by Year
in descending order

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Version: 2024-02-01

28	838	567247 15	501174 28
papers	citations	h-index	g-index

29	29	29	1527
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Evaluating the Performance of DFT Functionals in Assessing the Interaction Energy and Ground-State Charge Transfer of Donor/Acceptor Complexes: Tetrathiafulvaleneâ"Tetracyanoquinodimethane (TTFâ"TCNQ) as a Model Case. Journal of Chemical Theory and Computation, 2011, 7, 602-609.	5.3	143
2	Processable Star-Shaped Molecules with Triphenylamine Core as Hole-Transporting Materials: Experimental and Theoretical Approach. Journal of Physical Chemistry C, 2012, 116, 3765-3772.	3.1	95
3	Can hydrogen bonds improve the hole-mobility in amorphous organic semiconductors? Experimental and theoretical insights. Journal of Materials Chemistry C, 2015, 3, 11660-11674.	5.5	51
4	On the Molecular Origin of Charge Separation at the Donorâ€"Acceptor Interface. Advanced Energy Materials, 2018, 8, 1702232.	19.5	51
5	Characterization of intrinsic hole transport in single-crystal spiro-OMeTAD. Npj Flexible Electronics, 2017, 1, .	10.7	49
6	Aggregation, thermal annealing, and hosting effects on performances of an acridan-based TADF emitter. Organic Electronics, 2018, 63, 29-40.	2.6	49
7	Effect of Ethynyl Linkages on the Properties of the Derivatives of Triphenylamine and 1,8-Naphthalimide. Journal of Physical Chemistry C, 2015, 119, 28335-28346.	3.1	48
8	Structure and Disorder in Squaraineâ€"C₆₀ Organic Solar Cells: A Theoretical Description of Molecular Packing and Electronic Coupling at the Donorâ€"Acceptor Interface. Advanced Functional Materials, 2014, 24, 3790-3798.	14.9	43
9	Arylfluorenyl-substituted metoxytriphenylamines as deep blue exciplex forming bipolar semiconductors for white and blue organic light emitting diodes. Dyes and Pigments, 2017, 140, 187-202.	3.7	38
10	New derivatives of triphenylamine and naphthalimide as ambipolar organic semiconductors: Experimental and theoretical approach. Dyes and Pigments, 2014, 106, 58-70.	3.7	33
11	Influence of methoxy groups on the properties of 1,1-bis(4-aminophenyl)cyclohexane based arylamines: experimental and theoretical approach. Journal of Materials Chemistry, 2012, 22, 3015.	6.7	31
12	Can Fluorenone-Based Compounds Emit in the Blue Region? Impact of the Conjugation Length and the Ground-State Aggregation. Chemistry of Materials, 2017, 29, 1695-1707.	6.7	31
13	Interfacial and bulk properties of hole transporting materials in perovskite solar cells: spiro-MeTADversusspiro-OMeTAD. Journal of Materials Chemistry A, 2020, 8, 8527-8539.	10.3	28
14	Sensitivity of Redox and Optical Properties of Electroactive Carbazole Derivatives to the Molecular Architecture and Methoxy Substitutions. Journal of Physical Chemistry C, 2018, 122, 10138-10152.	3.1	24
15	Density functional theory for the description of charge-transfer processes at TTF/TCNQ interfaces. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	15
16	Understanding charge transport in donor/acceptor blends from large-scale device simulations based on experimental film morphologies. Energy and Environmental Science, 2020, 13, 601-615.	30.8	14
17	Impact of Imine Bond Orientations on the Geometric and Electronic Structures of Imineâ€based Covalent Organic Frameworks. Chemistry - an Asian Journal, 2021, 16, 3781-3789.	3.3	14
18	Hole transporting materials for perovskite solar cells: molecular versus polymeric carbazole-based derivatives. Journal of Materials Science, 2020, 55, 4820-4829.	3.7	13

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19	Controlled nâ€Doping of Naphthaleneâ€Diimideâ€Based 2D Polymers. Advanced Materials, 2022, 34, e2101932.	21.0	13
20	On the Physical Origins of Charge Separation at Donorâ€“Acceptor Interfaces in Organic Solar Cells: Energy Bending versus Energy Disorder. Advanced Theory and Simulations, 2020, 3, 1900230.	2.8	11
21	Blue versus yellow emission in bipolar fluorenone derivatives: the impact of aggregation and hydrogen bonding. Journal of Materials Chemistry C, 2018, 6, 1679-1692.	5.5	10
22	Interfacial versus Bulk Properties of Hole-Transporting Materials for Perovskite Solar Cells: Isomeric Triphenylamine-Based Enamines versus Spiro-OMeTAD. ACS Applied Materials & Interfaces, 2021, 13, 21320-21330.	8.0	8
23	Effect of methoxy-substitutions on the hole transport properties of carbazole-based compounds: pros and cons. Journal of Materials Chemistry C, 2021, 9, 9941-9951.	5.5	6
24	An experimental and theoretical study of exciplex-forming compounds containing trifluorobiphenyl and 3,6-di-tert-butylcarbazole units and their performance in OLEDs. Journal of Materials Chemistry C, 2020, 8, 14186-14195.	5.5	5
25	Enhancement of Hole Extraction Efficiency of Dibenzothiophenes by Substitution Engineering: Toward Additiveâ€Free Perovskite Solar Cells with Power Conversion Efficiency Exceeding 20%. Solar Rrl, 2022, 6, .	5.8	5
26	Assessing the effects of increasing conjugation length on exciton diffusion: from small molecules to the polymeric limit. Physical Chemistry Chemical Physics, 2021, 23, 15635-15644.	2.8	4
27	Satisfying both interfacial- and bulk requirements for organic photovoltaics: Bridged-triphenylamines with extended Ï€-conjugated systems as efficient new molecules. Organic Electronics, 2019, 73, 137-145.	2.6	3
28	Fast and Accurate Determination of the Singletâ€“Triplet Gap in Donorâ€“Acceptor and Multiresonance TADF Molecules by Using Holeâ€“Hole Tammâ€“Dancoff Approximated Density Functional Theory. Advanced Theory and Simulations, 2022, 5, .	2.8	3