

S M Bouzzine

List of Publications by Year in descending order

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62
papers

1,287
citations

331670

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395702

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times ranked

1149
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#	ARTICLE	IF	CITATIONS
1	DFT and TD-DFT calculation of new thienopyrazine-based small molecules for organic solar cells. <i>Chemistry Central Journal</i> , 2016, 10, 67.	2.6	97
2	Dielectric Properties, AC Conductivity, and Electric Modulus Analysis of Bulk Ethylcarbazole-Terphenyl. <i>Advances in Materials Science and Engineering</i> , 2020, 2020, 1-8.	1.8	83
3	Theoretical investigation of new thiazolothiazole-based D- π -A organic dyes for efficient dye-sensitized solar cell. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 124, 646-654.	3.9	79
4	Hybrid blind robust image watermarking technique based on DFT-DCT and Arnold transform. <i>Multimedia Tools and Applications</i> , 2018, 77, 27181-27214.	3.9	66
5	Density functional theory (B3LYP/6-31G*) study of oligothiophenes in their aromatic and polaronic states. <i>Computational and Theoretical Chemistry</i> , 2005, 726, 271-276.	1.5	61
6	Theoretical design of thiazolothiazole-based organic dyes with different electron donors for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 232-238.	3.9	61
7	Ground state geometries, UV/vis absorption spectra and charge transfer properties of triphenylamine-thiophenes based dyes for DSSCs: A TD-DFT benchmark study. <i>Computational and Theoretical Chemistry</i> , 2018, 1125, 39-48.	2.5	56
8	Identification of a novel dual-target scaffold for 3CLpro and RdRp proteins of SARS-CoV-2 using 3D-similarity search, molecular docking, molecular dynamics and ADMET evaluation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 4522-4535.	3.5	49
9	DFT/TD-DFT characterization of conjugational electronic structures and spectral properties of materials based on thieno[3,2-b][1]benzothiophene for organic photovoltaic and solar cell applications. <i>Journal of Saudi Chemical Society</i> , 2017, 21, 563-574.	5.2	44
10	The optoelectronic properties of organic materials based on triphenylamine that are relevant to organic solar photovoltaic cells. <i>New Journal of Chemistry</i> , 2017, 41, 13336-13346.	2.8	38
11	Designing Donor-Acceptor thienopyrazine derivatives for more efficient organic photovoltaic solar cell: A DFT study. <i>Physica B: Condensed Matter</i> , 2019, 560, 111-125.	2.7	38
12	DFT theoretical investigations of π -conjugated molecules based on thienopyrazine and different acceptor moieties for organic photovoltaic cells. <i>Journal of Saudi Chemical Society</i> , 2016, 20, S415-S425.	5.2	35
13	The bridged effect on the geometric, optoelectronic and charge transfer properties of the triphenylamine- π -bithiophene-based dyes: a DFT study. <i>Research on Chemical Intermediates</i> , 2018, 44, 2009-2023.	2.7	32
14	Density functional theory study of conformational and opto-electronic properties of oligo-para-phenylenes. <i>Computational and Theoretical Chemistry</i> , 2005, 725, 39-44.	1.5	29
15	Blind Robust 3D Mesh Watermarking Based on Mesh Saliency and Wavelet Transform for Copyright Protection. <i>Information (Switzerland)</i> , 2019, 10, 67.	2.9	27
16	Bridging effect on structural and optoelectronic properties of oligothiophene. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 254-262.	1.5	26
17	New organic materials based on D- π -A structure for application in dye-sensitized solar cells. <i>Research on Chemical Intermediates</i> , 2018, 44, 6071-6085.	2.7	25
18	DFT Study of Polythiophene Energy Band Gap and Substitution Effects. <i>Journal of Chemistry</i> , 2015, 2015, 1-12.	1.9	24

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19	Theoretical investigation on Ì€-spacer effect of the Dâ€™Ï€â€™A organic dyes for dye-sensitized solar cell applications: a DFT and TD-BHandH study. <i>Journal of Molecular Modeling</i> , 2019, 25, 92.	1.8	23
20	Bridge effect on the charge transfer and optoelectronic properties of triphenylamine-based organic dye sensitized solar cells: theoretical approach. <i>Research on Chemical Intermediates</i> , 2020, 46, 3961-3978.	2.7	23
21	Computational design of new organic (Dâ€™Ï€â€™A) dyes based on benzothiadiazole for photovoltaic applications, especially dye-sensitized solar cells. <i>Research on Chemical Intermediates</i> , 2020, 46, 3247-3262.	2.7	23
22	The optoelectronic properties of new dyes based onÂˆthienopyrazine. <i>Comptes Rendus Chimie</i> , 2017, 20, 461-466.	0.5	22
23	Theoretical study of structural and electronic properties of oligo(thiophene-phenylene)s in comparison with oligothiophenes and oligophenylenes. <i>Chinese Chemical Letters</i> , 2008, 19, 123-126.	9.0	21
24	Phenothiazine-based dyes containing imidazole with Ì€-linkers of benzene, furan and thiophene: Synthesis, photophysical, electrochemical and computational investigation. <i>Journal of Molecular Structure</i> , 2022, 1251, 131959.	3.6	19
25	New organic dyes based on phenylenevinylene for solar cells: DFT and TD-DFT investigation. <i>Karbala International Journal of Modern Science</i> , 2017, 3, 75-82.	1.0	18
26	Theoretical Investigations on the Electronic and Optical Properties of Bridged Oligothiophenes. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9730-9738.	2.5	17
27	The photophysical properties and electronic structures of bis[1]benzothieno[6,7- <i>d</i>]:6â€™,7â€™- <i>d</i>]benzo[1,2- <i>b</i> :4,5- <i>b</i>]dithiophene (BBTBDT) _{2,8} derivatives as hole-transporting materials for organic light-emitting diodes (OLEDs). <i>New Journal of Chemistry</i> , 2019, 43, 15899-15909.		17
28	DFT calculations of the local spin densities and oligomerization mechanism of thiopheneâ€™phenylene (TP) co-oligomers and derivatives. <i>Computational and Theoretical Chemistry</i> , 2007, 814, 25-32.	1.5	16
29	Vibrational and electronic properties of PPV-derived co-polymers: PPVâ€™ether and C1â€™4PPVâ€™ether. <i>Polymer</i> , 2005, 46, 9928-9940.	3.8	14
30	Synthesis, characterization and theoretical study of new organic copolymer based on PVK and PEDOT. <i>Journal of Non-Crystalline Solids</i> , 2010, 356, 467-473.	3.1	14
31	Quantitative structureâ€™activity relationship of antitumor and neurotoxic Î²-carbolines alkaloids: nine harmine derivatives. <i>Research on Chemical Intermediates</i> , 2013, 39, 2219-2236.	2.7	14
32	Density functional theory [B3LYP/6â€™311G(d,p)] study of a new copolymer based on carbazole and (3,4â€™ethylenedioxythiophene) in their aromatic and polaronic states. <i>Journal of Applied Polymer Science</i> , 2011, 122, 3351-3360.	2.6	13
33	Theoretical investigation of electroluminescent alkoxy substituted 4,4â€™-bis(2-phenylethenyl)biphenyls as guest in blue OLEDs. <i>Solar Energy Materials and Solar Cells</i> , 2006, 90, 1393-1402.	6.2	12
34	Study of the structural and optoelectronic properties of dye solar cells based on phosphonic acid anchoring by DFT functionals. <i>New Journal of Chemistry</i> , 2021, 45, 2723-2733.	2.8	12
35	Synthesis and characterization of co-polymers involving various thiophene and phenylene monomers. <i>Synthetic Metals</i> , 2004, 145, 237-243.	3.9	11
36	Molecular design of Dâ€™Aâ€™D conjugated molecules based on fluorene for organic solar cells. <i>Optical and Quantum Electronics</i> , 2019, 51, 1.	3.3	11

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37	Quantum chemical investigations study of the effect of electron donor units on the structural, electronic and optoelectronic properties of diarylthienopyrazine analogs. Computational and Theoretical Chemistry, 2014, 1036, 22-30.	2.5	10
38	Structural and photophysical studies of triphenylamine-based nonlinear optical dyes: effects of π -linker moieties on the D- π -A structure. Comptes Rendus Chimie, 2019, 22, 373-385.	0.5	10
39	Theoretical study of organic sensitizers based on 2, 6-diphenyl-4H-pyranylidene/1, 3, 4-oxadiazole for dye-sensitized solar cells. Journal of Molecular Modeling, 2020, 26, 346.	1.8	10
40	Effect of the alkyl chain length on the optoelectronic properties of organic dyes: theoretical approach. Journal of Computational Electronics, 2020, 19, 840-848.	2.5	9
41	Opto-electronic properties and molecular design of new materials based on pyrrole studied by DFT. Research on Chemical Intermediates, 2012, 38, 1375-1388.	2.7	8
42	New materials based on thiazolothiazole and thiophene candidates for optoelectronic device applications: theoretical investigations. Research on Chemical Intermediates, 2013, 39, 2679-2695.	2.7	8
43	Effects of adding cyanovinyl moiety on the photovoltaic DSSCs phosphonic acid based cells. Journal of Computational Electronics, 2020, 19, 1629-1644.	2.5	8
44	A theoretical investigation of the optoelectronic performance of some new carbazole dyes. Journal of Computational Electronics, 2019, 18, 951-961.	2.5	6
45	Computational study of the effect of π -spacers on the optoelectronic properties of carbazole-based organic dyes. Journal of Molecular Modeling, 2021, 27, 122.	1.8	6
46	Effects of auxiliary electron-withdrawing moieties on the photovoltaic properties of D- π -A TM - π -A phosphonic acid-based DSSCs. Computational and Theoretical Chemistry, 2022, 1210, 113645.	2.5	6
47	A Quantum Chemical Study On Structural And Electronic Properties Of New Pi-Conjugated Polymer Named Poly(4-Methylthioazole-2,5-Diyl). Advanced Materials Letters, 2012, 3, 15-20.	0.6	5
48	Improved photovoltaic performance of phosphonic acid π -based sensitized solar cells via an electron π -withdrawing moiety: A density of functional theory study. International Journal of Quantum Chemistry, 2021, 121, e26431.	2.0	5
49	New materials based on carbazole for optoelectronic device applications: Theoretical investigation. Chinese Chemical Letters, 2008, 19, 488-492.	9.0	4
50	DFT study of opto-electronic properties of benzothiazole derivatives for use in solar cells. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650023.	1.8	4
51	The computational study of bridge effect in D- π -A photosensitive dyes, based on triphenylamine. IOP Conference Series: Earth and Environmental Science, 2018, 161, 012021.	0.3	4
52	Study of low band gap DSSCs based on bridging bithiophene and biphenyl: theoretical investigation. Journal of the Iranian Chemical Society, 2016, 13, 37-44.	2.2	2
53	TUNING THE ELECTRONIC, PHOTOPHYSICAL AND CHARGE TRANSFER PROPERTIES OF SMALL D-A MOLECULES BASED ON THIENOPYRAZINE-TERTHIENYLS BY CHANGING THE DONOR FRAGMENT: A DFT STUDY. Journal of the Chilean Chemical Society, 2017, 62, 3637-3646.	1.2	2
54	Investigations of the Bridged Thiophene Derivative Effect on the Performance of N,N-diethylaniline-based Compounds for Organic Photovoltaic Cells. Orbital, 2018, 10, .	0.3	2

#	ARTICLE	IF	CITATIONS
55	OPTOELECTRONIC PROPERTIES OF TRIPHENYLAMINE BASED DYES FOR SOLAR CELL APPLICATIONS. A DFT STUDY. Quimica Nova, 0, , .	0.3	2
56	Étude structurale des systèmes dissymétriques de structure D-π-A à base de thiopyrazine destinés aux cellules solaires organiques de type « bulk heterojunction » (BHJ). Canadian Journal of Chemistry, 2019, 97, 745-755.	1.1	1
57	Theoretical investigation on the optoelectronic properties of non-centrosymmetric DπA hexaazatriphenylene derivatives for photovoltaic applications. Mediterranean Journal of Chemistry, 2015, 4, 168-175.	0.7	1
58	Effect of the Alkyl Chain Length Incorporated into Donor Part on the Optoelectronic Properties of the Carbazole Based Dyes: Theoretical Study. Orbital, 2017, 9, .	0.3	1
59	Study of the Effect of Substitution on Phtalocyanine Based Compounds for Photovoltaic Application. International Journal of Chemistry and Materials Research, 2015, 3, 65-78.	1.1	1
60	The opto-electronic properties and molecular design of new materials based on pyrrole. DFT study. Journal of Physical Studies, 2012, 16, .	0.5	1
61	Chemical Synthesis, Electronic Study, and Vibrational Analysis of a New Organic Copolymer Based on PVK and 3-nhexylthiophene. SRX Chemistry, 2010, 2010, 1-8.	0.2	1
62	Modulation on Dye/TiO ₂ Banding Energy and Charge Transfer to High Performance Triphenylamine Based Sensitizers in Solar Cells: A DFT Study. , 2018, , .		0