Shimaa Hussein

List of Publications by Year
in descending order

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21	296	933447	888059
papers	citations	10	17
		h-index	g-index

21	21	21	154
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis, DFT calculations, electronic structure, electronic absorption spectra, natural bond orbital (NBO) and nonlinear optical (NLO) analysis of the novel 5-methyl-8H-benzo[h]chromeno[2,3-b][1,6] naphthyridine-6(5H),8-dione (MBCND). Journal of Molecular Structure, 2017, 1130, 543-558.	3.6	44
2	TD-DFT calculations, NBO analysis and electronic absorption spectra of some thiazolo[3,2-a]pyridine derivatives. Journal of Molecular Structure, 2017, 1147, 651-667.	3.6	31
3	Theoretical approach for the performance of 4-mercapto-1-alkylpyridin-1-ium bromide as corrosion inhibitors using DFT. Egyptian Journal of Petroleum, 2018, 27, 695-699.	2.6	31
4	Synthesis, molecular, electronic structure, linear and non-linear optical and phototransient properties of 8-methyl-1,2-dihydro-4H-chromeno[2,3-b]quinoline-4,6(3H)-dione (MDCQD): Experimental and DFT investigations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 478-490.	3.9	29
5	Synthesis, DFT band structure calculations, optical and photoelectrical characterizations of the novel 5-hydroxy-4-methoxy-7-oxo-7H-furo[3,2-g]chromene-6-carbonitrile (HMOFCC). Optical Materials, 2017, 73, 290-305.	3.6	27
6	Synthesis, DFT study and photoelectrical characterizations of the novel 4-methoxyfuro[3`,2`:6,7]chromeno[2,3-e]benzo[b][1,4]diazepin-5(12H)-one. Optik, 2018, 166, 294-306.	2.9	21
7	Synthesis, spectral characterization, DFT and photosensitivity studies of 1-{[(4-methoxy-5-oxo-5H-furo) Tj ETQq1 1 0.784314 rgBT /Ov Optik, 2019, 178, 1163-1176.	2.9	16
8	Synthesis, DFT calculations, spectroscopic and photovoltaic of the novel Nâ€³, Nâ€´- bis [(4,9-dimethoxy-5-oxo-5 H -furo[3,2- g]chromen-6-yl)methylidene] thiocarbonohydrazide (BFCMT) and its photodiode application. Journal of Molecular Structure, 2018, 1156, 516-523.	3.6	13
9	Synthesis, FT-IR, structural, thermochemical, electronic absorption spectral, and NLO analysis of the novel 10-methoxy-10H-furo[3,2-g]chromeno[2,3-b][1,3]thiazolo[5,4-e]pyridine-2,10(3H)-dione (MFCTP): a DFT/TD-DFT study. RSC Advances, 2021, 11, 32047-32066.	3.6	13
10	DFT calculations and electronic absorption spectra of some, Î±- and Î³-pyrone derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 587-597.	3.9	11
11	Synthesis, spectral, structural, DFT and NLO studies of cerium(III) and thorium(IV) complexes of 1-(5-(1-(2-aminophenylimino)ethyl)-2,4-dihydroxyphenyl)ethanone. Journal of Coordination Chemistry, 2021, 74, 2984-3001.	2.2	11
12	Synthesis, DFT computational insights on structural, optical, photoelectrical characterizations and spectroscopic parameters of the novel (2E)-3-(4-methoxy-5-oxo-5H-furo[3,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 29 Td (2-g]chromen-6	3.6	10
13	Synthesis, Density Functional Theory Band Structure Calculations, Optical, and Photoelectrical Characterizations of the Novel (9â€Bromoâ€3â€cyanoâ€5â€oxoâ€1,5â€dihydroâ€2 H â€chromeno[4,3â€b) Tj ETQq1 1 0.784314 rgBT	2.6	8
14	Synthesis, spectral analysis, quantum studies, NLO, and thermodynamic properties of the novel 5-(6-hydroxy-4-methoxy-1-benzofuran-5-ylcarbonyl)-6-amino-3-methyl-1H-pyrazolo[3,4-b] pyridine (HMBPP). RSC Advances, 2022, 12, 13135-13153.	3.6	8
15	Integrated experimental and theoretical insights for Malachite Green Dye adsorption from wastewater using low cost adsorbent. Water Science and Technology, 2021, 84, 3833-3858.	2.5	7
16	Fabrication, DFT modeling, and photoelectronic characterizations of novel pyridinylcarbonylquinoline for promising potential energy conversion. Journal of Materials Research and Technology, 2021, 14, 3092-3110.	5.8	5
17	DFT Calculations, Spectroscopic Studies, Biological Activity and Non Linear Optical Properties (NLO) of Novel Ternary Cu(II)â€Chelates Derived from 5â€Acetylâ€4â€hydroxyâ€2Hâ€1,3â€thiazinedione. Applied Organometallic Chemistry, 2018, 32, e4435.	3.5	5
18	Simple quantum computation composition, DFT modeling, spectroscopic characterization, and charge, NLO analysis of the novel pyridopyrimidineamide. Journal of Molecular Structure, 2022, 1251, 132020.	3.6	2

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19	Theoretical Study and Experimental Analysis on 2-(1-Ethyl-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl)-2-oxoacetic Acid (3) Using the DFT Approach. Journal of Solution Chemistry, 2018, 47, 172-197.	1.2	1
20	TD-DFT calculations, electronic structure, natural bond orbital analysis, nonlinear optical properties electronic absorption spectra and antimicrobial activity application of new bis-spiropipridinon/pyrazole derivatives. European Journal of Chemistry, 2018, 9, 287-302.	0.6	1
21	Synthesis, Structure Investigation, DFT Analysis And Dielectric Characterization of Substituted Pyridinylidenepropanedinitrile (CMHQCPP) Nanostructure: Novel Approach. Journal of Inorganic and Organometallic Polymers and Materials, 0, , 1.	3.7	1