

# Shimaa Hussein

## List of Publications by Year in descending order

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21  
papers

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citations

933447

10  
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docs citations

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times ranked

154  
citing authors

#	ARTICLE	IF	CITATIONS
1	Simple quantum computation composition, DFT modeling, spectroscopic characterization, and charge, NLO analysis of the novel pyridopyrimidineamide. <i>Journal of Molecular Structure</i> , 2022, 1251, 132020.	3.6	2
2	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-1 <i>H</i> -pyrazolo[3,4- <i>b</i> ]pyridine (HMBPP). <i>RSC Advances</i> , 2022, 12, 13135-13153.	3.6	8
3	Synthesis, DFT computational insights on structural, optical, photoelectrical characterizations and spectroscopic parameters of the novel (2 <i>E</i> )-3-(4-methoxy-5-oxo-5 <i>H</i> -furo[3,2- <i>g</i> ]chromeno[2,3- <i>b</i> ][1,3]thiazolo[5,4- <i>e</i> ]pyridine-2,10(3- <i>H</i> )-dione (MECTP): a DFT/TD-DFT study. <i>RSC Advances</i> , 2021, 11, 32047-32066.	3.6	13
4	Fabrication, DFT modeling, and photoelectronic characterizations of novel pyridinylcarbonylquinoline for promising potential energy conversion. <i>Journal of Materials Research and Technology</i> , 2021, 14, 3092-3110.	5.8	5
5	Synthesis, FT-IR, structural, thermochemical, electronic absorption spectral, and NLO analysis of the novel 10-methoxy-10 <i>H</i> -furo[3,2- <i>g</i> ]chromeno[2,3- <i>b</i> ][1,3]thiazolo[5,4- <i>e</i> ]pyridine-2,10(3- <i>H</i> )-dione (MECTP): a DFT/TD-DFT study. <i>RSC Advances</i> , 2021, 11, 32047-32066.	3.6	13
6	Integrated experimental and theoretical insights for Malachite Green Dye adsorption from wastewater using low cost adsorbent. <i>Water Science and Technology</i> , 2021, 84, 3833-3858.	2.5	7
7	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. <i>Journal of Coordination Chemistry</i> , 2021, 74, 2984-3001.	2.2	11
8	Synthesis, Density Functional Theory Band Structure Calculations, Optical, and Photoelectrical Characterizations of the Novel (9 <i>α</i> -Bromo-3 <i>α</i> -Cyano-5 <i>α</i> -oxo-1,5 <i>α</i> -dihydro-2 <i>H</i> -chromeno[4,3- <i>b</i> ]thiazolo[5,4- <i>e</i> ]pyridine-2,10(3- <i>H</i> )-dione (MECTP): a DFT/TD-DFT study. <i>RSC Advances</i> , 2021, 11, 32047-32066.	3.6	13
9	Synthesis, spectral characterization, DFT and photosensitivity studies of 1-[(4-methoxy-5-oxo-5 <i>H</i> -furo[3,2- <i>g</i> ]chromeno[2,3- <i>b</i> ]quinoline-4,6(3 <i>H</i> )-dione (MDCQD): Experimental and DFT investigations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 478-490.	2.9	16
10	Synthesis, DFT study and photoelectrical characterizations of the novel 4-methoxyfuro[3,2- <i>g</i> ]chromeno[2,3- <i>e</i> ]benzo[ <i>b</i> ][1,4]diazepin-5(12 <i>H</i> )-one. <i>Optik</i> , 2018, 166, 294-306.	2.9	21
11	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. <i>Journal of Solution Chemistry</i> , 2018, 47, 172-197.	1.2	1
12	Synthesis, molecular, electronic structure, linear and non-linear optical and phototransient properties of 8-methyl-1,2-dihydro-4 <i>H</i> -chromeno[2,3- <i>b</i> ]quinoline-4,6(3 <i>H</i> )-dione (MDCQD): Experimental and DFT investigations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 478-490.	3.9	29
13	Synthesis, DFT calculations, spectroscopic and photovoltaic of the novel <i>N</i> <sup>3</sup> , <i>N</i> <sup>6</sup> -bis [(4,9-dimethoxy-5-oxo-5 <i>H</i> -furo[3,2- <i>g</i> ]chromen-6-yl)methylidene] thiocarbonohydrazide (BFCMT) and its photodiode application. <i>Journal of Molecular Structure</i> , 2018, 1156, 516-523.	3.6	13
14	Theoretical approach for the performance of 4-mercapto-1-alkylpyridin-1-ium bromide as corrosion inhibitors using DFT. <i>Egyptian Journal of Petroleum</i> , 2018, 27, 695-699.	2.6	31
15	DFT Calculations, Spectroscopic Studies, Biological Activity and Non Linear Optical Properties (NLO) of Novel Ternary Cu(II)-Chelates Derived from 5 <i>α</i> -Acetyl-4 <i>α</i> -hydroxy-2 <i>H</i> -1,3 <i>α</i> -thiazinedione. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4435.	3.5	5
16	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. <i>European Journal of Chemistry</i> , 2018, 9, 287-302.	0.6	1
17	Synthesis, DFT band structure calculations, optical and photoelectrical characterizations of the novel 5-hydroxy-4-methoxy-7-oxo-7 <i>H</i> -furo[3,2- <i>g</i> ]chromene-6-carbonitrile (HMOFCC). <i>Optical Materials</i> , 2017, 73, 290-305.	3.6	27
18	TD-DFT calculations, NBO analysis and electronic absorption spectra of some thiazolo[3,2- <i>a</i> ]pyridine derivatives. <i>Journal of Molecular Structure</i> , 2017, 1147, 651-667.	3.6	31

#	ARTICLE	IF	CITATIONS
19	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
20	DFT calculations and electronic absorption spectra of some, $\hat{1}\pm$ - and $\hat{1}^3$ -pyrone derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 587-597.	3.9	11
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