

# Shamsa Bibi

## List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Fine Tuning the Optoelectronic Properties of Triphenylamine Based Donor Molecules for Organic Solar Cells. <i>Zeitschrift Fur Physikalische Chemie</i> , 2017, 231, 1127-1139.	1.4	67
2	X-Shaped donor molecules based on benzo[2,1-b:3,4-b'']dithiophene as organic solar cell materials with PDIs as acceptors. <i>Journal of Materials Chemistry A</i> , 2013, 1, 13828.	5.2	40
3	Exploring the impact of central core modifications among several push-pull configurations to enhance nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107665.	1.3	34
4	Theoretical study on hydrogen storage capacity of expanded h-BN systems. <i>Computational Materials Science</i> , 2017, 139, 335-340.	1.4	32
5	Experimental and theoretical studies of Rhodamine B direct dye sorption onto clay-cellulose composite. <i>Journal of Molecular Liquids</i> , 2021, 328, 115165.	2.3	32
6	Effect of different topological structures (D- $\pi$ -D and D- $\pi$ -A- $\pi$ -D) on the optoelectronic properties of benzo[2,1-B:3,4-B']dithiophene based donor molecules toward organic solar cells. <i>Solar Energy</i> , 2019, 186, 311-322.	2.9	31
7	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021, 6, 24602-24613.	1.6	31
8	Investigation of the adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug-delivery carrier: a DFT study. <i>RSC Advances</i> , 2022, 12, 2873-2887.	1.7	31
9	Investigation of LaAlO <sub>3</sub> pervoskite compound for optoelectronic and thermoelectric devices under pressure. <i>Materials Research Express</i> , 2020, 7, 015907.	0.8	29
10	Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021, 43, 128079.	1.0	29
11	Metal doped fullerene complexes as promising drug delivery materials against COVID-19. <i>Chemical Papers</i> , 2021, 75, 6487-6497.	1.0	19
12	Evaluation of a NIAB Gold castor variety for biodiesel production and bio-pesticide. <i>Industrial Crops and Products</i> , 2019, 130, 634-641.	2.5	17
13	Insighting the functionally modified C60 fullerenes as an efficient nonlinear optical materials: A quantum chemical study. <i>Materials Science in Semiconductor Processing</i> , 2022, 141, 106421.	1.9	17
14	Theoretical studies of heteroatom-doping in TiO <sub>2</sub> to enhance the electron injection in dye-sensitized solar cells. <i>RSC Advances</i> , 2015, 5, 79868-79873.	1.7	16
15	Electronic, optical and magnetic properties of low concentration Ni-doped CdSe by first principle method. <i>Bulletin of Materials Science</i> , 2020, 43, 1.	0.8	16
16	Graphene oxide and Fe <sub>3</sub> O <sub>4</sub> composite synthesis, characterization and adsorption efficiency evaluation for NO <sub>3</sub> <sup>-</sup> and PO <sub>4</sub> <sup>3-</sup> ions in aqueous medium. <i>Journal of Molecular Liquids</i> , 2021, 339, 116746.	2.3	14
17	The ratio and topology effects of benzodithiophene donor and benzooxadiazole acceptor fragments on the optoelectronic properties of donor molecules toward solar cell materials. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7986-7999.	1.3	13
18	Theoretical studies to investigate the effect of different cores and two different topologies on the optical and charge transfer properties of donor materials for organic solar cells. <i>New Journal of Chemistry</i> , 2016, 40, 3693-3704.	1.4	13

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19	Synthesis and Characterization of Mg <sup>2+</sup> /Zn Bimetallic Nanoparticles: Selective Hydrogenation of p-Nitrophenol, Degradation of Reactive Carbon Black 5 and Fuel Additive. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 438-450.	1.9	13
20	Designing and comparative analysis of 3D subphthalocyanines based non-fullerene acceptor molecules as an efficient material for organic solar cells. <i>Optik</i> , 2021, 246, 167845.	1.4	13
21	Designing Benzodithiophene-Based Donor Materials with Favorable Photovoltaic Parameters for Bulk Heterojunction Organic Solar Cells. <i>ChemistrySelect</i> , 2017, 2, 5628-5639.	0.7	12
22	Dipoles in 4,12,4-graphyne. <i>Applied Surface Science</i> , 2021, 545, 148991.	3.1	12
23	The phosphorescence properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization. <i>Organic Chemistry Frontiers</i> , 2017, 4, 2191-2201.	2.3	11
24	Fuzzy logic-based intelligent control for hydrostatic journal bearing. <i>Measurement and Control</i> , 2019, 52, 229-243.	0.9	11
25	Designation and Match of Non-Fullerene Acceptors with X-Shaped Donors toward Organic Solar Cells. <i>ChemistrySelect</i> , 2019, 4, 3654-3664.	0.7	10
26	Excited State Complexes of Coumarin Derivatives. <i>Journal of Fluorescence</i> , 2022, 32, 1-17.	1.3	10
27	Structural and computational analysis, spectroscopic and electrochemical elucidation of a Schiff base. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 3845-3860.	1.2	10
28	Theoretical Investigation of Perylene Diimide derivatives as Acceptors to Match with Benzodithiophene based Donors for Organic Photovoltaic Devices. <i>Zeitschrift Fur Physikalische Chemie</i> , 2021, 235, 427-449.	1.4	9
29	DFT and TD-DFT studies of phenothiazine based derivatives as fluorescent materials for semiconductor applications. <i>Materials Science in Semiconductor Processing</i> , 2021, 134, 106036.	1.9	9
30	DFT analysis of different substitutions on optoelectronic properties of carbazole-based small acceptor materials for Organic Photovoltaics. <i>Materials Science in Semiconductor Processing</i> , 2022, 140, 106381.	1.9	9
31	The effect of different aromatic conjugated bridges on optoelectronic properties of diketopyrrolopyrrole-based donor materials for organic photovoltaics. <i>Journal of Molecular Modeling</i> , 2020, 26, 154.	0.8	8
32	Zirconium nanoparticles-poly (N-isopropylacrylamide-methacrylic acid) hybrid microgels decorated graphene sheets for catalytic reduction of organic pollutants. <i>Chemical Physics Letters</i> , 2021, 780, 138915.	1.2	8
33	A Versatile Material: Perovskite Bismuth Ferrite Microparticles as a Potential Catalyst for Enhancing Fuel Efficiency and Degradation of Various Organic Dyes. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 3761-3770.	1.9	7
34	Review of recent advancements in fluorescent chemosensor for ion detection via coumarin derivatives. <i>Chemical Papers</i> , 2022, 76, 3303-3349.	1.0	7
35	DFT and TDDFT Studies of Non-Fullerene Organometallic Based Acceptors for Organic Photovoltaics. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2021, 31, 1676-1687.	1.9	6
36	Investigation analysis of optoelectronic and structural properties of cis- and trans-structures of azo dyes: density functional theory study. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4183.	0.9	6

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37	A New Type of Aerostatic Thrust Bearing Controlled by High-speed Pneumatic Valve and a Novel Pressure Transducer. <i>International Journal of Automotive and Mechanical Engineering</i> , 2019, 16, 7430-7446.	0.5	6
38	Efficient Adsorption of Lead Ions from Synthetic Wastewater Using Agrowaste-Based Mixed Biomass (Potato Peels and Banana Peels). <i>Water (Switzerland)</i> , 2021, 13, 3344.	1.2	6
39	Comparison of catalytic and fuel additive properties of bimetallic nanoparticles and its composite: FeMnO <sub>3</sub> and PANI-FeMnO <sub>3</sub> . <i>Materials Science in Semiconductor Processing</i> , 2022, 144, 106630.	1.9	6
40	Insighting the systematic impact of shape, size and substitution of heteroatoms in quinoidal oligomers to tune their optoelectronic properties. <i>Optical and Quantum Electronics</i> , 2022, 54, .	1.5	5
41	Substitutional effect of different bridging groups on optical and charge transfer properties of small bipolar molecules for OLEDs. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e4000.	0.9	4
42	Exploring the quinoidal oligothiophenes to their robust limit for efficient linear and nonlinear optical response properties. <i>Chemical Papers</i> , 2022, 76, 4273-4288.	1.0	4
43	Control of oil film thickness for hydrostatic journal bearing using PID disturbance rejection controller. , 2017, , .		3
44	Techniques in the synthesis of organometallic compounds of tungsten. <i>Reviews in Inorganic Chemistry</i> , 2020, 40, 1-45.	1.8	3
45	Role of capping agent in the synthesis of zinc-cobalt bimetallic nanoparticles and its application as catalyst and fuel additive. <i>Applied Nanoscience (Switzerland)</i> , 2022, 12, 2169-2181.	1.6	2
46	Organometallic complexes of neodymium: an overview of synthetic methodologies based on coordinating elements. <i>Reviews in Inorganic Chemistry</i> , 2021, 41, 77-130.	1.8	1