Muhammad Usman Khan

List of Publications by Year
in descending order

96	4,814	57758	106344
papers	citations	44 h-index	65 g-index

96	96	96	1056
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis and characterization of ferrocene-based thiosemicarbazones along with their computational studies for potential as inhibitors for SARS-CoV-2. Journal of the Iranian Chemical Society, 2022, 19, 839-846.	2.2	11
2	Computational engineering to enhance the photovoltaic by <scp>endâ€capped</scp> and bridging core alterations: Empowering the future with solar energy through synergistic effect in <scp>Dâ€A</scp> materials. International Journal of Quantum Chemistry, 2022, 122, e26821.	2.0	14
3	A facile synthesis and structural elucidation for furfural based chromophores: Prediction of linear and nonlinear optical properties. Journal of Molecular Structure, 2022, 1249, 131543.	3.6	5
4	Antibacterial metal complexes of oâ€sulfamoylbenzoic acid: Synthesis, characterization, and DFT study. Applied Organometallic Chemistry, 2022, 36, .	3.5	32
5	Novel Starâ€Shaped Benzotriindoleâ€Based Nonfullerene Donor Materials: Toward the Development of Promising Photovoltaic Compounds for Highâ€Performance Organic Solar Cells. Energy Technology, 2022, 10, .	3.8	18
6	Physicalâ€organic aspects along with linear and nonlinear optical properties of benzene sulfonamide compounds: In silico analysis. Journal of Physical Organic Chemistry, 2022, 35, .	1.9	13
7	Influence of acceptor tethering on the performance of nonlinear optical properties for pyrene-based materials with A-Ï€-D-Ï€-D architecture. Arabian Journal of Chemistry, 2022, 15, 103673.	4.9	29
8	Isolation of Thioinosine and Butenolides from a Terrestrial Actinomycetes sp. GSCWâ€51 and Their in Silico Studies for Potential against SARSâ€CoVâ€2. Chemistry and Biodiversity, 2022, 19, .	2.1	3
9	Ab Initio Study of Two-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells. ACS Omega, 2022, 7, 10638-10648.	3.5	30
10	First example of vinylbenzene based small photovoltaic molecules: Towards the development of efficient D-Ï€-A configured optoelectronic materials for bulk heterojunction solar cells. Physica B: Condensed Matter, 2022, 633, 413769.	2.7	18
11	Novel quad-rotor-shaped photovoltaic materials: first example of fused-ring non-fullerene acceptors with proficient photovoltaic properties for high-performance solar cells. Journal of Molecular Modeling, 2022, 28, 18.	1.8	2
12	Quinoline based thiosemicarbazones as colorimetric chemosensors for fluoride and cyanide ions and DFT studies. Scientific Reports, 2022, 12, 4927.	3.3	23
13	First example of N-shaped dipyrrolo[2,3-b:2â€²,3â€²-e]pyrazine-2,6(1H,5H)-dione based small acceptor materials: Role of cyano (â^'C‰¡N) free guest acceptors for developing environmental friendly organic solar cells. European Physical Journal Plus, 2022, 137, .	2.6	4
14	Efficient designing of half-moon-shaped chalcogen heterocycles as non-fullerene acceptors for organic solar cells. Journal of Molecular Modeling, 2022, 28, 125.	1.8	28
15	Heterometallic decanuclear [Fe₆â€“Ln₄] coordination clusters with enzymatic mimic activity: Synthesis, structures, magnetic properties, and evaluation of catecholase activity. Applied Organometallic Chemistry, 2022, 36, .	3.5	6
16	Exploration of Nonlinear Optical Properties for the First Theoretical Framework of Non-Fullerene DTS(FBTTh₂)₂-Based Derivatives. ACS Omega, 2022, 7, 18027-18040.	3.5	14
17	Computational study of 2N-atom functionalized corannulene by alkali metals doping: Towards the development of highly efficient nonlinear optical materials. Physica B: Condensed Matter, 2022, 640, 414041.	2.7	14
18	Exploration of nonlinear optical enhancement and interesting optical behavior with pyrene moiety as the conjugated donor and efficient modification in acceptor moieties. Optical and Quantum Electronics, 2022, 54, .	3.3	16

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19	Deciphering the Role of Alkali Metals (Li, Na, K) Doping for Triggering Nonlinear Optical (NLO) Properties of T-Graphene Quantum Dots: Toward the Development of Giant NLO Response Materials. ACS Omega, 2022, 7, 24396-24414.	3.5	15
20	Theoretical and Conceptual Framework to Design Efficient Dye-Sensitized Solar Cells (DSSCs): Molecular Engineering by DFT Method. Journal of Cluster Science, 2021, 32, 243-253.	3.3	80
21	Persistent prevalence of supramolecular architectures of novel ultrasonically synthesized hydrazones due to hydrogen bonding [Xâ€“Hâ‹¯O; X=N]: Experimental and density functional theory analyses. Journal of Physics and Chemistry of Solids, 2021, 148, 109679.	4.0	53
22	Molecular designing of highâ€performance 3D starâ€shaped electron acceptors containing a truxene core for nonfullerene organic solar cells. Journal of Physical Organic Chemistry, 2021, 34, .	1.9	85
23	Designing of benzodithiophene core-based small molecular acceptors for efficient non-fullerene organic solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 244, 118873.	3.9	102
24	First theoretical framework of Z-shaped acceptor materials with fused-chrysene core for high performance organic solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 245, 118938.	3.9	84
25	Efficient Cu Decorated Inorganic B₁₂P₁₂Nanoclusters for Sensing Toxic COCl₂Gas: A Detailed DFT Study. Journal of Computational Biophysics and Chemistry, 2021, 20, 85-97.	1.7	36
26	Efficient designing of triphenylamine-based hole transport materials with outstanding photovoltaic characteristics for organic solar cells. Journal of Materials Science, 2021, 56, 5113-5131.	3.7	86
27	Exploration of CHâ‹¯F & CFâ‹¯H mediated supramolecular arrangements into fluorinated terphenyls and theoretical prediction of their third-order nonlinear optical response. RSC Advances, 2021, 11, 7766-7778.	3.6	36
28	Structural parameter-modulated nonlinear optical amplitude of acceptorâ€“Ï€â€“Dâ€“Ï€â€“donor-configured pyrene derivatives: a DFT approach. RSC Advances, 2021, 11, 14237-14250.	3.6	83
29	Quantum chemical design of nearâ€infrared sensitive fused ring electron acceptors containing selenophene as Ï€â€bridge for highâ€performance organic solar cells. Journal of Physical Organic Chemistry, 2021, 34, e4204.	1.9	58
30	2-Amino-6-methylpyridine based co-crystal salt formation using succinic acid: Single-crystal analysis and computational exploration. Journal of Molecular Structure, 2021, 1230, 129893.	3.6	29
31	Non-covalent interactions abetted supramolecular arrangements of N-Substituted benzylidene acetohydrazide to direct its solid-state network. Journal of Molecular Structure, 2021, 1230, 129827.	3.6	32
32	Key Electronic, Linear and Nonlinear Optical Properties of Designed Disubstituted Quinoline with Carbazole Compounds. Molecules, 2021, 26, 2760.	3.8	23
33	High-throughput calculations and experimental insights towards the development of potent thiazoline based functional materials. Materials Today Communications, 2021, 27, 102485.	1.9	5
34	An Efficient Synthesis, Spectroscopic Characterization, and Optical Nonlinearity Response of Novel Salicylaldehyde Thiosemicarbazone Derivatives. ACS Omega, 2021, 6, 16058-16065.	3.5	31
35	Novel W-Shaped Oxygen Heterocycle-Fused Fluorene-Based Non-Fullerene Acceptors: First Theoretical Framework for Designing Environment-Friendly Organic Solar Cells. Energy & Fuels, 2021, 35, 12436-12450.	5.1	67
36	Structural modulation of Ï€-conjugated linkers in Dâ€“Ï€â€“A dyes based on triphenylamine dicyanovinylene framework to explore the NLO properties. Royal Society Open Science, 2021, 8, 210570.	2.4	45

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37	Exploration of Nonlinear Optical Properties of Triphenylamine-Dicyanovinylene Coexisting Donor-Ï€-Acceptor Architecture by the Modification of Ï€-Conjugated Linker. Frontiers in Materials, 2021, 8, .	2.4	9
38	NLO potential exploration for Dâ€“Ï€â€“A heterocyclic organic compounds by incorporation of various Ï€-linkers and acceptor units. Arabian Journal of Chemistry, 2021, 14, 103295.	4.9	72
39	Efficient tuning of small acceptor chromophores with A1-Ï€-A2-Ï€-A1 configuration for high efficacy of organic solar cells via end group manipulation. Journal of Saudi Chemical Society, 2021, 25, 101305.	5.2	53
40	Exploration of second and third order nonlinear optical properties for theoretical framework of organic Dâ€“Ï€â€“Dâ€“Ï€â€“A type compounds. Optical and Quantum Electronics, 2021, 53, 1.	3.3	15
41	Facile Synthesis of Diversely Functionalized Peptoids, Spectroscopic Characterization, and DFT-Based Nonlinear Optical Exploration. ACS Omega, 2021, 6, 26016-26025.	3.5	14
42	Theoretical investigation of nonlinear optical behavior for rod and T-Shaped phenothiazine based D-Ï€-A organic compounds and their derivatives. Journal of Saudi Chemical Society, 2021, 25, 101339.	5.2	37
43	An effective strategy for tuning nonlinear optical response of N-atom functionalized corannulene by alkali metals doping: First theoretical insight. Computational and Theoretical Chemistry, 2021, 1205, 113430.	2.5	19
44	Synthesis, characterization and DFT calculated properties of electron-rich hydrazinylthiazoles: Experimental and computational synergy. Journal of Molecular Structure, 2021, 1245, 131043.	3.6	19
45	Exploration of efficient electron acceptors for organic solar cells: rational design of indacenodithiophene based non-fullerene compounds. Scientific Reports, 2021, 11, 19931.	3.3	63
46	2-Nitro- and 4-fluorocinnamaldehyde based receptors as naked-eye chemosensors to potential molecular keypad lock. Scientific Reports, 2021, 11, 20847.	3.3	6
47	Exploration of promising optical and electronic properties of (non-polymer) small donor molecules for organic solar cells. Scientific Reports, 2021, 11, 21540.	3.3	46
48	Structural parameters, electronic, linear and nonlinear optical exploration of thiopyrimidine derivatives: A comparison between DFT/TDDFT and experimental study. Journal of Molecular Structure, 2020, 1201, 127183.	3.6	53
49	Synthesis, crystal structure, spectroscopic, electronic and nonlinear optical properties of potent thiazole based derivatives: Joint experimental and computational insight. Journal of Molecular Structure, 2020, 1202, 127354.	3.6	30
50	A facile microwave assisted synthesis and structure elucidation of (3R)-3-alkyl-4,1-benzoxazepine-2,5-diones by crystallographic, spectroscopic and DFT studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 230, 117995.	3.9	26
51	Synthesis and structural analysis of novel indole derivatives by XRD, spectroscopic and DFT studies. Journal of Molecular Structure, 2020, 1203, 127438.	3.6	51
52	Designing spirobifullerene core based threeâ€dimensional cross shape acceptor materials with promising photovoltaic properties for <scp>highâ€efficiency</scp> organic solar cells. International Journal of Quantum Chemistry, 2020, 120, e26377.	2.0	84
53	Exploration of Chromone-Based Thiosemicarbazone Derivatives: SC-XRD/DFT, Spectral (IR, UVâ€“Vis) Characterization, and Quantum Chemical Analysis. ACS Omega, 2020, 5, 30176-30188.	3.5	28
54	Molecular engineering of Aâ€“Dâ€“Câ€“Dâ€“A configured small molecular acceptors (SMAs) with promising photovoltaic properties for high-efficiency fullerene-free organic solar cells. Optical and Quantum Electronics, 2020, 52, 1.	3.3	96

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55	An Experimental and Computational Exploration on the Electronic, Spectroscopic, and Reactivity Properties of Novel Halo-Functionalized Hydrazones. ACS Omega, 2020, 5, 18907-18918.	3.5	14
56	Palladium-catalyzed synthesis of pyrimidine substituted diaryl ethers through Suzuki Miyaura coupling reactions: Experimental and DFT studies. Optik, 2020, 219, 165285.	2.9	11
57	Exploration of adsorption behavior, electronic nature and NLO response of hydrogen adsorbed Alkali metals (Li, Na and K) encapsulated Al12N12 nanocages. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050031.	1.8	40
58	Synthesis of needle like nano composite of rGO-Mn2O and their applications as photo-catalyst. Chemical Physics Letters, 2020, 757, 137874.	2.6	4
59	In Silico Modeling of New â€œY-Seriesâ€•Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. ACS Omega, 2020, 5, 24125-24137.	3.5	103
60	Designing Star-Shaped Subphthalocyanine-Based Acceptor Materials with Promising Photovoltaic Parameters for Non-fullerene Solar Cells. ACS Omega, 2020, 5, 23039-23052.	3.5	61
61	Designing of near-infrared sensitive asymmetric small molecular donors for high-efficiency organic solar cells. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050034.	1.8	67
62	Stabilization of Supramolecular Assembly of Nâ€Substituted Benzylidene Acetohydrazide Analogs by Nonâ€Covalent Interactions: A Concise Experimental and Theoretical Approach. ChemistrySelect, 2020, 5, 10618-10631.	1.5	17
63	Facile Ultrasoundâ€Based Synthesis, SCâ€XRD, DFT Exploration of the Substituted Acylâ€Hydrazones: An Experimental and Theoretical Slant towards Supramolecular Chemistry. ChemistrySelect, 2020, 5, 14844-14856.	1.5	47
64	Enhancement in Photovoltaic Properties of N,Nâ€diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. ChemistrySelect, 2020, 5, 5022-5034.	1.5	95
65	Designing indenothiophene-based acceptor materials with efficient photovoltaic parameters for fullerene-free organic solar cells. Journal of Molecular Modeling, 2020, 26, 137.	1.8	97
66	Density functional theory study of palladium cluster adsorption on a graphene support. RSC Advances, 2020, 10, 20595-20607.	3.6	86
67	An efficient synthesis, structural (SC-XRD) and spectroscopic (FTIR, 1HNMR, MS spectroscopic) characterization of novel benzofuran-based hydrazones: An experimental and theoretical studies. Journal of Molecular Structure, 2020, 1216, 128318.	3.6	35
68	Exploration of Noncovalent Interactions, Chemical Reactivity, and Nonlinear Optical Properties of Piperidone Derivatives: A Concise Theoretical Approach. ACS Omega, 2020, 5, 13236-13249.	3.5	38
69	Designing N-phenylaniline-triazol configured donor materials with promising optoelectronic properties for high-efficiency solar cells. Computational and Theoretical Chemistry, 2020, 1186, 112908.	2.5	119
70	First principles study of electronic and nonlinear optical properties of Aâ€“Dâ€“Ïâ€“A and Dâ€“Aâ€“Dâ€“Ïâ€“A configured compounds containing novel quinolineâ€“carbazole derivatives. RSC Advances, 2020, 10, 22273-22283.	3.6	122
71	Adsorption of Phosgene Gas on Pristine and Copper-Decorated B₁₂N₁₂ Nanocages: A Comparative DFT Study. ACS Omega, 2020, 5, 7641-7650.	3.5	114
72	Benzenesulfonohydrazides inhibiting urease: Design, synthesis, their inÂvitro and in silico studies. Journal of Molecular Structure, 2020, 1220, 128740.	3.6	54

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73	Spectroscopic and DFT/TDDFT insights of the novel phosphonate imine compounds. Journal of Molecular Structure, 2020, 1207, 127838.	3.6	15
74	Facile preparation, characterization, SC-XRD and DFT/DTDFT study of diversely functionalized unsymmetrical bis-aryl-Î±, Î²-unsaturated ketone derivatives. Journal of Molecular Structure, 2020, 1206, 127755.	3.6	51
75	Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. Computational and Theoretical Chemistry, 2020, 1181, 112833.	2.5	94
76	Experimental and computational investigations of new indole derivatives: A combined spectroscopic, SC-XRD, DFT/TD-DFT and QTAIM analysis. Journal of Molecular Structure, 2020, 1207, 127803.	3.6	50
77	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells. RSC Advances, 2019, 9, 26402-26418.	3.6	115
78	Synthesis, XRD, spectral (IR, UVâ€“Vis, NMR) characterization and quantum chemical exploration of benzoimidazoleâ€based hydrazones: A synergistic experimentalâ€computational analysis. Applied Organometallic Chemistry, 2019, 33, e5182.	3.5	42
79	Efficient Synthesis by Monoâ€Carboxy Methylation of 4,4â€²â€Biphenol, Xâ€ray Diffraction, Spectroscopic Characterization and Computational Study of the Crystal Packing of Ethyl 2â€((4â€²â€hydroxyâ€[1,1â€²â€biphenyl]â€4â€yl)oxy)acetate. ChemistrySelect, 2019, 4, 9274-9284.	1.5	32
80	Electron Donor and Acceptor Influence on the Nonlinear Optical Response of Diacetylene-Functionalized Organic Materials (DFOMs): Density Functional Theory Calculations. Molecules, 2019, 24, 2096.	3.8	48
81	Synthesis, spectroscopic, SC-XRD characterizations and DFT based studies of ethyl2-(substituted-(2-benzylidenehydrazinyl))thiazole-4-carboxylate derivatives. Journal of Molecular Structure, 2019, 1187, 164-171.	3.6	55
82	Quantum chemical designing of indolo[3,2,1-jk]carbazole-based dyes for highly efficient nonlinear optical properties. Chemical Physics Letters, 2019, 719, 59-66.	2.6	108
83	Synthesis, crystal structure analysis, spectral characterization and nonlinear optical exploration of potent thiosemicarbazones based compounds: A DFT refine experimental study. Inorganica Chimica Acta, 2019, 486, 162-171.	2.4	56
84	First theoretical probe for efficient enhancement of nonlinear optical properties of quinacridone based compounds through various modifications. Chemical Physics Letters, 2019, 715, 222-230.	2.6	125
85	Prediction of Second-Order Nonlinear Optical Properties of Dâ€“Ïâ€“A Compounds Containing Novel Fluorene Derivatives: A Promising Route to Giant Hyperpolarizabilities. Journal of Cluster Science, 2019, 30, 415-430.	3.3	110
86	Synthesis, crystal structure analysis, spectral IR, UVâ€“Vis, NMR assessments, electronic and nonlinear optical properties of potent quinoline based derivatives: Interplay of experimental and DFT study. Journal of Saudi Chemical Society, 2019, 23, 546-560.	5.2	98
87	Synthesis, single crystal analysis and DFT based computational studies of 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrim idin-1-ium 3,4,5-trihydroxybenzoate -methanol (DETM). Journal of Molecular Structure, 2019, 1180, 119-126.	3.6	57
88	A combined experimental and computational study of 3-bromo-5-(2,5-difluorophenyl) pyridine and 3,5-bis(naphthalen-1-yl)pyridine: Insight into the synthesis, spectroscopic, single crystal XRD, electronic, nonlinear optical and biological properties. Journal of Molecular Structure, 2018, 1160, 129-141.	3.6	70
89	First Theoretical Framework of Triphenylamineâ€“Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of Ïâ€-Linkers. Journal of Physical Chemistry C, 2018, 122, 4009-4018.	3.1	193
90	Synthetic, XRD, non-covalent interactions and solvent dependent nonlinear optical studies of Sulfadiazine-Ortho-Vanillin Schiff base: (E)-4-((2-hydroxy-3-methoxy- benzylidene)) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 57 Td (amino)-N	3.6	28

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91	Synthesis and XRD, FT-IR vibrational, UVâ€“vis, and nonlinear optical exploration of novel tetra substituted imidazole derivatives: A synergistic experimental-computational analysis. Journal of Physics and Chemistry of Solids, 2018, 115, 265-276.	4.0	77
92	Synthesis and study of catalytic application of l-methionine protected gold nanoparticles. Applied Nanoscience (Switzerland), 2017, 7, 429-437.	3.1	16
93	Effect of Ï€-conjugation spacer (CC) on the first hyperpolarizabilities of polymeric chain containing polyoxometalate cluster as a side-chain pendant: A DFT study. Computational and Theoretical Chemistry, 2012, 994, 34-40.	2.5	138
94	A DFT Study on The Twoâ€Dimensional Secondâ€Order Nonlinear Optical (NLO) Response of Terpyridineâ€Substituted Hexamolybdates: Physical Insight on 2D Inorganicâ€“Organic Hybrid Functional Materials. European Journal of Inorganic Chemistry, 2012, 2012, 705-711.	2.0	109
95	In Silico Modelling of Viscoelastic Surfactants: Towards NLO Response and Novel Physical Insights through Bridging Acceptor. Journal of Cluster Science, 0, , 1.	3.3	1
96	Theoretical Investigation of Jack-in-the-Box Electro-Optical Compounds: In-Silico Design of Mixed-Argon Benzonitriles Towards the Template of Clusters. Journal of Cluster Science, 0, , 1.	3.3	1