

Muhammad Usman Khan

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8091269/publications.pdf>

Version: 2024-02-01

96
papers

4,814
citations

57758

44
h-index

106344

65
g-index

96
all docs

96
docs citations

96
times ranked

1056
citing authors

#	ARTICLE	IF	CITATIONS
1	First Theoretical Framework of Triphenylamine- π -Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of π -Linkers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4009-4018.	3.1	193
2	Effect of π -conjugation spacer (CC) on the first hyperpolarizabilities of polymeric chain containing polyoxometalate cluster as a side-chain pendant: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2012, 994, 34-40.	2.5	138
3	First theoretical probe for efficient enhancement of nonlinear optical properties of quinacridone based compounds through various modifications. <i>Chemical Physics Letters</i> , 2019, 715, 222-230.	2.6	125
4	First principles study of electronic and nonlinear optical properties of π -conjugated A and B configured compounds containing novel quinoline-carbazole derivatives. <i>RSC Advances</i> , 2020, 10, 22273-22283.	3.6	122
5	Designing N-phenylaniline-triazol configured donor materials with promising optoelectronic properties for high-efficiency solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1186, 112908.	2.5	119
6	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells. <i>RSC Advances</i> , 2019, 9, 26402-26418.	3.6	115
7	Adsorption of Phosgene Gas on Pristine and Copper-Decorated $B_{12}N_{12}$ Nanocages: A Comparative DFT Study. <i>ACS Omega</i> , 2020, 5, 7641-7650.	3.5	114
8	Prediction of Second-Order Nonlinear Optical Properties of π -Conjugated Compounds Containing Novel Fluorene Derivatives: A Promising Route to Giant Hyperpolarizabilities. <i>Journal of Cluster Science</i> , 2019, 30, 415-430.	3.3	110
9	A DFT Study on The Two-Dimensional Second-Order Nonlinear Optical (NLO) Response of Terpyridine-Substituted Hexamolybdates: Physical Insight on 2D Inorganic-Organic Hybrid Functional Materials. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 705-711.	2.0	109
10	Quantum chemical designing of indolo[3,2,1-jk]carbazole-based dyes for highly efficient nonlinear optical properties. <i>Chemical Physics Letters</i> , 2019, 719, 59-66.	2.6	108
11	In Silico Modeling of New π -Series-Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. <i>ACS Omega</i> , 2020, 5, 24125-24137.	3.5	103
12	Designing of benzodithiophene core-based small molecular acceptors for efficient non-fullerene organic solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 244, 118873.	3.9	102
13	Synthesis, crystal structure analysis, spectral IR, UV-Vis, NMR assessments, electronic and nonlinear optical properties of potent quinoline based derivatives: Interplay of experimental and DFT study. <i>Journal of Saudi Chemical Society</i> , 2019, 23, 546-560.	5.2	98
14	Designing indenothiophene-based acceptor materials with efficient photovoltaic parameters for fullerene-free organic solar cells. <i>Journal of Molecular Modeling</i> , 2020, 26, 137.	1.8	97
15	Molecular engineering of π -conjugated A configured small molecular acceptors (SMAs) with promising photovoltaic properties for high-efficiency fullerene-free organic solar cells. <i>Optical and Quantum Electronics</i> , 2020, 52, 1.	3.3	96
16	Enhancement in Photovoltaic Properties of π -Diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. <i>ChemistrySelect</i> , 2020, 5, 5022-5034.	1.5	95
17	Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1181, 112833.	2.5	94
18	Density functional theory study of palladium cluster adsorption on a graphene support. <i>RSC Advances</i> , 2020, 10, 20595-20607.	3.6	86

#	ARTICLE	IF	CITATIONS
19	Efficient designing of triphenylamine-based hole transport materials with outstanding photovoltaic characteristics for organic solar cells. <i>Journal of Materials Science</i> , 2021, 56, 5113-5131.	3.7	86
20	Molecular designing of high-performance 3D star-shaped electron acceptors containing a truxene core for nonfullerene organic solar cells. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, .	1.9	85
21	Designing spirobifullerene core based three-dimensional cross shape acceptor materials with promising photovoltaic properties for high-efficiency organic solar cells. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26377.	2.0	84
22	First theoretical framework of Z-shaped acceptor materials with fused-chrysene core for high performance organic solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 245, 118938.	3.9	84
23	Structural parameter-modulated nonlinear optical amplitude of acceptor-donor-configured pyrene derivatives: a DFT approach. <i>RSC Advances</i> , 2021, 11, 14237-14250.	3.6	83
24	Theoretical and Conceptual Framework to Design Efficient Dye-Sensitized Solar Cells (DSSCs): Molecular Engineering by DFT Method. <i>Journal of Cluster Science</i> , 2021, 32, 243-253.	3.3	80
25	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 ETQq1 1 0.784314 rgBT /Overlook 10 Tf50 497 Td	3.3	80
26	Synthesis and XRD, FT-IR vibrational, UV-vis, and nonlinear optical exploration of novel tetra substituted imidazole derivatives: A synergistic experimental-computational analysis. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 115, 265-276.	4.0	77
27	NLO potential exploration for A heterocyclic organic compounds by incorporation of various linkers and acceptor units. <i>Arabian Journal of Chemistry</i> , 2021, 14, 103295.	4.9	72
28	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. <i>Journal of Molecular Structure</i> , 2018, 1160, 129-141.	3.6	70
29	Designing of near-infrared sensitive asymmetric small molecular donors for high-efficiency organic solar cells. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2050034.	1.8	67
30	Novel W-Shaped Oxygen Heterocycle-Fused Fluorene-Based Non-Fullerene Acceptors: First Theoretical Framework for Designing Environment-Friendly Organic Solar Cells. <i>Energy & Fuels</i> , 2021, 35, 12436-12450.	5.1	67
31	Exploration of efficient electron acceptors for organic solar cells: rational design of indacenodithiophene based non-fullerene compounds. <i>Scientific Reports</i> , 2021, 11, 19931.	3.3	63
32	Designing Star-Shaped Subphthalocyanine-Based Acceptor Materials with Promising Photovoltaic Parameters for Non-fullerene Solar Cells. <i>ACS Omega</i> , 2020, 5, 23039-23052.	3.5	61
33	Quantum chemical design of near-infrared sensitive fused ring electron acceptors containing selenophene as bridge for high-performance organic solar cells. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4204.	1.9	58
34	Synthesis, single crystal analysis and DFT based computational studies of 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrimidin-1-ium 3,4,5-trihydroxybenzoate-methanol (DETM). <i>Journal of Molecular Structure</i> , 2019, 1180, 119-126.	3.6	57
35	Synthesis, crystal structure analysis, spectral characterization and nonlinear optical exploration of potent thiosemicarbazones based compounds: A DFT refine experimental study. <i>Inorganica Chimica Acta</i> , 2019, 486, 162-171.	2.4	56
36	Synthesis, spectroscopic, SC-XRD characterizations and DFT based studies of ethyl-2-(substituted-(2-benzylidenehydrazinyl))thiazole-4-carboxylate derivatives. <i>Journal of Molecular Structure</i> , 2019, 1187, 164-171.	3.6	55

#	ARTICLE	IF	CITATIONS
37	Benzenesulfonohydrazides inhibiting urease: Design, synthesis, their in vitro and in silico studies. Journal of Molecular Structure, 2020, 1220, 128740.	3.6	54
38	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
39	Persistent prevalence of supramolecular architectures of novel ultrasonically synthesized hydrazones due to hydrogen bonding [X=O; X=N]: Experimental and density functional theory analyses. Journal of Physics and Chemistry of Solids, 2021, 148, 109679.	4.0	53
40	Efficient tuning of small acceptor chromophores with A1-A2-A1 configuration for high efficacy of organic solar cells via end group manipulation. Journal of Saudi Chemical Society, 2021, 25, 101305.	5.2	53
41	Synthesis and structural analysis of novel indole derivatives by XRD, spectroscopic and DFT studies. Journal of Molecular Structure, 2020, 1203, 127438.	3.6	51
42	Facile preparation, characterization, SC-XRD and DFT/DTDF study of diversely functionalized unsymmetrical bis-aryl-1,2-unsaturated ketone derivatives. Journal of Molecular Structure, 2020, 1206, 127755.	3.6	51
43	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
44	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
45	Facile Ultrasound-Based Synthesis, SC-XRD, DFT Exploration of the Substituted Acyl-Hydrazones: An Experimental and Theoretical Slant towards Supramolecular Chemistry. ChemistrySelect, 2020, 5, 14844-14856.	1.5	47
46	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
47	Structural modulation of π -conjugated linkers in D-A dyes based on triphenylamine dicyanovinylene framework to explore the NLO properties. Royal Society Open Science, 2021, 8, 210570.	2.4	45
48	Synthesis, XRD, spectral (IR, UV-Vis, NMR) characterization and quantum chemical exploration of benzoimidazole-based hydrazones: A synergistic experimental-computational analysis. Applied Organometallic Chemistry, 2019, 33, e5182.	3.5	42
49	Exploration of adsorption behavior, electronic nature and NLO response of hydrogen adsorbed Alkali metals (Li, Na and K) encapsulated Al ₁₂ N ₁₂ nanocages. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050031.	1.8	40
50	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
51	Theoretical investigation of nonlinear optical behavior for rod and T-Shaped phenothiazine based D-A organic compounds and their derivatives. Journal of Saudi Chemical Society, 2021, 25, 101339.	5.2	37
52	Efficient Cu Decorated Inorganic B ₁₂ P ₁₂ Nanoclusters for Sensing Toxic COCl ₂ Gas: A Detailed DFT Study. Journal of Computational Biophysics and Chemistry, 2021, 20, 85-97.	1.7	36
53	Exploration of CH ₂ F & CF ₂ 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
54	An efficient synthesis, structural (SC-XRD) and spectroscopic (FTIR, ¹ HNMR, MS spectroscopic) characterization of novel benzofuran-based hydrazones: An experimental and theoretical studies. Journal of Molecular Structure, 2020, 1216, 128318.	3.6	35

#	ARTICLE	IF	CITATIONS
55	Efficient Synthesis by Mono- <i>o</i> -Carboxy Methylation of 4,4'-Biphenol, X-ray Diffraction, Spectroscopic Characterization and Computational Study of the Crystal Packing of Ethyl 2-((4'-hydroxy-[1,1'-biphenyl]-4-yl)oxy)acetate. <i>ChemistrySelect</i> , 2019, 4, 9274-9284.	1.5	32
56	Non-covalent interactions abetted supramolecular arrangements of N-Substituted benzylidene acetohydrazide to direct its solid-state network. <i>Journal of Molecular Structure</i> , 2021, 1230, 129827.	3.6	32
57	Antibacterial metal complexes of <i>o</i> -sulfamoylbenzoic acid: Synthesis, characterization, and DFT study. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	3.5	32
58	An Efficient Synthesis, Spectroscopic Characterization, and Optical Nonlinearity Response of Novel Salicylaldehyde Thiosemicarbazone Derivatives. <i>ACS Omega</i> , 2021, 6, 16058-16065.	3.5	31
59	Synthesis, crystal structure, spectroscopic, electronic and nonlinear optical properties of potent thiazole based derivatives: Joint experimental and computational insight. <i>Journal of Molecular Structure</i> , 2020, 1202, 127354.	3.6	30
60	Ab Initio Study of Two-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells. <i>ACS Omega</i> , 2022, 7, 10638-10648.	3.5	30
61	2-Amino-6-methylpyridine based co-crystal salt formation using succinic acid: Single-crystal analysis and computational exploration. <i>Journal of Molecular Structure</i> , 2021, 1230, 129893.	3.6	29
62	Influence of acceptor tethering on the performance of nonlinear optical properties for pyrene-based materials with A- <i>h</i> -D- <i>h</i> -D architecture. <i>Arabian Journal of Chemistry</i> , 2022, 15, 103673.	4.9	29
63	Exploration of Chromone-Based Thiosemicarbazone Derivatives: SC-XRD/DFT, Spectral (IR, UV-Vis) Characterization, and Quantum Chemical Analysis. <i>ACS Omega</i> , 2020, 5, 30176-30188.	3.5	28
64	Efficient designing of half-moon-shaped chalcogen heterocycles as non-fullerene acceptors for organic solar cells. <i>Journal of Molecular Modeling</i> , 2022, 28, 125.	1.8	28
65	A facile microwave assisted synthesis and structure elucidation of (3 <i>R</i>)-3-alkyl-4,1-benzoxazepine-2,5-diones by crystallographic, spectroscopic and DFT studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 230, 117995.	3.9	26
66	Key Electronic, Linear and Nonlinear Optical Properties of Designed Disubstituted Quinoline with Carbazole Compounds. <i>Molecules</i> , 2021, 26, 2760.	3.8	23
67	Quinoline based thiosemicarbazones as colorimetric chemosensors for fluoride and cyanide ions and DFT studies. <i>Scientific Reports</i> , 2022, 12, 4927.	3.3	23
68	An effective strategy for tuning nonlinear optical response of N-atom functionalized corannulene by alkali metals doping: First theoretical insight. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113430.	2.5	19
69	Synthesis, characterization and DFT calculated properties of electron-rich hydrazinylthiazoles: Experimental and computational synergy. <i>Journal of Molecular Structure</i> , 2021, 1245, 131043.	3.6	19
70	Novel Star-Shaped Benzotriindole-Based Nonfullerene Donor Materials: Toward the Development of Promising Photovoltaic Compounds for High-Performance Organic Solar Cells. <i>Energy Technology</i> , 2022, 10, .	3.8	18
71	First example of vinylbenzene based small photovoltaic molecules: Towards the development of efficient D-A configured optoelectronic materials for bulk heterojunction solar cells. <i>Physica B: Condensed Matter</i> , 2022, 633, 413769.	2.7	18
72	Stabilization of Supramolecular Assembly of <i>N</i> -Substituted Benzylidene Acetohydrazide Analogs by Non-Covalent Interactions: A Concise Experimental and Theoretical Approach. <i>ChemistrySelect</i> , 2020, 5, 10618-10631.	1.5	17

#	ARTICLE	IF	CITATIONS
73	Synthesis and study of catalytic application of L-methionine protected gold nanoparticles. Applied Nanoscience (Switzerland), 2017, 7, 429-437.	3.1	16
74	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
75	Spectroscopic and DFT/TDDFT insights of the novel phosphonate imine compounds. Journal of Molecular Structure, 2020, 1207, 127838.	3.6	15
76	Exploration of second and third order nonlinear optical properties for theoretical framework of organic Dâ€“â€“A type compounds. Optical and Quantum Electronics, 2021, 53, 1.	3.3	15
77	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
78	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
79	Facile Synthesis of Diversely Functionalized Peptoids, Spectroscopic Characterization, and DFT-Based Nonlinear Optical Exploration. ACS Omega, 2021, 6, 26016-26025.	3.5	14
80	Computational engineering to enhance the photovoltaic by <sc>endâ€“capped</sc> and bridging core alterations: Empowering the future with solar energy through synergistic effect in <sc>Dâ€“A</sc> materials. International Journal of Quantum Chemistry, 2022, 122, e26821.	2.0	14
81	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
82	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
83	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
84	Palladium-catalyzed synthesis of pyrimidine substituted diaryl ethers through Suzuki Miyaura coupling reactions: Experimental and DFT studies. Optik, 2020, 219, 165285.	2.9	11
85	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
86	Exploration of Nonlinear Optical Properties of Triphenylamine-Dicyanovinylene Coexisting Donor-â€“Acceptor Architecture by the Modification of â€“Conjugated Linker. Frontiers in Materials, 2021, 8, .	2.4	9
87	2-Nitro- and 4-fluorocinnamaldehyde based receptors as naked-eye chemosensors to potential molecular keypad lock. Scientific Reports, 2021, 11, 20847.	3.3	6
88	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
89	High-throughput calculations and experimental insights towards the development of potent thiazoline based functional materials. Materials Today Communications, 2021, 27, 102485.	1.9	5
90	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

#	ARTICLE	IF	CITATIONS
91	Synthesis of needle like nano composite of rGO-Mn ₂ O and their applications as photo-catalyst. Chemical Physics Letters, 2020, 757, 137874.	2.6	4
92	First example of N-shaped dipyrrolo[2,3-b:2',3'-e]pyrazine-2,6(1H,5H)-dione based small acceptor materials: Role of cyano (≡C%)N free guest acceptors for developing environmental friendly organic solar cells. European Physical Journal Plus, 2022, 137, .	2.6	4
93	Isolation of Thioinosine and Butenolides from a Terrestrial <i>Actinomycetes</i> sp. GSCW51 and Their <i>In Silico</i> Studies for Potential against SARS-CoV2. Chemistry and Biodiversity, 2022, 19, .	2.1	3
94	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
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