Muhammad Ramzan Saeed Ashraf Janju

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Green Synthesis of Silver Nanoparticles through Reduction with Solanum xanthocarpum L. Berry Extract: Characterization, Antimicrobial and Urease Inhibitory Activities against Helicobacter pylori. International Journal of Molecular Sciences, 2012, 13, 9923-9941.	4.1	286
2	First Theoretical Framework of Triphenylamine–Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of π-Linkers. Journal of Physical Chemistry C, 2018, 122, 4009-4018.	3.1	193
3	Chemical Cosubstitution-Oriented Design of Rare-Earth Borates as Potential Ultraviolet Nonlinear Optical Materials. Journal of the American Chemical Society, 2017, 139, 18397-18405.	13.7	187
4	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
5	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
6	A DFT Study on The Twoâ€Dimensional Secondâ€Order Nonlinear Optical (NLO) Response of Terpyridineâ€Substituted Hexamolybdates: Physical Insight on 2D Inorganic–Organic Hybrid Functional Materials. European Journal of Inorganic Chemistry, 2012, 2012, 705-711.	2.0	109
7	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
8	Quantum chemical study of benzimidazole derivatives to tune the second-order nonlinear optical molecular switching by proton abstraction. Physical Chemistry Chemical Physics, 2010, 12, 4791.	2.8	106
9	In Silico Modeling of New "Y-Series―Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. ACS Omega, 2020, 5, 24125-24137.	3.5	103
10	Prediction of Remarkably Large Second-Order Nonlinear Optical Properties of Organoimido-Substituted Hexamolybdates. Journal of Physical Chemistry A, 2009, 113, 3576-3587.	2.5	102
11	Effect of thiophene rings on UV/visible spectra and non-linear optical (NLO) properties of triphenylamine based dyes: a quantum chemical perspective. Journal of Physical Organic Chemistry, 2015, 28, 418-422.	1.9	99
12	How Does Bridging Core Modification Alter the Photovoltaic Characteristics of Triphenylamineâ€Based Hole Transport Materials? Theoretical Understanding and Prediction. Chemistry - A European Journal, 2021, 27, 4197-4210.	3.3	97
13	Investigation of Dibenzoboroles Having π-Electrons: Toward a New Type of Two-Dimensional NLO Molecular Switch?. Journal of Physical Chemistry C, 2009, 113, 12551-12557.	3.1	94
14	Quantum Mechanical Design of Efficient Second-Order Nonlinear Optical Materials Based on Heteroaromatic Imido-Substituted Hexamolybdates: First Theoretical Framework of POM-Based Heterocyclic Aromatic Rings. Inorganic Chemistry, 2012, 51, 11306-11314.	4.0	86
15	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
16	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
17	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
18	Theoretical Understanding and Role of Guest π-Bridges in Triphenylamine-Based Donor Materials for High-Performance Solar Cells. Energy & Fuels, 2021, 35, 12451-12460.	5.1	57

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#	Article	IF	CITATIONS
19	Deciphering the role of invited guest bridges in non-fullerene acceptor materials for high performance organic solar cells. Synthetic Metals, 2021, 279, 116865.	3.9	55
20	Compositional difference in antioxidant and antibacterial activity of all parts of the Carica papaya using different solvents. Chemistry Central Journal, 2016, 10, 5.	2.6	54
21	First Principle Study of Electronic and Non-Linear Optical (NLO) Properties of Triphenylamine Dyes: Interactive Design Computation of New NLO Compounds. Australian Journal of Chemistry, 2016, 69, 467.	0.9	54
22	Synthesis of Co3O4 Nano Aggregates by Co-precipitation Method and its Catalytic and Fuel Additive Applications. Open Chemistry, 2019, 17, 865-873.	1.9	49
23	Quantum Chemical Design of D–π–Aâ€Type Donor Materials for Highly Efficient, Photostable, and Vacuumâ€Processed Organic Solar Cells. Energy Technology, 2021, 9, 2100489.	3.8	46
24	Theoretical Framework for Encapsulation of Inorganic B ₁₂ N ₁₂ Nanoclusters with Alkaline Earth Metals for Efficient Hydrogen Adsorption: A Step Forward toward Hydrogen Storage Materials. Inorganic Chemistry, 2021, 60, 2816-2828.	4.0	43
25	Quantum chemical perspective of efficient NLO materials based on dipolar trans-tetraammineruthenium (II) complexes with pyridinium and thiocyanate ligands: First theoretical framework. Computational and Theoretical Chemistry, 2014, 1033, 6-13.	2.5	42
26	Solvent-Dependent Non-Linear Optical Properties of 5,5′-Disubstituted-2,2′-bipyridine Complexes of Ruthenium(II): A Quantum Chemical Perspective. Australian Journal of Chemistry, 2015, 68, 1502.	0.9	42
27	Machineâ€Learning Analysis of Smallâ€Molecule Donors for Fullerene Based Organic Solar Cells. Energy Technology, 2022, 10, .	3.8	42
28	Quantum Chemical Designing of Efficient Sensitizers for Dye Sensitized Solar Cells. Bulletin of the Korean Chemical Society, 2013, 34, 2093-2098.	1.9	41
29	Solvent effects on nonlinear optical response of certain tetrammineruthenium(II) complexes of modified 1,10-phenanthrolines. Canadian Journal of Chemistry, 2013, 91, 1303-1309.	1.1	37
30	All-small-molecule organic solar cells with high fill factor and enhanced open-circuit voltage with 18.25 % PCE: Physical insights from quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 279, 121487.	3.9	36
31	Tuning Second-Order Non-linear (NLO) Optical Response of Organoimido-Substituted Hexamolybdates through Halogens: Quantum Design of Novel Organic-Inorganic Hybrid NLO Materials. Australian Journal of Chemistry, 2010, 63, 836.	0.9	35
32	Prediction and Understanding: Quantum Chemical Framework of Transition Metals Enclosed in a B ₁₂ N ₁₂ Inorganic Nanocluster for Adsorption and Removal of DDT from the Environment. Inorganic Chemistry, 2021, 60, 10837-10847.	4.0	35
33	Prediction of robustly large molecular second-order nonlinear optical properties of terpyridine-substituted hexamolybdates: Structural modelling towards a rational entry to NLO materials. Journal of Molecular Graphics and Modelling, 2010, 28, 735-745.	2.4	30
34	Quantum Chemical Designing of Efficient TC4-Based Sensitizers by Modification of Auxiliary Donor and π-Spacer. Bulletin of the Chemical Society of Japan, 2013, 86, 1272-1281.	3.2	30
35	Synthesis of ferric oxyhydroxide nanoparticles and ferric oxide nanorods by reflux assisted coprecipitation method and comparative study of their thermal properties. Materials Research Express, 2017, 4, 115019.	1.6	29
36	Insights into endâ€capped modifications effect on the photovoltaic and optoelectronic properties of Sâ€shaped fullereneâ€free acceptor molecules: A density functional theory computational study for organic solar cells. Journal of Physical Organic Chemistry, 2022, 35, .	1.9	28

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#	Article	IF	CITATIONS
37	Learning from Fullerenes and Predicting for Y6: Machine Learning and Highâ€Throughput Screening of Small Molecule Donors for Organic Solar Cells. Energy Technology, 2022, 10, .	3.8	28
38	Quantum Chemical Design for Enhanced Secondâ€Order NLO Response of Terpyridineâ€Substituted Hexamolybdates. European Journal of Inorganic Chemistry, 2010, 2010, 3466-3472.	2.0	26
39	Synthesis, characterization and catalytic application of polyhedron zinc oxide microparticles. Materials Research Express, 2017, 4, 015902.	1.6	26
40	First theoretical framework of di-substituted donor moieties of triphenylamine and carbazole for NLO properties: quantum paradigms of interactive molecular computation. Molecular Simulation, 2017, 43, 1539-1545.	2.0	26
41	Exploring the effect of end-capped modifications of carbazole-based fullerene-free acceptor molecules for high-performance indoor organic solar cell applications. Journal of Computational Electronics, 2022, 21, 40-51.	2.5	25
42	Nonlinear optical response of a series of small molecules: quantum modification of π-spacer and acceptor. Journal of the Iranian Chemical Society, 2017, 14, 2041-2054.	2.2	24
43	DFT Molecular Simulation for Design and Effect of Core Bridging Acceptors (BA) on NLO Response: First Theoretical Framework to Enhance Nonlinearity Through BA. Journal of Cluster Science, 2017, 28, 3175-3183.	3.3	24
44	Agar and egg shell derived calcium carbonate and calcium hydroxide nanoparticles: Synthesis, characterization and applications. Chemical Physics Letters, 2019, 732, 136662.	2.6	24
45	Hydrogen as an energy currency: Encapsulation of inorganic Ga12N12 with alkali metals for efficient H2 adsorption as hydrogen storage materials. Journal of Physics and Chemistry of Solids, 2022, 160, 110352.	4.0	23
46	First Synthetic Study of Cube-Like Cobalt Hydroxystannate Nanoparticles as Photocatalyst for Drimarene Red K-4BL Degradation and Fuel Additive. Journal of Cluster Science, 2018, 29, 685-696.	3.3	21
47	Zinc oxide hollow micro spheres and nano rods: Synthesis and applications in gas sensor. Materials Chemistry and Physics, 2014, 147, 225-231.	4.0	20
48	Radiation assisted synthesis of dumb bell shaped calcium hydroxide nanostructures from egg shells and study of its thermal and catalytic applications. Chemical Physics Letters, 2018, 710, 45-53.	2.6	20
49	Synthesis of Saucer Shaped Manganese Oxide Nanoparticles by Co-precipitation Method and the Application as Fuel Additive. Journal of Cluster Science, 2018, 29, 1099-1106.	3.3	20
50	High-Throughput Designing and Investigation of D–Aâ~π–A -Type Donor Materials for Potential Application in Greenhouse-Integrated Solar Cells. Energy & Fuels, 2021, 35, 12461-12472.	5.1	20
51	A Quantum Mechanical Study of the Second-Order Nonlinear Optical Properties of Aryldiazenido-Substituted Hexamolybdates: A Surprising Charge Transfer. European Journal of Inorganic Chemistry, 2009, 2009, 5181-5188.	2.0	19
52	In silico modelling of acceptor materials by End-capped and π-linker modifications for High-Performance organic solar Cells: Estimated PCEÂ>Â18%. Computational and Theoretical Chemistry, 2022, 1208, 113555.	2.5	19
53	A DFT study on the electronic and redox properties of [X ₈ V ₁₄ O ₅₀] ^{<i>n</i>–} (X = Si ^{IV} ,) Tj ETQq1 434-442.	1 0.784314 1.1	4 rgBT /Overle
54	The synthesis of flower shaped microstructures of Co 3 O 4 by solvothermal approach and	3.2	18

investigation of its catalytic activity. Solid State Sciences, 2014, 36, 73-79.

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55	Synthetic Study and Merits of Fe3O4 Nanoparticles as Emerging Material. Journal of Cluster Science, 2017, 28, 2369-2400.	3.3	18
56	Computational Study on Non-linear Optical and Absorption Properties of Benzothiazole based Dyes: Tunable Electron-Withdrawing Strength and Reverse Polarity. Open Chemistry, 2017, 15, 139-146.	1.9	18
57	Quantum chemical design and prediction that complements understanding: How do the transition metals enhance the CO2 sensing ability of inorganic Mg12O12 nanoclusters?. Journal of Physics and Chemistry of Solids, 2022, 167, 110789.	4.0	18
58	The influence of hydrogen bonding on the nonlinear optical properties of a semiorganic material NH ₄ B[<scp>d</scp> -(+)-C ₄ H ₄ O ₅] ₂ ·H _{2· a theoretical perspective. Physical Chemistry Chemical Physics, 2014, 16, 20089.}	<td>17</td>	17
59	An Interesting Behavior and Nonlinear Optical (NLO) Response of Hexamolybdate Metal Cluster: Theoretical Insight into Electro-Optic Modulation of Hybrid Composites. Journal of Cluster Science, 2017, 28, 2693-2708.	3.3	17
60	Photocatalytic degradation of reactive black 5 on the surface of tin oxide microrods. Journal of Water and Health, 2018, 16, 773-781.	2.6	16
61	QUANTUM CHEMICAL DESIGNING OF TRIPHENYLAMINE DYES WITH D-A-Π-Α CONFIGURATION FOR DYE SENSITIZED SOLAR CELLS: MOLECULAR ENGINEERING THROUGH FIRST-PRINCIPLES CALCULATIONS. Journal of the Chilean Chemical Society, 2018, 63, 3850-3854.	1.2	16
62	Morphologically controlled synthesis, characterization and application of zinc-aluminum layered double hydroxide nano needles. Chemical Physics, 2020, 528, 110530.	1.9	16
63	Theoretical modelling of novel indandione-based donor molecules for organic solar cell applications. Journal of Physics and Chemistry of Solids, 2022, 162, 110508.	4.0	16
64	Doping of superalkali and superhalogen on graphene quantum dot surfaces to enhance nonlinear optical response: An efficient strategy for fabricating novel electro-optical materials. Journal of Physics and Chemistry of Solids, 2022, 169, 110859.	4.0	16
65	Synthesis and structural investigation of polyhedron Co3O4 nanoparticles: Catalytic application and as fuel additive. Materials Chemistry and Physics, 2018, 216, 82-92.	4.0	15
66	Morphologically controlled synthesis of ferric oxide nano/micro particles and their catalytic application in dry and wet media: a new approach. Chemistry Central Journal, 2017, 11, 49.	2.6	14
67	Bioactivity and DNA/BSA Interactions of Selenium Nâ€Heterocyclic Carbene Adducts. ChemistrySelect, 2020, 5, 10970-10981.	1.5	14
68	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
69	Structure–Property Relationship and Systematic Study of a Series of Terpyridine Based Nonlinear Optical Compounds: DFT Computation of Interactive Design. Journal of Cluster Science, 2019, 30, 45-51.	3.3	13
70	Synthesis and Characterization of Mg–Zn Bimetallic Nanoparticles: Selective Hydrogenation of p-Nitrophenol, Degradation of Reactive Carbon Black 5 and Fuel Additive. Journal of Inorganic and Organometallic Polymers and Materials, 2020, 30, 438-450.	3.7	13
71	Prediction of NLO response of substituted organoimido hexamolybedate: First theoretical framework based on p-anisidine adduct [Mo6O18(p-MeOC6H4N)]2 Materials Today Communications, 2021, 26, 101880.	1.9	13
72	Quantum design of transition metals decorated on boron phosphide inorganic nanocluster for Favipiravir adsorption: a possible treatment for COVID-19. New Journal of Chemistry, 2022, 46, 1720-1730.	2.8	13

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73	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
74	Synthesis, spectroscopic characterization, and computed optical analysis of green fluorescent cyclohexenone derivatives. Journal of Physical Organic Chemistry, 2016, 29, 152-160.	1.9	12
75	Synthesis of Self-Assembled Co3O4 Nanoparticles with Porous Sea Urchin-Like Morphology and their Catalytic and Electrochemical Applications. Australian Journal of Chemistry, 2017, 70, 908.	0.9	11
76	Synthesis of manganese–tin oxide microparticles by the solvothermal method and study of application as a catalyst and additive. Environmental Technology (United Kingdom), 2021, 42, 1187-1195.	2.2	11
77	Synthesis and characterization of polyaniline/nickel oxide composites for fuel additive and dyes reduction. Chemical Physics Letters, 2021, 776, 138713.	2.6	11
78	Electronic absorption spectra and nonlinear optical properties of ruthenium acetylide complexes: a DFT study toward the designing of new high NLO response compounds. Acta Chimica Slovenica, 2014, 61, 382-90.	0.6	11
79	Synthesis and structure of calcium-tin hybrid microparticles from egg shell and investigation of their thermal behavior and catalytic application. Chemical Physics, 2020, 530, 110613.	1.9	10
80	4-Nitrophenol imprinted core-shell poly(N-isopropylacrylamide-acrylic acid)/poly(acrylic acid) microgels loaded with cadmium nanoparticles: A novel catalyst. Materials Chemistry and Physics, 2021, 260, 124156.	4.0	10
81	Role of Terminal Positions of Aryl Ring Towards Second-Order Nonlinearity in Arylimido-Substituted Molybdates: An Interesting Quantum Study of Organic-Inorganic Hybrid Composites. Current Physical Chemistry, 2011, 1, 99-105.	0.2	10
82	Structural Properties and Nonlinear Optical Responses of Halogenated Compounds: A DFT Investigation on Molecular Modelling. Open Chemistry, 2018, 16, 978-985.	1.9	9
83	Investigation of catalytic and fuel additive applications of copper/copper(I) oxide/copper(II) oxide (Cu/CuO/Cu ₂ O) microspheres synthesized by hydrothermal method using sucrose as template. Materials Research Express, 2020, 7, 025036.	1.6	9
84	Synthesis and structural analysis of mesoporous magnesium hydroxide nanoparticles as efficient catalyst. Journal of the Chinese Chemical Society, 2018, 65, 1495-1503.	1.4	8
85	Template free synthesis of calcium-tin (CaSn3) bimetallic micro cubes: Characterization, catalytic activity, adsorption and additive properties. Chemical Physics Letters, 2020, 739, 136917.	2.6	8
86	Zirconium nanoparticles-poly (N-isopropylacrylamide-methacrylic acid) hybrid microgels decorated graphene sheets for catalytic reduction of organic pollutants. Chemical Physics Letters, 2021, 780, 138915.	2.6	8
87	The first morphologically controlled synthesis of a nanocomposite of graphene oxide with cobalt tin oxide nanoparticles. RSC Advances, 2018, 8, 36647-36661.	3.6	7
88	A Versatile Material: Perovskite Bismuth Ferrite Microparticles as a Potential Catalyst for Enhancing Fuel Efficiency and Degradation of Various Organic Dyes. Journal of Inorganic and Organometallic Polymers and Materials, 2020, 30, 3761-3770.	3.7	7
89	Synthesis of WSe2 Nanorods by Selenium Powder Precursor for Photocatalytic Application and Fuel Additive. Journal of Cluster Science, 2021, 32, 1061-1073.	3.3	6
90	Comparison of catalytic and fuel additive properties of bimetallic nanoparticles and its composite: FeMnO3 and PANI-FeMnO3. Materials Science in Semiconductor Processing, 2022, 144, 106630.	4.0	6

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91	The NLO properties of hybrid materials based on molybdate/hexamolybdate derivatives: A theoretical perspective for electro-optic modulation. Synthetic Metals, 2014, 198, 277-284.	3.9	5
92	First-Principle Study on the Effect of Pi-Spacers on Small Molecule Acceptors: Quantum Design of Organic Solar Cells and NLO Compounds. Journal of Cluster Science, 2017, 28, 2419-2431.	3.3	5
93	Phase diagram and surface adsorption behavior of benzyl dimethyl hexadecyl ammonium bromide in a binary surfactant-water system. Journal of Molecular Liquids, 2019, 285, 403-407.	4.9	5
94	Chromogenic and fluorogenic detection of copper ions in the solution and intracellular media. Journal of the Chinese Chemical Society, 2019, 66, 500-505.	1.4	5
95	High-throughput calculations and experimental insights towards the development of potent thiazoline based functional materials. Materials Today Communications, 2021, 27, 102485. A comparative DFT study on the mechanism of olefin epoxidation catalyzed by substituted binuclear	1.9	5
96	peroxotungstates ([SeO ₄ WO(O ₂) ₂ MO(O ₂) ₂₂₂) _{222<td>sup>â^'<td>sup>) Tj E</td></td>}	sup>â^' <td>sup>) Tj E</td>	sup>) Tj E
97	458-462. Synthesis of monetite micro particles from egg shell waste and study of its environmental applications: Fuel additive and catalyst. Chemical Physics Letters, 2020, 755, 137804.	2.6	4
98	Synthesis of needle like nano composite of rGO-Mn2O and their applications as photo-catalyst. Chemical Physics Letters, 2020, 757, 137874.	2.6	4
99	Structural Characterization, Synthesis and Application of Zincite Nanoparticles as Fuel Additive. Journal of Cluster Science, 2022, 33, 1165-1176.	3.3	3
100	UV-absorbing benzamide-based dendrimer precursors: synthesis, theoretical calculation, and spectroscopic characterization. New Journal of Chemistry, 2021, 46, 75-85.	2.8	3
101	Computationally assisted design and prediction of remarkably boosted NLO response of organoimido $\hat{a} \in s$ ubstituted hexamolybdates. Journal of Physical Organic Chemistry, 2022, 35, .	1.9	3
102	Role of capping agent in the synthesis of zinc–cobalt bimetallic nanoparticles and its application as catalyst and fuel additive. Applied Nanoscience (Switzerland), 2022, 12, 2169-2181.	3.1	2
103	Physicochemical insights into the rational designing of new acceptor molecules by donor bridge modifications for efficient solar cells: In silico chemistry. Journal of Physical Organic Chemistry, 0, , .	1.9	2
104	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
105	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
106	Synthesis and structure of calcium-tin hybrid microparticles from egg shell and investigation of their thermal behavior and catalytic application. , 2020, 530, 110613-110613.		1
107	Synthesis of Rod Like Chromium/Manganese Layer Double Hydroxide and Applications. Russian Journal of Physical Chemistry A, 2022, 96, 1215-1227.	0.6	1
108	Physicochemical insights and in silico designing of new fullerene-free acceptor molecules for highly efficient and stable organic solar cells. Journal of Physics and Chemistry of Solids, 2022, 169, 110842.	4.0	1

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109	Recent advances in morphologically controlled synthesis of graphene oxideâ€based nanocomposite as catalyst and fuel additive. Journal of Physical Organic Chemistry, 0, , .	1.9	0