

# Tariq Mahmood

## List of Publications by Year in descending order

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Version: 2024-02-01

210  
papers

4,938  
citations

94433

37  
h-index

149698

56  
g-index

213  
all docs

213  
docs citations

213  
times ranked

4177  
citing authors

| #  | ARTICLE   | IF  | CITATIONS |
|----|---|-----|-----------|
| 1  | An intelligent fault detection approach based on reinforcement learning system in wireless sensor network. <i>Journal of Supercomputing</i> , 2022, 78, 3646-3675.  | 3.6 | 29        |
| 2  | Remarkable nonlinear optical response of Mn@C20 (M = Na & K and n = 1-6); a DFT outcome. <i>Materials Science in Semiconductor Processing</i> , 2022, 138, 106269.  | 4.0 | 20        |
| 3  | Nano-porous C4N as a toxic pesticide's scavenger: A quantum chemical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 111, 108078.  | 2.4 | 24        |
| 4  | Effect of high pressure on structural, electrical, and optical properties of graphene-like zinc oxide (g-ZnO) structure. <i>Materials Science in Semiconductor Processing</i> , 2022, 142, 106465.                    | 4.0 | 6         |
| 5  | Breast lesions classifications of mammographic images using a deep convolutional neural network-based approach. <i>PLoS ONE</i> , 2022, 17, e0263126.   | 2.5 | 30        |
| 6  | Superalkali (Li2F, Li3F) doped Al12N12 electrides with enhanced static, dynamic nonlinear optical responses and refractive indices. <i>Materials Science in Semiconductor Processing</i> , 2022, 143, 106518.         | 4.0 | 23        |
| 7  | In memory of Professor Iain Wilkinson: cognitive and neuroimaging endophenotypes in a consanguineous schizophrenia multiplex family. <i>Psychological Medicine</i> , 2022, , 1-9.                                     | 4.5 | 1         |
| 8  | Association between the physical activity and metabolic syndrome in residents of a foot-hill area in India. <i>Diabetes and Metabolic Syndrome: Clinical Research and Reviews</i> , 2022, 16, 102471.                 | 3.6 | 1         |
| 9  | Sensing behaviour of monocyclic C18 and B9N9 analogues toward chemical warfare agents (CWAs); quantum chemical approach. <i>Surfaces and Interfaces</i> , 2022, 30, 101912.   | 3.0 | 13        |
| 10 | Olympicene as a high-performance sensor for lung irritants: A dispersion corrected DFT insight. <i>Materials Science in Semiconductor Processing</i> , 2022, 144, 106620.   | 4.0 | 17        |
| 11 | First-principles study for electrochemical sensing of neurotoxin hydrazine derivatives via h-g-C3N4 quantum dot. <i>Surfaces and Interfaces</i> , 2022, 30, 101913.   | 3.0 | 12        |
| 12 | DFT studies on electrochemical properties of halide ions doped GDY-28 nanoflake for Na-ion battery applications. <i>Materials Science in Semiconductor Processing</i> , 2022, 145, 106651.                            | 4.0 | 5         |
| 13 | Mixed superalkalis are a better choice than pure superalkalis for B <sub>12</sub> N <sub>12</sub> nanocages to design high-performance nonlinear optical materials. <i>Dalton Transactions</i> , 2022, 51, 8437-8453. | 3.3 | 10        |
| 14 | Static, dynamic nonlinear optical (NLO) response and electride characteristics of superalkalis doped star like C6S6Li6. <i>Surfaces and Interfaces</i> , 2022, 31, 102044.  | 3.0 | 9         |
| 15 | Electrochemical sensing of heptazine graphitic C3N4 quantum dot for chemical warfare agents; a quantum chemical approach. <i>Materials Science in Semiconductor Processing</i> , 2022, 148, 106753.                   | 4.0 | 18        |
| 16 | Ab initio study for superior sensitivity of graphyne nanoflake towards nitrogen halides over ammonia. <i>Journal of Molecular Modeling</i> , 2022, 28, .  | 1.8 | 5         |
| 17 | Benchmark Density Functional Theory Approach for the Calculation of Bond Dissociation Energies of the O <sub>2</sub> Bond: A Key Step in Water Splitting Reactions. <i>ACS Omega</i> , 2022, 7, 20800-20808.          | 3.5 | 9         |
| 18 | Aggregation induced emission based fluorenes as dual-channel fluorescent probes for rapid detection of cyanide: applications of smartphones and logic gates. <i>RSC Advances</i> , 2022, 12, 18897-18910.             | 3.6 | 10        |

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|----|---|-----|-----------|
| 19 | Superhalogen doping of aromatic heterocycles; effective approach for the enhancement of static and dynamic NLO response. <i>Vacuum</i> , 2022, 203, 111301.   | 3.5 | 4         |
| 20 | A Recessively Inherited Risk Locus on Chromosome 13q22-31 Conferring Susceptibility to Schizophrenia. <i>Schizophrenia Bulletin</i> , 2021, 47, 796-802.  | 4.3 | 3         |
| 21 | Fundus image-based cataract classification using a hybrid convolutional and recurrent neural network. <i>Visual Computer</i> , 2021, 37, 2407-2417.   | 3.5 | 27        |
| 22 | Electronic, optical and elastic properties of cubic zirconia (c-ZrO <sub>2</sub> ) under pressure: A DFT study. <i>Physica B: Condensed Matter</i> , 2021, 604, 412462.   | 2.7 | 12        |
| 23 | Surface functionalization of twisted graphene C <sub>32</sub> H <sub>15</sub> and C <sub>104</sub> H <sub>52</sub> derivatives with alkalis and superalkalis for NLO response; a DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107794.             | 2.4 | 34        |
| 24 | Silver cluster (Ag <sub>6</sub> ) decorated coronene as non-enzymatic sensor for glucose and H <sub>2</sub> O <sub>2</sub> . <i>Journal of Molecular Graphics and Modelling</i> , 2021, 103, 107824.  | 2.4 | 16        |
| 25 | Hybrid vector similarity measures based on complex hesitant fuzzy sets and their applications to pattern recognition and medical diagnosis. <i>Journal of Intelligent and Fuzzy Systems</i> , 2021, 40, 625-646.  | 1.4 | 37        |
| 26 | Remarkable static and dynamic NLO response of alkali and superalkali doped macrocyclic [hexa-]thiophene complexes; a DFT approach. <i>RSC Advances</i> , 2021, 11, 4118-4128.   | 3.6 | 35        |
| 27 | Alteration impact of electronic properties of c-SrTiO <sub>3</sub> on optical response due to Ca inclusion: A DFT study. <i>Physica B: Condensed Matter</i> , 2021, 602, 412553.  | 2.7 | 9         |
| 28 | Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake: a DFT study. <i>Journal of Molecular Modeling</i> , 2021, 27, 117.  | 1.8 | 26        |
| 29 | DFT studies of single and multiple alkali metals doped C <sub>24</sub> fullerene for electronics and nonlinear optical applications. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107867.  | 2.4 | 33        |
| 30 | Breast Mass Detection and Classification Using Deep Convolutional Neural Networks for Radiologist Diagnosis Assistance. , 2021, , .   |     | 9         |
| 31 | Computer Vision-Based Microcalcification Detection in Digital Mammograms Using Fully Connected Depthwise Separable Convolutional Neural Network. <i>Sensors</i> , 2021, 21, 4854.   | 3.8 | 26        |
| 32 | Electrochemical sensing behavior of graphdiyne nanoflake towards uric acid: a quantum chemical approach. <i>Journal of Molecular Modeling</i> , 2021, 27, 244.  | 1.8 | 4         |
| 33 | An Automated In-Depth Feature Learning Algorithm for Breast Abnormality Prognosis and Robust Characterization from Mammography Images Using Deep Transfer Learning. <i>Biology</i> , 2021, 10, 859.   | 2.8 | 29        |
| 34 | Impact of even number of alkaline earth metal doping on the NLO response of C <sub>20</sub> nanocluster; a DFT outcome. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113386.  | 2.5 | 16        |
| 35 | DFT based investigations of BAWO <sub>4</sub> : Electronic and optical properties. <i>Physica B: Condensed Matter</i> , 2021, 621, 413309.  | 2.7 | 9         |
| 36 | First example of lanthanum as dopant on Al <sub>12</sub> N <sub>12</sub> and Al <sub>12</sub> P <sub>12</sub> nanocages for improved electronic and nonlinear optical properties with high stability. <i>Materials Science in Semiconductor Processing</i> , 2021, 135, 106122. | 4.0 | 22        |

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|----|--|-----|-----------|
| 37 | Sensing of toxic Lewisite ( $L_{1}$ , $L_{2}$ , and $L_{3}$ ) molecules by graphdiyne nanoflake using density functional theory calculations and quantum theory of atoms in molecule analysis. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4181. | 1.9 | 18        |
| 38 | Demonstrating the Potential of Alkali Metal-Doped Cyclic $C_{6}O_{6}Li_{6}$ Organometallics as Electrides and High-Performance NLO Materials. <i>ACS Omega</i> , 2021, 6, 29852-29861.   | 3.5 | 26        |
| 39 | An Automatic Detection and Localization of Mammographic Microcalcifications ROI with Multi-Scale Features Using the Radiomics Analysis Approach. <i>Cancers</i> , 2021, 13, 5916.  | 3.7 | 9         |
| 40 | Natural and semisynthetic polymers blended orodispersible films of citalopram. <i>Natural Product Research</i> , 2020, 34, 16-25.  | 1.8 | 11        |
| 41 | Synthesis, crystal structures, computational studies and $\hat{I}\pm$ -amylase inhibition of three novel 1,3,4-oxadiazole derivatives. <i>Journal of Molecular Structure</i> , 2020, 1200, 127085.   | 3.6 | 33        |
| 42 | Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. <i>Optics and Laser Technology</i> , 2020, 122, 105855.   | 4.6 | 73        |
| 43 | Structural, spectroscopic and nonlinear optical properties of sulfonamide derivatives; experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2020, 1202, 127393.   | 3.6 | 22        |
| 44 | Benchmark approach to search of cost-effective and accurate density functional for homolytic cleavage of $C\text{---}Mg$ bond of Grignard reagent. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26106.                                      | 2.0 | 4         |
| 45 | Sentiment analysis on IMDB using lexicon and neural networks. <i>SN Applied Sciences</i> , 2020, 2, 1.   | 2.9 | 41        |
| 46 | Alkaline earth metal decorated phosphide nanoclusters for potential applications as high performance NLO materials; A first principle study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 118, 113906.                                 | 2.7 | 38        |
| 47 | Design of novel inorganic alkaline earth metal doped aluminum nitride complexes (AEM@Al <sub>12</sub> N <sub>12</sub> ) with high chemical stability, improved electronic properties and large nonlinear optical response. <i>Optik</i> , 2020, 207, 163792.   | 2.9 | 27        |
| 48 | Significant nonlinear optical response of alkaline earth metals doped beryllium and magnesium oxide nanocages. <i>Materials Chemistry and Physics</i> , 2020, 242, 122507.   | 4.0 | 44        |
| 49 | Permeation of second row neutral elements through Al <sub>12</sub> P <sub>12</sub> and B <sub>12</sub> P <sub>12</sub> nanocages; a first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 101, 107748.                            | 2.4 | 5         |
| 50 | Biomarkers in psychiatry: a clinician's viewpoint. <i>British Medical Bulletin</i> , 2020, 135, 23-27.   | 6.9 | 7         |
| 51 | Feature Selection Optimization in Software Product Lines. <i>IEEE Access</i> , 2020, 8, 160231-160250.   | 4.2 | 5         |
| 52 | A Brief Survey on Breast Cancer Diagnostic With Deep Learning Schemes Using Multi-Image Modalities. <i>IEEE Access</i> , 2020, 8, 165779-165809.   | 4.2 | 52        |
| 53 | Superhalogen doping: a new and effective approach to design materials with excellent static and dynamic NLO responses. <i>New Journal of Chemistry</i> , 2020, 44, 16358-16369.  | 2.8 | 35        |
| 54 | Energy routing algorithm based on OSPF protocol and virtual circuit switching mode in energy local area network. <i>International Journal of Computational Complexity and Intelligent Algorithms</i> , 2020, 1, 292.   | 0.2 | 1         |

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|----|---|-----|-----------|
| 55 | Synergic effect of pore size engineering and an applied electric field on the controlled permeation of alkali metal atoms and ions across pristine and defect-containing h-BN sheets. <i>New Journal of Chemistry</i> , 2020, 44, 7891-7901.  | 2.8 | 4         |
| 56 | Remarkable second and third order nonlinear optical properties of organometallic $C_{60}Li_6 \cdot M_3O$ electrides. <i>New Journal of Chemistry</i> , 2020, 44, 9822-9829.   | 2.8 | 43        |
| 57 | A computational insight of electronic and optical properties of Cd-doped BaZrO <sub>3</sub> . <i>Chinese Journal of Physics</i> , 2020, 66, 318-326.  | 3.9 | 15        |
| 58 | Outstanding NLO response of thermodynamically stable single and multiple alkaline earth metals doped C <sub>20</sub> fullerene. <i>Journal of Molecular Liquids</i> , 2020, 305, 112875.  | 4.9 | 43        |
| 59 | Theoretical study on novel superalkali doped graphdiyne complexes: Unique approach for the enhancement of electronic and nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107573.   | 2.4 | 68        |
| 60 | Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107569.   | 2.4 | 66        |
| 61 | High selectivity of cyclic tetrapyrrole over tetrafulan and tetrathiophene toward toxic chemicals; A first-principles study. <i>Microporous and Mesoporous Materials</i> , 2020, 299, 110126.   | 4.4 | 48        |
| 62 | Theoretical investigation on radical anion promoted electrocyclization in photochromes. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107550.  | 2.4 | 1         |
| 63 | Silver-graphene quantum dots based electrochemical sensor for trinitrotoluene and p-nitrophenol. <i>Journal of Molecular Liquids</i> , 2020, 306, 112878.   | 4.9 | 65        |
| 64 | Exceptionally high NLO response and deep ultraviolet transparency of superalkali doped macrocyclic oligofuran rings. <i>New Journal of Chemistry</i> , 2020, 44, 2609-2618.   | 2.8 | 58        |
| 65 | Studies on genetic divergence of rapeseed genotypes using SSR markers. <i>Pakistan Journal of Botany</i> , 2020, 52, .  | 0.5 | 3         |
| 66 | Introducing robustness in DBR routing protocol. <i>International Journal of Communication Networks and Distributed Systems</i> , 2020, 24, 316.   | 0.4 | 3         |
| 67 | Fabrication and <i>in vitro</i> characterization of fenofibric acid-loaded hyaluronic acid-polyethylene glycol polymeric composites with enhanced drug solubility and dissolution rate. <i>International Journal of Polymeric Materials and Polymeric Biomaterials</i> , 2019, 68, 510-515. | 3.4 | 14        |
| 68 | Synthesis of novel metal complexes of 2-((phenyl (2-(4-sulfophenyl) hydrazono) methyl) diazenyl) benzoic acid formazan dyes: Characterization, antimicrobial and optical properties studies on leather. <i>Journal of Molecular Structure</i> , 2019, 1175, 73-89.                          | 3.6 | 15        |
| 69 | Cellulosic and acrylic polymers based composites for controlled drug release. <i>Iranian Polymer Journal (English Edition)</i> , 2019, 28, 769-776.   | 2.4 | 2         |
| 70 | A comprehensive DFT study on the sensing abilities of cyclic oligothiophenes (n-CTs). <i>New Journal of Chemistry</i> , 2019, 43, 14120-14133.  | 2.8 | 45        |
| 71 | Role of Pyridine Nitrogen in Palladium-Catalyzed Imine Hydrolysis: A Case Study of (E)-1-(3-bromothiophen-2-yl)-N-(4-methylpyridin-2-yl)methanimine. <i>Molecules</i> , 2019, 24, 2609.   | 3.8 | 18        |
| 72 | Preparation and <i>in vitro</i> characterization of polyvinylpyrrolidone-ploxamer polymeric synergy for oral drug delivery. <i>Journal of Polymer Research</i> , 2019, 26, 1.   | 2.4 | 4         |

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|----|--|-----|-----------|
| 73 | Density functional theory study of structural, electronic and CO adsorption properties of anionic Scnâ” (nâ€=â€2â€13) clusters. Computational and Theoretical Chemistry, 2019, 1163, 112511.                                       | 2.5 | 8         |
| 74 | Theoretical study on design of novel superalkalis doped graphdiyne: A new donorâ€acceptor (D-Ï€-A) strategy for enhancing NLO response. Applied Surface Science, 2019, 492, 255-263.   | 6.1 | 66        |
| 75 | Highly selective acridinium based cyanine dyes for the detection of DNA base pairs (adenine, cytosine,) Tj ETQq1 1 0.784314 rgBT /Ov   | 2.5 | 78        |
| 76 | Cobalt Phosphide Ultrathin and Freestanding Sheets Prepared through Microwave Chemical Vapor Deposition: A Highly Efficient Oxygen Evolution Reaction Catalyst. ChemElectroChem, 2019, 6, 5469-5478.                               | 3.4 | 16        |
| 77 | An efficient and improved scheme for handwritten digit recognition based on convolutional neural network. SN Applied Sciences, 2019, 1, 1.   | 2.9 | 49        |
| 78 | Doping superalkali on Zn12O12 nanocage constitutes a superior approach to fabricate stable and high-performance nonlinear optical materials. Optics and Laser Technology, 2019, 120, 105753.                                       | 4.6 | 64        |
| 79 | Benchmark DFT studies on Câ€CN homolytic cleavage and screening the substitution effect on bond dissociation energy. Journal of Molecular Modeling, 2019, 25, 47.  | 1.8 | 18        |
| 80 | Extended Version of Linguistic Picture Fuzzy TOPSIS Method and Its Applications in Enterprise Resource Planning Systems. Mathematical Problems in Engineering, 2019, 2019, 1-8.  | 1.1 | 20        |
| 81 | Design, synthesis and anti-bacterial studies of piperazine derivatives against drug resistant bacteria. European Journal of Medicinal Chemistry, 2019, 166, 224-231.   | 5.5 | 31        |
| 82 | &lt;p&gt;Dexibuprofen amide derivatives as potential anticancer agents: synthesis, in silico docking, bioevaluation, and molecular dynamic simulation&lt;/p&gt;. Drug Design, Development and Therapy, 2019, Volume 13, 1643-1657. | 4.3 | 16        |
| 83 | Synthesis and Reactivities of Triphenyl Acetamide Analogs for Potential Nonlinear Optical Material Uses. Symmetry, 2019, 11, 622.  | 2.2 | 9         |
| 84 | Fuzzy hyperideals of hyperquantaes. Journal of Intelligent and Fuzzy Systems, 2019, 36, 5605-5615.   | 1.4 | 6         |
| 85 | Pythagorean cubic fuzzy aggregation information based on confidence levels and its application to multi-criteria decision making process. Journal of Intelligent and Fuzzy Systems, 2019, 36, 5669-5683.                           | 1.4 | 15        |
| 86 | Comparative investigation of sensor application of polypyrrole for gaseous analytes. Journal of Physical Organic Chemistry, 2019, 32, e3960.   | 1.9 | 39        |
| 87 | Synthesis, structural properties, DFT studies, antimicrobial activities and DNA binding interactions of two newly synthesized organotin(IV) carboxylates. Journal of Molecular Structure, 2019, 1191, 291-300.                     | 3.6 | 32        |
| 88 | Halides encapsulation in aluminum/boron phosphide nanoclusters: An effective strategy for high cell voltage in Na-ion battery. Materials Science in Semiconductor Processing, 2019, 97, 71-79.                                     | 4.0 | 26        |
| 89 | Theoretical study on a boron phosphide nanocage doped with superalkalis: novel electrides having significant nonlinear optical response. New Journal of Chemistry, 2019, 43, 5727-5736.  | 2.8 | 73        |
| 90 | Isolation, characterization and DFT studies of epoxy ring containing new withanolides from Withania coagulans Dunal. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 217, 113-121.                    | 3.9 | 6         |

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|-----|--|-----|-----------|
| 91  | Superalkalis as a source of diffuse excess electrons in newly designed inorganic electrides with remarkable nonlinear response and deep ultraviolet transparency: A DFT study. <i>Applied Surface Science</i> , 2019, 483, 1118-1128.  | 6.1 | 105       |
| 92  | A Novel UV-Spectrophotometric Method for Simultaneous Estimation of Amlodipine and Captopril. <i>Pharmaceutical Chemistry Journal</i> , 2019, 52, 952-958.   | 0.8 | 4         |
| 93  | Density functional theory-supported studies of structural and electronic properties of substituted-phenol derivatives synthesized by efficient O- or C-arylation via Chan-Lam or Suzuki cross-coupling reactions. <i>Turkish Journal of Chemistry</i> , 2019, 43, 1306-1321. | 1.2 | 4         |
| 94  | Spherical fuzzy sets and their applications in multi-attribute decision making problems. <i>Journal of Intelligent and Fuzzy Systems</i> , 2019, 36, 2829-2844.  | 1.4 | 246       |
| 95  | Assessment of mold and yeast in some bakery products of Lahore, Pakistan based on LM and SEM. <i>Microscopy Research and Technique</i> , 2019, 82, 85-91.  | 2.2 | 6         |
| 96  | Effect of magnesium on structural and optical properties of CaTiO <sub>3</sub> : A DFT study. <i>Physica B: Condensed Matter</i> , 2019, 568, 88-91.   | 2.7 | 19        |
| 97  | Design, synthesis and bioevaluation of tricyclic fused ring system as dual binding site acetylcholinesterase inhibitors. <i>Bioorganic Chemistry</i> , 2019, 83, 336-347.  | 4.1 | 72        |
| 98  | Numerical treatment for Darcy-Forchheimer flow of nanofluid due to a rotating disk with slip effects. <i>Canadian Journal of Physics</i> , 2019, 97, 856-863.  | 1.1 | 14        |
| 99  | Silymarin-laden PVP-PEG polymeric composite for enhanced aqueous solubility and dissolution rate: Preparation and in vitro characterization. <i>Journal of Pharmaceutical Analysis</i> , 2019, 9, 34-39.   | 5.3 | 43        |
| 100 | Isolation, spectroscopic and density functional theory of two withanolide glycosides. <i>Journal of Molecular Structure</i> , 2019, 1177, 449-456.   | 3.6 | 9         |
| 101 | A Comprehensive Survey on the Performance Analysis of Underwater Wireless Sensor Networks (UWSN) Routing Protocols. <i>International Journal of Advanced Computer Science and Applications</i> , 2019, 10, .   | 0.7 | 3         |
| 102 | Risk of psychosis in Yorkshire South Asians. <i>Journal of Psychiatric Intensive Care</i> , 2019, 15, 117-121.   | 0.6 | 4         |
| 103 | New Perspectives on the Efficacy of Gallic Acid in Cosmetics & Nanocosmeceuticals. <i>Current Pharmaceutical Design</i> , 2019, 24, 5181-5187.   | 1.9 | 48        |
| 104 | Impact of Magnetic Field and Second-Order Slip Flow of Casson Liquid with Heat Transfer Subject to Suction/Injection and Convective Boundary Condition. <i>Journal of Magnetism</i> , 2019, 24, 81-89.   | 0.4 | 13        |
| 105 | Study and Analysis of Delay Sensitive and Energy Efficient Routing Approach. <i>International Journal of Advanced Computer Science and Applications</i> , 2019, 10, .  | 0.7 | 1         |
| 106 | Comparative efficacy of two anti-aging products containing retinyl palmitate in healthy human volunteers. <i>Journal of Cosmetic Dermatology</i> , 2018, 17, 454-460.  | 1.6 | 4         |
| 107 | Palladium(0) catalyzed Suzuki cross-coupling reaction of 2,5-dibromo-3-methylthiophene: selectivity, characterization, DFT studies and their biological evaluations. <i>Chemistry Central Journal</i> , 2018, 12, 49.  | 2.6 | 18        |
| 108 | Visible light photocatalytic degradation of crystal violet dye and electrochemical detection of ascorbic acid & glucose using BaWO <sub>4</sub> nanorods. <i>Materials Research Bulletin</i> , 2018, 104, 38-43.   | 5.2 | 32        |

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|-----|---|-----|-----------|
| 109 | Copper-doped Al <sub>12</sub> N <sub>12</sub> nano-cages: potential candidates for nonlinear optical materials. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.  | 2.3 | 38        |
| 110 | High sensitivity of polypyrrole sensor for uric acid over urea, acetamide and sulfonamide: A density functional theory study. <i>Synthetic Metals</i> , 2018, 235, 49-60.   | 3.9 | 66        |
| 111 | Synthesis, crystal structures, computational studies and antimicrobial activity of new designed bis((5-aryl-1,3,4-oxadiazol-2-yl)thio)alkanes. <i>Journal of Molecular Structure</i> , 2018, 1155, 403-413.   | 3.6 | 31        |
| 112 | Impact of processing methods on the dissolution of artemether from two non-ordered mesoporous silicas. <i>European Journal of Pharmaceutical Sciences</i> , 2018, 112, 139-145.   | 4.0 | 13        |
| 113 | Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations. <i>Journal of Molecular Structure</i> , 2018, 1156, 193-200. | 3.6 | 20        |
| 114 | Influence of polymer ratio and surfactants on controlled drug release from cellulosic microsponges. <i>International Journal of Biological Macromolecules</i> , 2018, 109, 963-970.   | 7.5 | 40        |
| 115 | (M, N)-Double framed soft ideals of Abel Grassmann's groupoids. <i>Journal of Intelligent and Fuzzy Systems</i> , 2018, 35, 6313-6327.  | 1.4 | 2         |
| 116 | Synthesis of 3,4-Biaryl-2,5-Dichlorothiophene through Suzuki Cross-Coupling and Theoretical Exploration of Their Potential Applications as Nonlinear Optical Materials. <i>Symmetry</i> , 2018, 10, 766.  | 2.2 | 10        |
| 117 | Sensor applications of polypyrrole for oxynitrogen analytes: a DFT study. <i>Journal of Molecular Modeling</i> , 2018, 24, 308.   | 1.8 | 29        |
| 118 | First principles investigation of electronic and optical properties of AgAlO <sub>2</sub> . <i>Chinese Journal of Physics</i> , 2018, 56, 2186-2190.  | 3.9 | 8         |
| 119 | Theoretical insight into structural and electronic properties of cationic Sc <sup>n+</sup> (n=2-13): A benchmark study. <i>Solid State Sciences</i> , 2018, 86, 60-68.  | 3.2 | 3         |
| 120 | Detailed Mechanistic Study of Radical Mediated Chemoselective Phosphination of Aryl Halide. <i>ChemistrySelect</i> , 2018, 3, 11302-11308.  | 1.5 | 2         |
| 121 | Facile synthesis of N-(4-bromophenyl)-1-(3-bromothiophen-2-yl)methanimine derivatives via Suzuki cross-coupling reaction: their characterization and DFT studies. <i>Chemistry Central Journal</i> , 2018, 12, 84.  | 2.6 | 16        |
| 122 | Synthesis, quantum chemical, in vitro acetyl cholinesterase inhibition and molecular docking studies of four new coumarin based pyrazolylthiazole nuclei. <i>Journal of Molecular Structure</i> , 2018, 1168, 175-186.  | 3.6 | 17        |
| 123 | Accurate theoretical method for homolytic cleavage of C-Sn bond: A benchmark approach. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 134-144.  | 2.5 | 11        |
| 124 | Scorpion Venom Peptides as a Potential Source for Human Drug Candidates. <i>Protein and Peptide Letters</i> , 2018, 25, 702-708.  | 0.9 | 25        |
| 125 | Enhancing food security in arid areas of Pakistan through newly developed drought tolerant and short duration mustard ( <i>Brassica juncea</i> L.) Canola. <i>Genetika</i> , 2018, 50, 21-31.   | 0.4 | 6         |
| 126 | Multivariate analysis for adaptability and yield stability of rapeseed ( <i>Brassica napus</i> L.) strains in different agro-climatic zones. <i>Genetika</i> , 2018, 50, 369-378.   | 0.4 | 2         |



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|-----|--|-----|-----------|
| 127 | Selective arylation of phenol protected propargyl bromide via Pd-catalysed Suzuki coupling reaction: synthesis, mechanistic studies by DFT calculations and Their Pharmacological Aspects". <i>Acta Poloniae Pharmaceutica</i> , 2018, 75, 911-919.    | 0.1 | 2         |
| 128 | Benchmark study of structural and vibrational properties of scandium clusters. <i>Journal of Molecular Structure</i> , 2017, 1142, 139-147.  | 3.6 | 6         |
| 129 | Synthesis, molecular structure, quantum mechanical studies and urease inhibition assay of two new isatin derived sulfonylhydrazides. <i>Journal of Molecular Structure</i> , 2017, 1133, 80-89.  | 3.6 | 26        |
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