Asif Mahmood

List of Publications by Year
in descending order

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64 papers	3,898 citations	93792 39 h-index	139680 61 g-index
64 all docs	64 docs citations	64 times ranked	2903 citing authors

#	Article	IF	Citations
1	Non-fullerene acceptors with hetero-dihalogenated terminals induce significant difference in single crystallography and enable binary organic solar cells with 17.5% efficiency. Energy and Environmental Science, 2022, 15, 320-333.	15.6	95
2	Developing Efficient Small Molecule Acceptors with sp²â€Hybridized Nitrogen at Different Positions by Density Functional Theory Calculations, Molecular Dynamics Simulations and Machine Learning. Chemistry - A European Journal, 2022, 28, .	1.7	94
3	Machine learning and molecular dynamics simulation-assisted evolutionary design and discovery pipeline to screen efficient small molecule acceptors for PTB7-Th-based organic solar cells with over 15% efficiency. Journal of Materials Chemistry A, 2022, 10, 4170-4180.	5.2	124
4	Separation of Fe from wastewater and its use for NOx reduction; a sustainable approach for environmental remediation. Chemosphere, 2022, 303, 135103.	4.2	11
5	Machine Learning for Organic Photovoltaic Polymers: A Minireview. Chinese Journal of Polymer Science (English Edition), 2022, 40, 870-876.	2.0	77
6	Machine learning for high performance organic solar cells: current scenario and future prospects. Energy and Environmental Science, 2021, 14, 90-105.	15.6	207
7	A time and resource efficient machine learning assisted design of non-fullerene small molecule acceptors for P3HT-based organic solar cells and green solvent selection. Journal of Materials Chemistry A, 2021, 9, 15684-15695.	5.2	142
8	Selenium-containing two-dimensional conjugated fused-ring electron acceptors for enhanced crystal packing, charge transport, and photovoltaic performance. Journal of Materials Chemistry A, 2021, 9, 15665-15677.	5.2	18
9	Synergistic effect of the selenophene-containing central core and the regioisomeric monochlorinated terminals on the molecular packing, crystallinity, film morphology, and photovoltaic performance of selenophene-based nonfullerene acceptors. Journal of Materials Chemistry C, 2021, 9, 1923-1935.	2.7	21
10	A Synergistic Strategy of Manipulating the Number of Selenophene Units and Dissymmetric Central Core of Small Molecular Acceptors Enables Polymer Solar Cells with 17.5â€‰% Efficiency. Angewandte Chemie - International Edition, 2021, 60, 19241-19252.	7.2	129
11	A Synergistic Strategy of Manipulating the Number of Selenophene Units and Dissymmetric Central Core of Small Molecular Acceptors Enables Polymer Solar Cells with 17.5â€‰% Efficiency. Angewandte Chemie, 2021, 133, 19390-19401.	1.6	22
12	Twoâ€Dimensional Conjugated Benzo[1,2â€b:4,5â€bâ€²]diselenopheneâ€Based Copolymer Donor Enables Large Openâ€Circuit Voltage and High Efficiency in Selenopheneâ€based Organic Solar Cells. ChemSusChem, 2021, 14, 4454-4465.	3.6	10
13	Quantum chemical analysis and molecular dynamics simulations to study the impact of electron-deficient substituents on electronic behavior of small molecule acceptors. Computational and Theoretical Chemistry, 2021, 1204, 113387.	1.1	71
14	Machine learning-integrated omics for the risk and safety assessment of nanomaterials. Biomaterials Science, 2021, 9, 1598-1608.	2.6	44
15	A Review of Grazing Incidence Smallâ€and Wideâ€Angle Xâ€Ray Scattering Techniques for Exploring the Film Morphology of Organic Solar Cells. Solar Rrl, 2020, 4, 2000337.	3.1	112
16	Electronâ€Deficient and Quinoid Central Unit Engineering for Unfused Ringâ€Based A₁â€“Dâ€“A₂â€“Dâ€“A₁â€Type Acceptor Enables High Performance Nonfullerene Polymer Solar Cells with High V_{oc} and PCE Simultaneously. Small, 2020, 16, e1907681.	5.2	31
17	A bromine and chlorine concurrently functionalized end group for benzo[1,2-b:4,5-bâ€²]diselenophene-based non-fluorinated acceptors: a new hybrid strategy to balance the crystallinity and miscibility of blend films for enabling highly efficient polymer solar cells. Journal of Materials Chemistry A, 2020, 8, 4856-4867.	5.2	51
18	Computational analysis to understand the performance difference between two small-molecule acceptors differing in their terminal electron-deficient group. Journal of Computational Electronics, 2020, 19, 931-939.	1.3	73

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19	Effect of fluorination on exciton binding energy and electronic coupling in small molecule acceptors for organic solar cells. Computational and Theoretical Chemistry, 2020, 1179, 112797.	1.1	79
20	First-principles theoretical designing of planar non-fullerene small molecular acceptors for organic solar cells: manipulation of noncovalent interactions. Physical Chemistry Chemical Physics, 2019, 21, 2128-2139.	1.3	82
21	Experimental and theoretical study of planar small molecule acceptor for organic solar cells. Journal of Molecular Structure, 2019, 1196, 169-175.	1.8	24
22	Photovoltaic and Charge Transport Behavior of Diketopyrrolopyrrole Based Compounds with Aâ€“Dâ€“Aâ€“Dâ€“A Skeleton. Journal of Cluster Science, 2019, 30, 1123-1130.	1.7	80
23	pH-Dependent Antibiotic Gatifloxacin Interacting with Cationic Surfactant: Insights from Spectroscopic and Chromatographic Measurements. Journal of Solution Chemistry, 2019, 48, 936-948.	0.6	5
24	Impact of electronâ€withdrawing and electronâ€donating substituents on the electrochemical and charge transport properties of indacenodithiopheneâ€based small molecule acceptors for organic solar cells. Journal of Physical Organic Chemistry, 2019, 32, e3909.	0.9	35
25	Red shifting of absorption maxima of phenothiazine based dyes by incorporating electron-deficient thiadiazole derivatives as Ï€-spacer. Arabian Journal of Chemistry, 2019, 12, 1447-1453.	2.3	89
26	Quinoxaline-Containing Nonfullerene Small-Molecule Acceptors with a Linear A₂-A₁-D-A₁-A₂ Skeleton for Poly(3-hexylthiophene)-Based Organic Solar Cells. ACS Applied Materials & Interfaces, 2018, 10, 10254-10261.	4.0	60
27	Designing of Efficient Acceptors for Organic Solar Cells: Molecular Modelling at DFT Level. Journal of Cluster Science, 2018, 29, 359-365.	1.7	46
28	Theoretical and experimental study of electron-deficient core substitution effect of diketopyrrolopyrrole derivatives on optoelectrical and charge transport properties. Chemical Physics, 2018, 500, 67-73.	0.9	12
29	A novel thiazole based acceptor for fullerene-free organic solar cells. Dyes and Pigments, 2018, 149, 470-474.	2.0	81
30	Introducing Four 1,1-Dicyanomethylene-3-indanone End-Capped Groups as an Alternative Strategy for the Design of Small-Molecular Nonfullerene Acceptors. Journal of Physical Chemistry C, 2018, 122, 29122-29128.	1.5	79
31	Recent progress in porphyrin-based materials for organic solar cells. Journal of Materials Chemistry A, 2018, 6, 16769-16797.	5.2	215
32	Achievement of High V_{oc} of 1.02 V for P3HTâ€Based Organic Solar Cell Using a Benzotriazoleâ€Containing Nonâ€Fullerene Acceptor. Advanced Energy Materials, 2017, 7, 1602269.	10.2	191
33	Non-linear Optical Response of Triphenylamine Dyes with D-A-Ï€-A Structure. Asian Journal of Chemistry, 2016, 28, 1985-1988.	0.1	1
34	Synthesis, spectroscopic characterization, and computed optical analysis of green fluorescent cyclohexenone derivatives. Journal of Physical Organic Chemistry, 2016, 29, 152-160.	0.9	12
35	pH-dependent probing of levofloxacin assimilated in surfactant mediated assemblies: Insights from photoluminescent and chromatographic measurements. Journal of Molecular Liquids, 2016, 220, 26-32.	2.3	22
36	Effect of fluorination and symmetry on the properties of polymeric photovoltaic materials based on an asymmetric building block. RSC Advances, 2016, 6, 90051-90060.	1.7	23

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37	Triphenylamine based dyes for dye sensitized solar cells: A review. Solar Energy, 2016, 123, 127-144.	2.9	218
38	Optimization of Phospholipid Nanoparticle Formulations Using Response Surface Methodology. Journal of Surfactants and Detergents, 2016, 19, 67-74.	1.0	8
39	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.	0.5	54
40	Theoretical Investigation for Exploring the Antioxidant Potential of Chlorogenic Acid: A Density Functional Theory Study. International Journal of Food Properties, 2016, 19, 745-751.	1.3	41
41	Fluoro-silicon (FSi) interaction as a promising force for the formation of thermodynamically stabilized Brook-type silabenzene: A quantum chemical approach. Journal of Fluorine Chemistry, 2015, 176, 51-56.	0.9	1
42	Computational Designing of Triphenylamine Dyes with Broad and Redâ€shifted Absorption Spectra for Dyeâ€sensitized Solar Cells using Multiâ€Thiophene Rings in Ï€â€Spacer. Bulletin of the Korean Chemical Society, 2015, 36, 2615-2620.	1.0	77
43	Heterocyclic azo dyes for dye sensitized solar cells: A quantum chemical study. Computational and Theoretical Chemistry, 2015, 1066, 94-99.	1.1	64
44	Synthesis, structureâ€“activity relationship and molecular docking of cyclohexenone based analogous as potent non-nucleoside reverse-transcriptase inhibitors. Journal of Molecular Structure, 2015, 1086, 8-16.	1.8	22
45	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.	0.9	99
46	Spectral-luminescent properties of pH-sensitive azo fluorophore in complexes with quaternary ammonium disinfectants. Colloid and Polymer Science, 2015, 293, 3145-3156.	1.0	3
47	Solvent-Dependent Non-Linear Optical Properties of 5,5â€²-Disubstituted-2,2â€²-bipyridine Complexes of Ruthenium(II): A Quantum Chemical Perspective. Australian Journal of Chemistry, 2015, 68, 1502.	0.5	42
48	Recent research progress on quasi-solid-state electrolytes for dye-sensitized solar cells. Journal of Energy Chemistry, 2015, 24, 686-692.	7.1	59
49	Enhancement of nonlinear optical (NLO) properties of indigo through modification of auxiliary donor, donor and acceptor. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 139, 425-430.	2.0	87
50	Assessing the quantum mechanical level of theory for prediction of UV/Visible absorption spectra of some aminoazobenzene dyes. Journal of Saudi Chemical Society, 2015, 19, 436-441.	2.4	70
51	Utilization of electronâ€deficient thiadiazole derivatives as Ï€-spacer for the red shifting of absorption maxima of diarylamine-fluorene based dyes. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	43
52	Synthesis, characterization, theoretical, anti-bacterial and molecular docking studies of quinoline based chalcones as a DNA gyrase inhibitor. Bioorganic Chemistry, 2014, 54, 31-37.	2.0	79
53	Synthesis, characterization of novel cyclohexenone derivatives and computation of their optical response. Journal of Molecular Structure, 2014, 1071, 103-110.	1.8	12
54	Theoretical designing of novel heterocyclic azo dyes for dye sensitized solar cells. Journal of Computational Electronics, 2014, 13, 1033-1041.	1.3	77

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55	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.	1.1	42
56	Quantum Chemical Designing of Novel Organic Non-Linear Optical Compounds. Bulletin of the Korean Chemical Society, 2014, 35, 1391-1396.	1.0	73
57	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.	0.2	11
58	Theoretical investigation for the designing of novel antioxidants. Canadian Journal of Chemistry, 2013, 91, 126-130.	0.6	58
59	Solvent effects on nonlinear optical response of certain tetramminеruthenium(II) complexes of modified 1,10-phenanthrolines. Canadian Journal of Chemistry, 2013, 91, 1303-1309.	0.6	37
60	Quantum Chemical Designing of Efficient TC4-Based Sensitizers by Modification of Auxiliary Donor and Ï€-Spacer. Bulletin of the Chemical Society of Japan, 2013, 86, 1272-1281.	2.0	30
61	Quantum Chemical Designing of Efficient Sensitizers for Dye Sensitized Solar Cells. Bulletin of the Korean Chemical Society, 2013, 34, 2093-2098.	1.0	41
62	DFT for exploring the antioxidant potential of homogentisic and orsellinic acids. Pakistan Journal of Pharmaceutical Sciences, 2013, 26, 1209-14.	0.2	4
63	Optimized biodiesel production and environmental assessment of produced biodiesel. Biotechnology and Bioprocess Engineering, 2012, 17, 617-623.	1.4	31
64	A Comparative Study on the Physicochemical Parameters of Milk Samples Collected from Buffalo, Cow, Goat and Sheep of Gujrat, Pakistan. Pakistan Journal of Nutrition, 2010, 9, 1192-1197.	0.2	47