

Rahim Ghadari

List of Publications by Year in descending order

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72
papers

1,310
citations

304743
22
h-index

395702
33
g-index

81
all docs

81
docs citations

81
times ranked

1456
citing authors

#	ARTICLE	IF	CITATIONS
1	Heteroatom engineering on spiro-type hole transporting materials for perovskite solar cells. Journal of Energy Chemistry, 2022, 67, 19-26.	12.9	22
2	The strategy for high-efficiency hole conductors by engineering short-range intramolecular interactions. Dyes and Pigments, 2022, 197, 109889.	3.7	6
3	Effect of the substitution position and extending the conjugation in naphthalene-triphenylamine hole transport materials for perovskite solar cells. Synthetic Metals, 2022, 284, 116990.	3.9	4
4	Multifunctional organic semiconductor for dopant-free perovskite solar cells. Synthetic Metals, 2022, 285, 117027.	3.9	4
5	Modulated bonding interaction in propanediol electrolytes toward stable aqueous zinc-ion batteries. Science China Materials, 2022, 65, 1156-1164.	6.3	37
6	Isomeric D-A- π -D Dopant-Free Hole Transport Materials: Effect of the Substitution Position and Heteroatom on the Performance of Perovskite Solar Cells. ChemistrySelect, 2022, 7, .	1.5	2
7	Pyridine-triphenylamine hole transport material for inverted perovskite solar cells. Journal of Energy Chemistry, 2021, 54, 395-402.	12.9	30
8	A computational study on the interactions between a layered imine-based COF structure and selected anticancer drugs. Journal of Molecular Modeling, 2021, 27, 44.	1.8	8
9	Hole transporting material with passivating group (C N) for perovskite solar cells with improved stability. Dyes and Pigments, 2021, 187, 109129.	3.7	17
10	Tetraphenylethylene-Arylamine Derivatives as Hole Transporting Materials for Perovskite Solar Cells. ACS Applied Materials & Interfaces, 2021, 13, 12322-12330.	8.0	21
11	Heteroatom effect on linear-shaped dopant-free hole transporting materials for perovskite solar cells. Solar Energy, 2021, 221, 323-331.	6.1	18
12	Molecular tailor-making of zinc phthalocyanines as dopant-free hole-transporting materials for efficient and stable perovskite solar cells. Journal of Power Sources, 2021, 505, 230095.	7.8	6
13	Effect of COF Presence on DNA Molecular Interactions: A QM/MM and MD Simulations Study. ChemistrySelect, 2021, 6, 9541-9551.	1.5	3
14	C N-based carbazole-arylamine hole transporting materials for perovskite solar cells: Substitution position matters. Journal of Energy Chemistry, 2021, 62, 563-571.	12.9	25
15	Plasmon-enhanced dye-sensitized solar cells through porphyrin-silver nanoparticle hybrid structures: Experimental and computational studies. Journal of Power Sources, 2021, 511, 230407.	7.8	6
16	The Design of Temperature and pH-Responsive Drug Delivery System Based on Cellulose and Aminated Cellulose by Computational and Experimental Methods. Journal of Computational Biophysics and Chemistry, 2021, 20, 189-200.	1.7	1
17	Dopant-free benzothiadiazole bridged hole transport materials for highly stable and efficient perovskite solar cells. Dyes and Pigments, 2020, 173, 107954.	3.7	19
18	Benzothiadiazole-based hole transport materials for high-efficiency dopant-free perovskite solar cells: Molecular planarity effect. Journal of Energy Chemistry, 2020, 44, 115-120.	12.9	23

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19	Two-dimensional triphenylene cored hole-transporting materials for efficient perovskite solar cells. Chemical Communications, 2020, 56, 1879-1882.	4.1	25
20	Introducing ammonium salt into hole transporting materials for perovskite solar cells. Chemical Communications, 2020, 56, 14471-14474.	4.1	14
21	Comparative Study of Linear and Starburst Ethane-Based Hole-Transporting Materials for Perovskite Solar Cells. Journal of Physical Chemistry C, 2020, 124, 2886-2894.	3.1	16
22	Phthalocyanine-silver nanoparticle structures for plasmon-enhanced dye-sensitized solar cells. Solar Energy, 2020, 198, 283-294.	6.1	24
23	Fused tetraphenylethylene-triphenylamine as an efficient hole transporting material in perovskite solar cells. Chemical Communications, 2020, 56, 3159-3162.	4.1	35
24	Enhanced phthalocyanine-sensitized solar cell efficiency via cooperation of nitrogen-doped carbon dots. Journal of Cleaner Production, 2020, 268, 122236.	9.3	19
25	Rhodanine-Furan Bis-Heterocyclic Frameworks Synthesis via Green One-Pot Sequential Six-Component Reactions: A Synthetic and Computational Study. ChemistrySelect, 2019, 4, 11893-11898.	1.5	20
26	In silico study on core-shell pseudodendrimeric glycoside structures in drug delivery related usages. Polyhedron, 2019, 160, 10-19.	2.2	3
27	Exploration of the Binding Properties of the Azo Dye Pollutants with Nitrogen-Doped Graphene Oxide by Computational Modeling for Wastewater Treatment Improvement. ChemistrySelect, 2019, 4, 5968-5978.	1.5	3
28	Facile synthesis of simple arylamine-substituted naphthalene derivatives as hole-transporting materials for efficient and stable perovskite solar cells. Journal of Power Sources, 2019, 425, 87-93.	7.8	26
29	Amino Acid Functionalized Single-Wall Carbon Nanotubes in Thermoresponsive Drug Delivery Systems: A Computational Study. ChemistrySelect, 2019, 4, 1516-1524.	1.5	5
30	Simply designed nonspiro fluorene-based hole-transporting materials for high performance perovskite solar cells. Synthetic Metals, 2019, 250, 42-48.	3.9	11
31	Computational DFT study on nickel symmetric bis(thiosemicarbazone) complexes: Electronic absorption and redox potentials. Polyhedron, 2019, 160, 35-41.	2.2	7
32	Synthesis, spectroscopic characterization, and DFT studies of 1,2,3-triazole-based organosilicon compounds. Journal of Molecular Structure, 2018, 1167, 200-208.	3.6	3
33	The inhibitory effect of farnesiferol C against catalase; Kinetics, interaction mechanism and molecular docking simulation. International Journal of Biological Macromolecules, 2018, 113, 1258-1265.	7.5	32
34	Synthesis of graphene oxide supported copper-cobalt ferrite material functionalized by arginine amino acid as a new high-performance catalyst. Applied Organometallic Chemistry, 2018, 32, e3965.	3.5	22
35	Highly efficient ruthenium complexes with acetyl electron-acceptor unit for dye sensitized solar cells. Journal of Power Sources, 2018, 396, 559-565.	7.8	23
36	A Computational Study on the Blocking Ability of Selected Commercially Available Anticancer Drugs and Their Hypothetic Derivatives on the CCR5. Assay and Drug Development Technologies, 2018, 16, 266-277.	1.2	2

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37	MD simulation studies on the effect of the temperature and protonation state on the imide-linked amino acid-based dendrimers. <i>Computational Materials Science</i> , 2018, 151, 124-131.	3.0	5
38	Ruthenium complexes as sensitizers with phenyl-based bipyridine anchoring ligands for efficient dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2018, 6, 9445-9452.	5.5	23
39	Synthesis and experimental/theoretical evaluations on redox potentials and electronic absorption spectra for copper symmetric bis(thiosemicarbazone) complexes. <i>Polyhedron</i> , 2018, 151, 221-232.	2.2	4
40	Nitrogen doped nanographene structures; study on the adsorption of nucleobases, nucleotides, and their triphosphate derivatives using mixed docking, MD, and QM/MM approaches. <i>Journal of Chemical Physics</i> , 2017, 146, 044105.	3.0	4
41	Unravelling the structural-electronic impact of arylamine electron-donating antennas on the performances of efficient ruthenium sensitizers for dye-sensitized solar cells. <i>Journal of Power Sources</i> , 2017, 346, 71-79.	7.8	26
42	Insight into Electron-Donating Ancillary Ligands in Ruthenium Terpyridyl Complexes Configuration on Performances of Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8752-8759.	3.1	9
43	Studies to reveal the nature of interactions between catalase and curcumin using computational methods and optical techniques. <i>International Journal of Biological Macromolecules</i> , 2017, 95, 550-556.	7.5	35
44	Thiophene- π -Arylamine Hole-Transporting Materials in Perovskite Solar Cells: Substitution Position Effect. <i>Energy Technology</i> , 2017, 5, 1788-1794.	3.8	44
45	Nickel- π -substituted cobalt ferrite nanoparticles supported on arginine- π -modified graphene oxide nanosheets: Synthesis and catalytic activity. <i>Applied Organometallic Chemistry</i> , 2017, 31, e3859.	3.5	6
46	A computational study on the usability of amino acid-functionalised nitrogen-doped graphene oxides as temperature-responsive drug delivery systems. <i>International Journal of Hyperthermia</i> , 2017, 33, 1-11.	2.5	3
47	Ferrocene based nonlinear optical chromophores: synthesis, characterization and study of optical properties. <i>Journal of Molecular Liquids</i> , 2017, 244, 322-329.	4.9	37
48	Design, synthesis and characterization of ferrocene based V-shaped chromophores with modified nonlinear effect. <i>Journal of Organometallic Chemistry</i> , 2017, 846, 397-406.	1.8	23
49	Anthracene- π -arylamine hole transporting materials for perovskite solar cells. <i>Chemical Communications</i> , 2017, 53, 9558-9561.	4.1	45
50	The role of human CYP2C8 in the metabolizing of montelukast-like compounds: a computational study. <i>Research on Chemical Intermediates</i> , 2017, 43, 4781-4794.	2.7	0
51	Destructive effect of non-enzymatic glycation on catalase and remediation via curcumin. <i>Archives of Biochemistry and Biophysics</i> , 2017, 630, 81-90.	3.0	27
52	Exploration of the binding properties of the human serum albumin sites with neurology drugs by docking and molecular dynamics simulation. <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 19-35.	2.2	5
53	In silico study to evaluate the governing criteria in the BF ₃ catalyzed Diels-Alder reaction. <i>Computational and Theoretical Chemistry</i> , 2016, 1091, 176-185.	2.5	1
54	A study on the interactions of amino acids with nitrogen doped graphene; docking, MD simulation, and QM/MM studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4352-4361.	2.8	17

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55	Synthesis, characterization, and electronic properties of novel Fc-DCM conjugated system; experimental and computational studies. <i>Journal of Organometallic Chemistry</i> , 2016, 811, 14-19.	1.8	22
56	Evaluation of the effect of the chiral centers of Taxol on binding to β -tubulin: A docking and molecular dynamics simulation study. <i>Computational Biology and Chemistry</i> , 2015, 56, 33-40.	2.3	12
57	Synthesis of a New Library of Pyrano-phenazine Derivatives via a Novel Three-Component Protocol. <i>Helvetica Chimica Acta</i> , 2014, 97, 228-236.	1.6	12
58	A computational study on the mechanism and the transition states of the cyclization of 1-trifluoromethyl-1,3-dicarbonyl compounds with azides to form 1,2,3-triazoles. <i>Computational and Theoretical Chemistry</i> , 2014, 1043, 64-70.	2.5	4
59	On-water-organic synthesis: l-proline catalyzed synthesis of pyrimidine-2,4-dione-, benzo[g]- and dihydropyrano[2,3-g]chromene derivatives in aqueous media. <i>Journal of the Iranian Chemical Society</i> , 2013, 10, 307-317.	2.2	14
60	A facile three- and four-component procedure toward the synthesis of functionalized pyrano- and benzo[f]quinoxaline derivatives. <i>Molecular Diversity</i> , 2012, 16, 453-461.	3.9	7
61	An in silico study on the ring-size effect in ring enlargement Bellus-Claisen rearrangement. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 25-30.	2.5	5
62	Investigation of origin of stereo-selectivity of $\text{BF}_3 \cdot \text{Et}_2\text{O}$ -promoted allylboration of aldehydes in the presence of (R)-pinanediol by computational method. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 28-33.	2.5	3
63	An unexpected route toward the synthesis of spiro-benzo[b]acridine-furan derivatives. <i>Tetrahedron Letters</i> , 2012, 53, 4018-4021.	1.4	18
64	A density functional theory approach toward substituent effect in Meerwein-Eschenmoser-Claisen rearrangement. <i>Journal of Molecular Modeling</i> , 2012, 18, 319-328.	1.8	3
65	An environmentally benign approach for the synthesis of bifunctional sulfonamide-amide compounds via isocyanide-based multicomponent reactions. <i>Green Chemistry</i> , 2011, 13, 582.	9.0	42
66	Pyridine-Functionalized MCM-41 as an Efficient and Recoverable Catalyst for the Synthesis of Pyran Annulated Heterocyclic Systems. <i>Chemical and Pharmaceutical Bulletin</i> , 2010, 58, 270-272.	1.3	16
67	Investigation of substituent effect on the Johnson-Claisen rearrangement: A DFT approach. <i>Computational and Theoretical Chemistry</i> , 2010, 961, 83-87.	1.5	6
68	Unexpected Knoevenagel self-condensation reaction of tetronic acid: synthesis of a new class of organic heterocyclic salts. <i>Tetrahedron</i> , 2010, 66, 1911-1914.	1.9	16
69	Direct Sulfonation of Methane to Methanesulfonic Acid. <i>Industrial & Engineering Chemistry Research</i> , 2010, 49, 7685-7686.	3.7	3
70	Coumarin synthesis via Knoevenagel condensation reaction in 1,1,3,3-tetramethylguanidinium trifluoroacetate ionic liquid. <i>Journal of the Iranian Chemical Society</i> , 2009, 6, 710-714.	2.2	50
71	Synthesis of Highly Functionalized Bis(4-h-chromene) and 4-Benzo[g]chromene Derivatives via an Isocyanide-Based Pseudo-Five-Component Reaction. <i>Journal of Organic Chemistry</i> , 2009, 74, 4372-4374.	3.2	112
72	Novel One-Pot Three- and Pseudo-Five-Component Reactions: Synthesis of Functionalized Benzo[g]- and Dihydropyrano[2,3-g]chromene Derivatives. <i>ACS Combinatorial Science</i> , 2009, 11, 956-959.	3.3	109