

Fu-Quan Bai

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198
papers

3,319
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204
ext. papers

3,964
ext. citations

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avg, IF

5.58
L-index

#	Paper	IF	Citations
198	Atomic Modulation of FeCo/Nitrogen-Carbon Bifunctional Oxygen Electrodes for Rechargeable and Flexible All-Solid-State Zinc-Air Battery. <i>Advanced Energy Materials</i> , 2017 , 7, 1602420	21.8	505
197	Hole Trapping by Iodine Interstitial Defects Decreases Free Carrier Losses in Perovskite Solar Cells: A Time-Domain Ab Initio Study. <i>ACS Energy Letters</i> , 2017 , 2, 1270-1278	20.1	114
196	Dimension-Matched Zinc Phthalocyanine/BiVO Ultrathin Nanocomposites for CO Reduction as Efficient Wide-Visible-Light-Driven Photocatalysts via a Cascade Charge Transfer. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 10873-10878	16.4	112
195	Quaternary ammonium hydroxide as a metal-free and halogen-free catalyst for the synthesis of cyclic carbonates from epoxides and carbon dioxide. <i>Catalysis Science and Technology</i> , 2015 , 5, 2314-2321	5.5	94
194	On the viability of cyclometalated Ru(II) complexes as dyes in DSSC regulated by COOH group, a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 2206-13	3.6	62
193	Solution-Processable Multiarmed Organic Molecules Containing Triphenylamine and DCM Moieties: Synthesis and Photovoltaic Properties. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 2636-2642	3.8	62
192	What Makes Hydroxamate a Promising Anchoring Group in Dye-Sensitized Solar Cells? Insights from Theoretical Investigation. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3992-9	6.4	58
191	Theoretical studies on spectroscopic properties of ruthenium sensitizers absorbed to TiO ₂ film surface with connection mode for DSSC. <i>Dyes and Pigments</i> , 2012 , 94, 459-468	4.6	56
190	Heterostructured Co ₃ O ₄ /PEI/CNTs composite: fabrication, characterization and CO gas sensors at room temperature. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 4558-4565	13	47
189	Enamine-Metal Lewis Acid Bifunctional Catalysis: Application to Direct Asymmetric Aldol Reaction of Ketones. <i>European Journal of Organic Chemistry</i> , 2009 , 2009, 4581-4585	3.2	46
188	White-Light-Emitting Materials and Highly Sensitive Detection of Fe ³⁺ and Polychlorinated Benzenes Based on Ln-Metal-Organic Frameworks. <i>Crystal Growth and Design</i> , 2018 , 18, 5353-5364	3.5	45
187	Theoretical investigation of triphenylamine-based sensitizers with different β spacers for DSSC. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 118, 1144-51	4.4	42
186	New organically templated chained and layered iodoplumbates. <i>CrystEngComm</i> , 2012 , 14, 4000	3.3	42
185	Theoretical studies of electronic and optical properties of the triphenylamine-based organic dyes with diketopyrrolopyrrole chromophore. <i>Dyes and Pigments</i> , 2015 , 113, 87-95	4.6	41
184	Planar amine-based dye features the rigidified O-bridged dithiophene β spacer: A potential high-efficiency sensitizer for dye-sensitized solar cells application. <i>Journal of Power Sources</i> , 2015 , 275, 207-216	8.9	39
183	Fine-tuning β spacer for high efficiency performance DSSC: A theoretical exploration with D β based organic dye. <i>Dyes and Pigments</i> , 2017 , 141, 251-261	4.6	37
182	Energy Platform for Directed Charge Transfer in the Cascade Z-Scheme Heterojunction: CO Photoreduction without a Cocatalyst. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 20906-20914	16.4	37

181	New photoluminescence acylhydrazidate-coordinated complexes. <i>Dalton Transactions</i> , 2012 , 41, 2382-924.3	4.3	35
180	Efficient blue-emitting Ir(III) complexes with phosphine carbanion-based ancillary ligand: a DFT study. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 11689-95	2.8	34
179	Stimuli-Responsive Luminescent Properties of Tetraphenylethene-Based Strontium and Cobalt Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 19716-19721	16.4	34
178	Theoretical investigation and design of high-efficiency dithiafulvenyl-based sensitizers for dye-sensitized solar cells: the impacts of elongating π spacers and rigidifying dithiophene. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 9458-68	3.6	33
177	Design of DAA organic dyes with different acceptor and auxiliary acceptor for highly efficient dye-sensitized solar cells: a computational study. <i>RSC Advances</i> , 2014 , 4, 50338-50350	3.7	32
176	Metal-Organic Frameworks Harness Cu Chelating and Photooxidation Against Amyloid β Aggregation in Vivo. <i>Chemistry - A European Journal</i> , 2019 , 25, 3489-3495	4.8	32
175	Dimension-Matched Zinc Phthalocyanine/BiVO ₄ Ultrathin Nanocomposites for CO ₂ Reduction as Efficient Wide-Visible-Light-Driven Photocatalysts via a Cascade Charge Transfer. <i>Angewandte Chemie</i> , 2019 , 131, 10989-10994	3.6	31
174	Anionic ancillary ligands in cyclometalated Ru(II) complex sensitizers improve photovoltaic efficiency of dye-sensitized solar cells: insights from theoretical investigations. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 15567-15577	13	29
173	Theoretical study and design of highly efficient platinum(II) complexes bearing tetradentate ligands for OLED. <i>RSC Advances</i> , 2016 , 6, 11648-11656	3.7	28
172	DFT and TD-DFT study on the electronic structures and phosphorescent properties of 6-phenyl-2,2'Pbipyridine tridentate iridium(III) complexes and their isomer. <i>Dalton Transactions</i> , 2012 , 41, 8441-6	4.3	28
171	Theoretical understanding of ruthenium(II) based fluoride sensor derived from 4,5-bis(benzimidazol-2-yl)imidazole (H3ImBzim) and bipyridine: electronic structure and binding nature. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 1985-91	2.8	28
170	Design of new benzothiadiazole-based linear and star molecules with different functional groups as solar cells materials: A theoretical approach. <i>Solar Energy Materials and Solar Cells</i> , 2011 , 95, 1800-1810	6.4	28
169	Promising pyridinium ylide based anchors towards high-efficiency dyes for dye-sensitized solar cells applications: Insights from theoretical investigations. <i>Electrochimica Acta</i> , 2018 , 283, 1798-1805	6.7	27
168	Crystal phase effect of iron oxides on the aerobic oxidative coupling of alcohols and amines under mild conditions: A combined experimental and theoretical study. <i>Journal of Catalysis</i> , 2019 , 377, 145-152	7.3	27
167	Comprehensive Investigation into Luminescent Properties of Ir(III) Complexes: An Integrated Computational Study of Radiative and Nonradiative Decay Processes. <i>Inorganic Chemistry</i> , 2018 , 57, 6561-6570	5.1	27
166	Theoretical research on the effect of regulated π conjugation on the photophysical properties of Ir(III) complexes. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 10014-21	3.6	26
165	New monoacylhydrazidate-coordinated Mn ²⁺ and Pb ²⁺ compounds. <i>Dalton Transactions</i> , 2012 , 41, 6137-447	4.7	25
164	Theoretical and experimental study on intramolecular charge-transfer in symmetric bi-1,3,4-oxadiazole derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015 , 312, 20-27	4.7	24

163	Theoretical studies on the spectroscopic properties of porphyrin derivatives for dye-sensitized solar cell application. <i>RSC Advances</i> , 2015 , 5, 33653-33665	3.7	24
162	Electronic structures and optical properties of neutral substituted fluorene-based cyclometalated platinum(II) π -acetylide complexes: A DFT exploration. <i>Journal of Organometallic Chemistry</i> , 2009 , 694, 1848-1860	2.3	24
161	Theoretical investigations on the unsymmetrical effect of π -link Zn-porphyrin sensitizers on the performance for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 3741-3751	3.6	23
160	Theoretical investigation of the adsorption, IR, and electron injection of hydroxamate anchor at the TiO ₂ anatase (1 0 1) surface. <i>RSC Advances</i> , 2014 , 4, 19690-19693	3.7	23
159	Synthesis, structural characterization and photoluminescence property of three Zn(2+)/Mn(2+)-acylhydrazidate complexes and two acylhydrazide molecules. <i>Dalton Transactions</i> , 2013 , 42, 16547-55	4.3	23
158	New Cd ²⁺ , Pb ²⁺ complexes with acylhydrazidate molecules from in situ acylation reactions. <i>Dalton Transactions</i> , 2013 , 42, 8771-80	4.3	23
157	The influence of an inner electric field on the performance of three types of Zn-porphyrin sensitizers in dye sensitized solar cells: a theoretical study. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 10130-10145	7.1	23
156	A highly selective fluorescent probe for cyanide ion and its detection mechanism from theoretical calculations. <i>Talanta</i> , 2018 , 185, 1-6	6.2	22
155	Theoretical study on the reaction mechanism of the thermal - isomerization of fluorine-substituted azobenzene derivatives.. <i>RSC Advances</i> , 2018 , 8, 11580-11588	3.7	22
154	Discovering the intermediate of dye regeneration in dye-sensitized solar cells: Theoretical investigations on the interaction between organic dye with different donors and . <i>Dyes and Pigments</i> , 2015 , 120, 74-84	4.6	21
153	Theoretical investigation on the photophysical properties of N-heterocyclic carbene iridium (III) complexes (fpmb)(x)Ir(bptz)(3-x) (x = 1-2). <i>Journal of Computational Chemistry</i> , 2012 , 33, 1038-46	3.5	21
152	Electron-withdrawing functional ligand promotes CO ₂ reduction catalysis in single atom catalyst. <i>Science China Chemistry</i> , 2020 , 63, 1727-1733	7.9	20
151	The influence of a dye/TiO ₂ interface on DSSC performance: a theoretical exploration with a ruthenium dye. <i>RSC Advances</i> , 2016 , 6, 81976-81982	3.7	20
150	Theoretical studies on structures and spectroscopic properties of cyclometalated gold(III) complexes. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 9396-403	2.8	20
149	Controllable molecular aggregation and fluorescence properties of 1,3,4-oxadiazole derivatives. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 11681-11688	7.1	19
148	Theoretical study on a series of iridium complexes with low efficiency roll-off property. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 134, 406-12	4.4	19
147	Oxalate-extended Cd ²⁺ π -acylhydrazidate coordination polymers: synthesis, structure and fluorescence property. <i>CrystEngComm</i> , 2013 , 15, 5919	3.3	19
146	Synthesis, structural characterization and photoluminescence property of four di(mono)acylhydrazidate-coordinated Cd ²⁺ and Zn ²⁺ compounds. <i>CrystEngComm</i> , 2012 , 14, 8162	3.3	19

145	DFT/TDDFT investigation of the electronic structures and optoelectronic properties of phosphorescent iridium (III) complexes with non-conjugated cyclometalated carbene ligands. <i>Molecular Physics</i> , 2011 , 109, 1657-1675	1.7	19
144	Effect of different topological structures (D- π D and D- π A- π D) on the optoelectronic properties of benzo[2,1-B:3,4-B']dithiophene based donor molecules toward organic solar cells. <i>Solar Energy</i> , 2019 , 186, 311-322	6.8	18
143	DFT/TD-DFT calculations on the sensing mechanism of a dual response near-infrared fluorescent chemosensor for superoxide anion and hydrogen polysulfides: photoinduced electron transfer. <i>RSC Advances</i> , 2016 , 6, 104735-104741	3.7	18
142	Theoretical description of dye regeneration on the TiO ₂ /dye/electrolyte model. <i>Computational Materials Science</i> , 2016 , 111, 239-246	3.2	18
141	Connection style and spectroscopic properties: Theoretical understanding of the interface between N749 and TiO ₂ in DSSCs. <i>Dyes and Pigments</i> , 2013 , 99, 201-208	4.6	17
140	New Mixed-C ^N Ligand Tris-Cyclometalated Ir(III) Complexes for Highly-Efficient Green Organic Light-Emitting Diodes with Low Efficiency Roll-Off. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 4614-4621	2.3	17
139	Theoretical investigation on the effect of ancillary ligand modification for highly efficient phosphorescent platinum(II) complex design. <i>RSC Advances</i> , 2017 , 7, 17368-17376	3.7	16
138	Molecular design of organic dyes with diketopyrrolopyrrole for dye-sensitized solar cell: A theoretical approach. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 560-567	2.1	15
137	New Zn ²⁺ coordination polymers constructed from acylhydrazidate molecules: synthesis and structural characterization. <i>Dalton Transactions</i> , 2014 , 43, 15617-27	4.3	15
136	Charge transport properties in organic D-A mixed-stack complexes based on corannulene and sumanene derivatives-a theoretical study. <i>Organic Electronics</i> , 2019 , 68, 35-44	3.5	14
135	How does graphene enhance the photoelectric conversion efficiency of dye sensitized solar cells? An insight from a theoretical perspective. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 2730-2740	13	14
134	Theoretical study on a high-efficient porphyrin-sensitizer in a local electric field: How does the local electric field affects the performance of dye-sensitized solar cells?. <i>Organic Electronics</i> , 2015 , 26, 164-173	3.5	14
133	Analysis of ethyl and methyl centralite vibrational spectra for mapping organic gunshot residues. <i>Analyst, The</i> , 2014 , 139, 4270-8	5	14
132	Excited states of a significantly ruffled porphyrin: computational study on structure-induced rapid decay mechanism via intersystem crossing. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 4184-94	2.8	14
131	An efficient fluorescent sensor for redox active species based on novel poly(aryl ether) containing electroactive pendant. <i>Journal of Materials Chemistry</i> , 2012 , 22, 3028		14
130	Density functional study on the effect of substituent group for the monomer of donor-acceptor copolymer. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2010 , 48, 2099-2107	2.6	14
129	Insights into the photocatalytic mechanism of the C ₄ N/MoS ₂ heterostructure: A first-principle study. <i>Chinese Chemical Letters</i> , 2020 , 31, 2319-2324	8.1	14
128	Performance Regulation of Thieno[3,2-b]benzothiophene π -Spacer-Based D- π A Organic Dyes for Dye-Sensitized Solar Cell Applications: Insights From Computational Study. <i>Frontiers in Chemistry</i> , 2018 , 6, 676	5	13

127	Disentangling the role of oxygen vacancies on the surface of Fe ₃ O ₄ and Fe ₂ O ₃ . <i>Inorganic Chemistry Frontiers</i> , 2019 , 6, 2660-2666	6.8	13
126	Theoretical study on thermal cis-to-trans isomerization of BF ₂ -coordinated azo compounds of the para-substitution with electron donating groups. <i>Dyes and Pigments</i> , 2016 , 129, 100-108	4.6	13
125	The theoretical study of substituent and charge effects in the conformational transformation process of molecular machine unit spiropyran. <i>Organic Electronics</i> , 2017 , 45, 33-41	3.5	12
124	A novel T-CN and seawater desalination. <i>Nanoscale</i> , 2020 , 12, 5055-5066	7.7	12
123	The effect of the embedded o-carborane ligand on the photophysical properties of a cyclometalated Pt(II) complex: a theoretical investigation. <i>Inorganic Chemistry Frontiers</i> , 2018 , 5, 1016-1025	6.8	12
122	First-principles investigation on the interfacial interaction and electronic structure of BiVO ₄ /WO ₃ heterostructure semiconductor material. <i>Applied Surface Science</i> , 2021 , 549, 149309	6.7	12
121	How the substituents in corannulene and sumanene derivatives alter their molecular assemblings and charge transport properties?—A theoretical study with a dimer model. <i>Journal of Computational Chemistry</i> , 2016 , 37, 813-24	3.5	12
120	Water-soluble fluorescent probe for multiple ions detection based on different pH moderation. <i>Organic Electronics</i> , 2019 , 70, 186-192	3.5	11
119	Theoretical studies of heteroatom-doping in TiO ₂ to enhance the electron injection in dye-sensitized solar cells. <i>RSC Advances</i> , 2015 , 5, 79868-79873	3.7	11
118	Theoretical studies on the interaction of ruthenium sensitizers and redox couple in different deprotonation situations. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 2244-52	2.8	11
117	Direct evidence for the effect of lateral hydrogen bonding on the smectic phase. <i>Liquid Crystals</i> , 2011 , 38, 767-774	2.3	11
116	An efficient proline-based homogeneous organocatalyst with recyclability. <i>New Journal of Chemistry</i> , 2018 , 42, 827-831	3.6	11
115	Influence of one-dimensional TiO ₂ nanotube on interfacial electron transfer in dye-sensitized solar cells: Insights from theoretical investigation. <i>Solar Energy</i> , 2018 , 176, 545-555	6.8	11
114	A complete evaluation from theoretical aspect on the phosphorescent efficiency improvement through ancillary ligands modifications of a blue Ir(III) complex. <i>Organic Electronics</i> , 2018 , 59, 293-300	3.5	11
113	A Computational Way To Achieve More Effective Candidates for Photodynamic Therapy. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 1089-1100	6.1	10
112	Role of Intermolecular Interactions in Molecular Packing of Alkoxy-Substituted Bis-1,3,4-oxadiazole Derivatives. <i>Crystal Growth and Design</i> , 2019 , 19, 6100-6113	3.5	10
111	The effect of molecular structure on intramolecular charge-transfer in 1,3,4-oxadiazole derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019 , 377, 309-317	4.7	10
110	Theoretical investigation on excited-state cyclization reactions of platinum-sensitized dithienylethene complexes. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 2819-28	2.8	10

109	Theoretical investigation on a series of novel S,S-dioxide diarylethenes with abnormal photochromic properties and design of new dyads. <i>New Journal of Chemistry</i> , 2015 , 39, 1634-1642	3.6	10
108	Arranging strategies for A-site cations: impact on the stability and carrier migration of hybrid perovskite materials. <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 1741-1749	6.8	10
107	Theoretical design of porphyrin sensitizers with different acceptors for application in dye-sensitized solar cells.. <i>RSC Advances</i> , 2018 , 8, 19804-19810	3.7	10
106	Iron oxides with a reverse spinel structure: impact of active sites on molecule adsorption. <i>Inorganic Chemistry Frontiers</i> , 2019 , 6, 2810-2816	6.8	10
105	Reaction-based fluorescent probe for differential detection of cyanide and bisulfite in the aqueous media. <i>Journal of Luminescence</i> , 2019 , 215, 116620	3.8	10
104	Bifunctional Phase-Transfer Catalysts Catalyzed Diastereo- and Enantioselective Aza-Henry Reaction of α,β -Unsaturated Nitroalkenes With Amidosulfones. <i>Advanced Synthesis and Catalysis</i> , 2017 , 359, 4111-4116	5.6	10
103	The impact of molecular stacking interactions on the electronic structure and charge transport properties in distyrylbenzene (DSB-) based D π A complexes: a theoretical study. <i>RSC Advances</i> , 2015 , 5, 47681-47691	3.7	10
102	Dihydrogen bond in C ₂ H ₄ h Cl _n NaH (n = 0, 1, 2, 3) complexes: ab initio, AIM and NBO studies. <i>Molecular Physics</i> , 2011 , 109, 645-653	1.7	10
101	Self-Adaptive Single-Atom Catalyst Boosting Selective Ferroptosis in Tumor Cells.. <i>ACS Nano</i> , 2022 ,	16.7	10
100	Regulating ancillary ligands of Ru(II) complexes with square-planar quadridentate ligands for more efficient sensitizers in dye-sensitized solar cells: insights from theoretical investigations. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 29591-29599	3.6	9
99	CASSCF/CASPT2 calculation of the low-lying electronic states of the CH ₃ Se neutral radical and its cation. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 7173-8	2.8	9
98	Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021 , 43, 128079	2.9	9
97	Theoretical investigation of N ₂ -coordinated Pt(II) and Pd(II) complexes for long-lived two-photon photodynamic therapy. <i>Dyes and Pigments</i> , 2017 , 142, 55-61	4.6	8
96	Study on the spectral complementary composite dye molecules designed for high performance dye-sensitized solar cells: A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2019 , 1154, 44-49	2	8
95	Theoretical study on organic dyes with tunable π spacers for dye-sensitized solar cells: Inspired by the organic polymer photovoltaics. <i>Chemical Physics Letters</i> , 2019 , 719, 39-44	2.5	8
94	Intrinsic quantum efficiency enhancement in well-known Ir(III) complexes by virtue of a simple and controllable deuteration strategy. <i>Materials Chemistry Frontiers</i> , 2018 , 2, 1215-1224	7.8	8
93	A series of pure orange-yellow iridium complexes with low efficiency roll-off: A computational study. <i>Chemical Research in Chinese Universities</i> , 2016 , 32, 451-454	2.2	8
92	Theoretical investigation on the spectroscopic properties of Zn porphyrin and Zn tetrapyrin. <i>Synthetic Metals</i> , 2016 , 213, 18-24	3.6	8

91	Theoretical study on fluorescent probes for cyanide based on the indolium functional group. <i>Organic Electronics</i> , 2016 , 30, 1-11	3.5	8
90	The phosphorescence properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization. <i>Organic Chemistry Frontiers</i> , 2017 , 4, 2191-2201	5.2	8
89	Theoretical study on the excited state decay properties of iron(ii) polypyridine complexes substituted by bromine and chlorine.. <i>RSC Advances</i> , 2019 , 9, 31621-31627	3.7	8
88	Theoretical Study on the Photoinduced Electron Transfer Mechanisms of Different Peroxynitrite Probes. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 217-223	2.8	8
87	Highly Conductive Alkaline-Earth Metal Electrodes: The Possibility of Maintaining Both Low Work Function and Surface Stability for Organic Electronics. <i>Advanced Optical Materials</i> , 2020 , 8, 2000206	8.1	7
86	Strategies on Cyclometalating Ligand Substitution of Several Ir(III) Complexes: Theoretical Investigation of Different Molecular Behaviors. <i>Organometallics</i> , 2018 , 37, 2491-2499	3.8	7
85	Efficiency difference between furan- and thiophene-based D-EA dyes in DSSCs explained by theoretical calculations.. <i>RSC Advances</i> , 2018 , 8, 29917-29923	3.7	7
84	Theoretical study on molecular packing and electronic structure of bi-1,3,4-oxadiazole derivatives. <i>RSC Advances</i> , 2014 , 4, 51942-51949	3.7	7
83	Experimental and theoretical study on molecular aggregation and its effect on the photo-physical properties of the mesogenic bi-1,3,4-thiadiazole derivative. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 9697-705	3.6	7
82	A DFT exploration of luminescent rhenium(I) tricarbonyl diimine complex with a triarylboron moiety and its F derivative. <i>Journal of Organometallic Chemistry</i> , 2011 , 696, 2943-2948	2.3	7
81	Stimuli-Responsive Luminescent Properties of Tetraphenylethene-Based Strontium and Cobalt Metal-Organic Frameworks. <i>Angewandte Chemie</i> , 2020 , 132, 19884-19889	3.6	7
80	Polymorphism dependent charge transport property of 9,10-bis((E)-2-(pyrid-2-yl)vinyl)anthracene: a theoretical study. <i>RSC Advances</i> , 2015 , 5, 18875-18880	3.7	6
79	Theoretical design of porphyrin dyes with electron-deficit heterocycles towards near-IR light sensitization in dye-sensitized solar cells. <i>Solar Energy</i> , 2019 , 188, 742-749	6.8	6
78	Theoretical study on the electronic structures and properties of diindolocarbazole isomers. <i>Journal of Physical Organic Chemistry</i> , 2014 , 27, 973-980	2.1	6
77	Enhancing Electron Injection in Dye-Sensitized Solar Cells by Adopting W6+-Doped TiO ₂ Nanowires: A Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2015 , 2015, 5563-5570	2.3	6
76	Computational studies on the spectroscopic properties of the 2-pyridylpyrazolate-based platinum(II) complexes with modified pyrazolate fragment. <i>International Journal of Quantum Chemistry</i> , 2009 , 109, 308-319	2.1	6
75	Theoretical studies on the structures and spectroscopic properties of rhenium(I) acetylide diimine complexes. <i>Computational and Theoretical Chemistry</i> , 2008 , 855, 52-63		6
74	Constructing High Efficiency CoZn Mn O Electrocatalyst by Regulating the Electronic Structure and Surface Reconstruction.. <i>Small</i> , 2022 , e2107268	11	6

73	Water-soluble fluorescent probe for simultaneous detection of cyanide, hypochlorite and bisulfite at different emission wavelengths. <i>Analytical Biochemistry</i> , 2020 , 591, 113539	3.1	6
72	DFT and TD-DFT study a series of blue and green iridium complexes with mesityl-phenyl-imidazole ligand. <i>Organic Electronics</i> , 2019 , 64, 181-187	3.5	6
71	Density functional theory investigation on iridium(III) complexes for efficient blue electrophosphorescence.. <i>RSC Advances</i> , 2018 , 8, 19437-19448	3.7	6
70	In Situ Fabrication of Cuprous Selenide Electrode via Selenization of Copper Current Collector for High-Efficiency Potassium-Ion and Sodium-Ion Storage.. <i>Advanced Science</i> , 2021 , e2104630	13.6	6
69	Theoretical study on the influence of electric field direction on the photovoltaic performance of aryl amine organic dyes for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2019 , 43, 651-661	3.6	5
68	Understanding the Diverse Coordination Modes of Thiocyanate Anion on Solid Surfaces. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 9282-9291	3.8	5
67	Novel sky blue heteroleptic iridium(III) complexes with finely-optimized emission spectra for highly efficient organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 5579-5583	7.1	5
66	The induced current strengths and aromatic pathways of heteroporphyrins and their antiaromatic derivatives. <i>International Journal of Quantum Chemistry</i> , 2015 , 115, 983-988	2.1	5
65	Accurate simulation of geometry, singlet-singlet and triplet-singlet excitation of cyclometalated iridium(III) complex. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2108	2	5
64	Theoretical studies on structural and spectroscopic properties of photoelectrochemical cell ruthenium sensitizers, derivatives of AR20. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 891-901	2.1	5
63	TD-DFT investigation of electronic structures, photophysical properties and the theoretical design of OLEDs based on phosphorescent Ir(III) complexes bearing the non- π -electron-conjugated carbene ligand. <i>Molecular Physics</i> , 2012 , 110, 185-197	1.7	5
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