Fu-Quan Bai

List of Publications by Year in Descending Order

198 papers	3,319 citations	28 h-index	47 g-index
204 ext. papers	3,964 ext. citations	4.6 avg, IF	5.58 L-index

#	Paper	IF	Citations
198	Investigation of the adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug-delivery carrier: a DFT study.. *RSC Advances*, **2022**, 12, 2873-2887	3.7	5
197	Constructing High Efficiency CoZn Mn O Electrocatalyst by Regulating the Electronic Structure and Surface Reconstruction.. *Small*, **2022**, e2107268	11	6
196	Self-Adaptive Single-Atom Catalyst Boosting Selective Ferroptosis in Tumor Cells.. *ACS Nano*, **2022**,	16.7	10
195	Neutral Pt(II) complexes containing diazafluorene derivative ligands and their electroluminescent properties. *Inorganic Chemistry Communication*, **2022**, 137, 109170	3.1	0
194	Pressure-Induced Restricting Intermolecular Vibration of a Herringbone Dimer for Significantly Enhanced Multicolor Emission in Rotor-Free Truxene Crystals.. *Journal of Physical Chemistry Letters*, **2022**, 2493-2499	6.4	2
193	Refine the evaluation of photophysical properties of organometallic chromophores under confined molecular crystal conditions.. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2022**, 275, 121168	4.4	
192	B N counterpart of biphenylene network: A theoretical investigation. *Applied Surface Science*, **2022**, 598, 153674	6.7	0
191	Accurate Analysis of Anisotropic Carrier Mobility and Structure-property Relationships in Organic BOXD Crystalline Materials. *Frontiers in Chemistry*, **2021**, 9, 775747	5	1
190	Computational insight into newly anomalous delayed fluorescence emitters based on D-A-A structures. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 250, 119392	4.4	
189	First-principles investigation on the interfacial interaction and electronic structure of BiVO4/WO3 heterostructure semiconductor material. *Applied Surface Science*, **2021**, 549, 149309	6.7	12
188	Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies. *Bioorganic and Medicinal Chemistry Letters*, **2021**, 43, 128079	2.9	9
187	Theoretical Investigation of Perylene Diimide derivatives as Acceptors to Match with Benzodithiophene based Donors for Organic Photovoltaic Devices. *Zeitschrift Fur Physikalische Chemie*, **2021**, 235, 427-449	3.1	4
186	Computational Studies on the Materials Combining Graphene Quantum Dots and Pt Complexes with Adjustable Luminescence Characteristics. *Inorganic Chemistry*, **2021**, 60, 1480-1490	5.1	4
185	Theoretical study on the molecular stacking interactions and charge transport properties of triazasumanene crystals - from explanation to prediction. *Physical Chemistry Chemical Physics*, **2021**, 23, 4681-4689	3.6	3
184	Investigating phosphorescence capability of halogen-substituted metal-free organic molecules: A theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 255, 119642	4.4	1
183	Energy Platform for Directed Charge Transfer in the Cascade Z-Scheme Heterojunction: CO2 Photoreduction without a Cocatalyst. *Angewandte Chemie*, **2021**, 133, 21074-21082	3.6	4
182	Energy Platform for Directed Charge Transfer in the Cascade Z-Scheme Heterojunction: CO Photoreduction without a Cocatalyst. *Angewandte Chemie - International Edition*, **2021**, 60, 20906-20914	16.4	37

181	In Situ Fabrication of Cuprous Selenide Electrode via Selenization of Copper Current Collector for High-Efficiency Potassium-Ion and Sodium-Ion Storage.. *Advanced Science*, **2021**, e2104630	13.6	6
180	Electron-withdrawing functional ligand promotes CO2 reduction catalysis in single atom catalyst. *Science China Chemistry*, **2020**, 63, 1727-1733	7.9	20
179	Highly Conductive Alkaline-Earth Metal Electrodes: The Possibility of Maintaining Both Low Work Function and Surface Stability for Organic Electronics. *Advanced Optical Materials*, **2020**, 8, 2000206	8.1	7
178	Arranging strategies for A-site cations: impact on the stability and carrier migration of hybrid perovskite materials. *Inorganic Chemistry Frontiers*, **2020**, 7, 1741-1749	6.8	10
177	A novel T-CN and seawater desalination. *Nanoscale*, **2020**, 12, 5055-5066	7.7	12
176	Probing the effect of substituent groups in Ir(III) bis-tridentate complexes during deep-blue phosphorescent illuminating. *Organic Electronics*, **2020**, 84, 105803	3.5	1
175	How does the porphyrin-like vacancy affect the spectral properties of graphene quantum dots? A theoretical study. *Journal of Physics Condensed Matter*, **2020**, 32, 155902	1.8	3
174	Water-soluble fluorescent probe for simultaneous detection of cyanide, hypochlorite and bisulfite at different emission wavelengths. *Analytical Biochemistry*, **2020**, 591, 113539	3.1	6
173	Stimuli-Responsive Luminescent Properties of Tetraphenylethene-Based Strontium and Cobalt Metal□Organic Frameworks. *Angewandte Chemie*, **2020**, 132, 19884-19889	3.6	7
172	Insights into the photocatalytic mechanism of the C4N/MoS2 heterostructure: A first-principle study. *Chinese Chemical Letters*, **2020**, 31, 2319-2324	8.1	14
171	Interesting spin state properties of iron(II) polypyridine complex substituted by fluorine: A theoretical study. *Organic Electronics*, **2020**, 85, 105884	3.5	0
170	Stability, Aromaticity, and Photophysical Behaviors of Macrocyclic Molecules: A Theoretical Analysis. *Frontiers in Chemistry*, **2020**, 8, 776	5	1
169	Stimuli-Responsive Luminescent Properties of Tetraphenylethene-Based Strontium and Cobalt Metal-Organic Frameworks. *Angewandte Chemie - International Edition*, **2020**, 59, 19716-19721	16.4	34
168	Role of Intermolecular Interactions in Molecular Packing of Alkoxy-Substituted Bis-1,3,4-oxadiazole Derivatives. *Crystal Growth and Design*, **2019**, 19, 6100-6113	3.5	10
167	Concentration-induced structural diversity and catalytic activity of BF3/n-BuOH complexes for n-decene polymerization. *Chinese Journal of Chemical Engineering*, **2019**, 27, 2687-2695	3.2	
166	Theoretical study on the influence of electric field direction on the photovoltaic performance of aryl amine organic dyes for dye-sensitized solar cells. *New Journal of Chemistry*, **2019**, 43, 651-661	3.6	5
165	Charge transport properties in organic D-A mixed-stack complexes based on corannulene and sumanene derivatives-a theoretical study. *Organic Electronics*, **2019**, 68, 35-44	3.5	14
164	How does graphene enhance the photoelectric conversion efficiency of dye sensitized solar cells? An insight from a theoretical perspective. *Journal of Materials Chemistry A*, **2019**, 7, 2730-2740	13	14

163	Dimension-Matched Zinc Phthalocyanine/BiVO4 Ultrathin Nanocomposites for CO2 Reduction as Efficient Wide-Visible-Light-Driven Photocatalysts via a Cascade Charge Transfer. *Angewandte Chemie*, **2019**, 131, 10989-10994	3.6	31
162	Disentangling the role of oxygen vacancies on the surface of Fe3O4 and Fe2O3. *Inorganic Chemistry Frontiers*, **2019**, 6, 2660-2666	6.8	13
161	Dimension-Matched Zinc Phthalocyanine/BiVO Ultrathin Nanocomposites for CO Reduction as Efficient Wide-Visible-Light-Driven Photocatalysts via a Cascade Charge Transfer. *Angewandte Chemie - International Edition*, **2019**, 58, 10873-10878	16.4	112
160	Effect of different topological structures (D-D and D-A-D) on the optoelectronic properties of benzo[2,1-B:3,4-B]dithiophene based donor molecules toward organic solar cells. *Solar Energy*, **2019**, 186, 311-322	6.8	18
159	Theoretical investigations of the aromaticity, stability and photophysical behaviors for expanded porphyrins. *Chemical Physics Letters*, **2019**, 728, 25-31	2.5	3
158	Water-soluble fluorescent probe for multiple ions detection based on different pH moderation. *Organic Electronics*, **2019**, 70, 186-192	3.5	11
157	Understanding the Diverse Coordination Modes of Thiocyanate Anion on Solid Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 9282-9291	3.8	5
156	Study on the spectral complementary composite dye molecules designed for high performance dye-sensitized solar cells: A theoretical investigation. *Computational and Theoretical Chemistry*, **2019**, 1154, 44-49	2	8
155	The effect of molecular structure on intramolecular charge-transfer in 1,3,4-oxadiazole derivatives. *Journal of Photochemistry and Photobiology A: Chemistry*, **2019**, 377, 309-317	4.7	10
154	Novel sky blue heteroleptic iridium(III) complexes with finely-optimized emission spectra for highly efficient organic light-emitting diodes. *Journal of Materials Chemistry C*, **2019**, 7, 5579-5583	7.1	5
153	Theoretical study on organic dyes with tunable spacers for dye-sensitized solar cells: Inspired by the organic polymer photovoltaics. *Chemical Physics Letters*, **2019**, 719, 39-44	2.5	8
152	Iron oxides with a reverse spinel structure: impact of active sites on molecule adsorption. *Inorganic Chemistry Frontiers*, **2019**, 6, 2810-2816	6.8	10
151	Reaction-based fluorescent probe for differential detection of cyanide and bisulfite in the aqueous media. *Journal of Luminescence*, **2019**, 215, 116620	3.8	10
150	Innentitelbild: Dimension-Matched Zinc Phthalocyanine/BiVO4 Ultrathin Nanocomposites for CO2 Reduction as Efficient Wide-Visible-Light-Driven Photocatalysts via a Cascade Charge Transfer (Angew. Chem. 32/2019). *Angewandte Chemie*, **2019**, 131, 10878-10878	3.6	
149	Crystal phase effect of iron oxides on the aerobic oxidative coupling of alcohols and amines under mild conditions: A combined experimental and theoretical study. *Journal of Catalysis*, **2019**, 377, 145-152	7.3	27
148	Theoretical design of porphyrin dyes with electron-deficit heterocycles towards near-IR light sensitization in dye-sensitized solar cells. *Solar Energy*, **2019**, 188, 742-749	6.8	6
147	Proline-derived Monodentate Organocatalyst for Asymmetric Reduction of Imine with HSiCl3. *ChemistrySelect*, **2019**, 4, 9590-9594	1.8	2
146	Theoretical study on the excited state decay properties of iron(ii) polypyridine complexes substituted by bromine and chlorine.. *RSC Advances*, **2019**, 9, 31621-31627	3.7	8

145	Metal-Organic Frameworks Harness Cu Chelating and Photooxidation Against Amyloid Aggregation in Vivo. *Chemistry - A European Journal*, **2019**, 25, 3489-3495	4.8	32
144	DFT and TD-DFT study a series of blue and green iridium complexes with mesityl-phenyl-imidazole ligand. *Organic Electronics*, **2019**, 64, 181-187	3.5	6
143	DFT and TD-DFT study of iridium complexes with low-color-temperature and low-efficiency roll-off properties. *Applied Organometallic Chemistry*, **2019**, 33, e4563	3.1	4
142	Performance Regulation of Thieno[3,2-b]benzothiophene Spacer-Based D-A Organic Dyes for Dye-Sensitized Solar Cell Applications: Insights From Computational Study. *Frontiers in Chemistry*, **2018**, 6, 676	5	13
141	The effect of the embedded o-carborane ligand on the photophysical properties of a cyclometalated Pt(II) complex: a theoretical investigation. *Inorganic Chemistry Frontiers*, **2018**, 5, 1016-1025	6.8	12
140	A highly selective fluorescent probe for cyanide ion and its detection mechanism from theoretical calculations. *Talanta*, **2018**, 185, 1-6	6.2	22
139	Intrinsic quantum efficiency enhancement in well-known Ir(III) complexes by virtue of a simple and controllable deuteriation strategy. *Materials Chemistry Frontiers*, **2018**, 2, 1215-1224	7.8	8
138	Theoretical investigations on the unsymmetrical effect of -link Zn-porphyrin sensitizers on the performance for dye-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2018**, 20, 3741-3751	3.6	23
137	Influences of donor/acceptor ratio on the optical and electrical properties of the D/A alternating model oligomers: A density functional theory study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 199, 260-270	4.4	
136	Theoretical study on the reaction mechanism of the thermal - isomerization of fluorine-substituted azobenzene derivatives.. *RSC Advances*, **2018**, 8, 11580-11588	3.7	22
135	Promising pyridinium ylide based anchors towards high-efficiency dyes for dye-sensitized solar cells applications: Insights from theoretical investigations. *Electrochimica Acta*, **2018**, 283, 1798-1805	6.7	27
134	Strategies on Cyclometalating Ligand Substitution of Several Ir(III) Complexes: Theoretical Investigation of Different Molecular Behaviors. *Organometallics*, **2018**, 37, 2491-2499	3.8	7
133	Efficiency difference between furan- and thiophene-based D-A dyes in DSSCs explained by theoretical calculations.. *RSC Advances*, **2018**, 8, 29917-29923	3.7	7
132	White-Light-Emitting Materials and Highly Sensitive Detection of Fe3+ and Polychlorinated Benzenes Based on Ln-Metal Organic Frameworks. *Crystal Growth and Design*, **2018**, 18, 5353-5364	3.5	45
131	Theoretical design of porphyrin sensitizers with different acceptors for application in dye-sensitized solar cells.. *RSC Advances*, **2018**, 8, 19804-19810	3.7	10
130	An efficient proline-based homogeneous organocatalyst with recyclability. *New Journal of Chemistry*, **2018**, 42, 827-831	3.6	11
129	Theoretical Study on the Photoinduced Electron Transfer Mechanisms of Different Peroxynitrite Probes. *Journal of Physical Chemistry A*, **2018**, 122, 217-223	2.8	8
128	New Mixed-C^N Ligand Tris-Cyclometalated IrIII Complexes for Highly-Efficient Green Organic Light-Emitting Diodes with Low Efficiency Roll-Off. *European Journal of Inorganic Chemistry*, **2018**, 2018, 4614-4621	2.3	17

127	Accurate Control of Deuterated Locations and Amount of Deep Blue Ir(dfpypy)2pic for Phosphorescent Efficiency Enhancement: Evaluations from Theoretical Aspect. *Chemical Research in Chinese Universities*, **2018**, 34, 781-785	2.2	0
126	Influence of one-dimensional TiO2 nanotube on interfacial electron transfer in dye-sensitized solar cells: Insights from theoretical investigation. *Solar Energy*, **2018**, 176, 545-555	6.8	11
125	Density functional theory investigation on iridium(iii) complexes for efficient blue electrophosphorescence.. *RSC Advances*, **2018**, 8, 19437-19448	3.7	6
124	Comprehensive Investigation into Luminescent Properties of Ir(III) Complexes: An Integrated Computational Study of Radiative and Nonradiative Decay Processes. *Inorganic Chemistry*, **2018**, 57, 6561-6570	5.1	27
123	A complete evaluation from theoretical aspect on the phosphorescent efficiency improvement through ancillary ligands modifications of a blue Ir(III) complex. *Organic Electronics*, **2018**, 59, 293-300	3.5	11
122	Fine-tuning π-spacer for high efficiency performance DSSC: A theoretical exploration with D-A-π-A based organic dye. *Dyes and Pigments*, **2017**, 141, 251-261	4.6	37
121	Atomic Modulation of Fe-Co-Nitrogen-Carbon Bifunctional Oxygen Electrodes for Rechargeable and Flexible All-Solid-State Zinc-Air Battery. *Advanced Energy Materials*, **2017**, 7, 1602420	21.8	505
120	The theoretical study of substituent and charge effects in the conformational transformation process of molecular machine unit spiropyran. *Organic Electronics*, **2017**, 45, 33-41	3.5	12
119	Hole Trapping by Iodine Interstitial Defects Decreases Free Carrier Losses in Perovskite Solar Cells: A Time-Domain Ab Initio Study. *ACS Energy Letters*, **2017**, 2, 1270-1278	20.1	114
118	Theoretical analysis of electrochromism under redox of bis(3-thienyl)/(2-thienyl)hexafluorocyclopentene: effects of charged and substituted systems. *Physical Chemistry Chemical Physics*, **2017**, 19, 9281-9291	3.6	2
117	A Computational Way To Achieve More Effective Candidates for Photodynamic Therapy. *Journal of Chemical Information and Modeling*, **2017**, 57, 1089-1100	6.1	10
116	Theoretical investigation on the effect of ancillary ligand modification for highly efficient phosphorescent platinum(II) complex design. *RSC Advances*, **2017**, 7, 17368-17376	3.7	16
115	Theoretical investigation of NCN-coordinated Pt(II) and Pd(II) complexes for long-lived two-photon photodynamic therapy. *Dyes and Pigments*, **2017**, 142, 55-61	4.6	8
114	Bifunctional Phase-Transfer Catalysts Catalyzed Diastereo- and Enantioselective Aza-Henry Reaction of β,γ-Unsaturated Nitroalkenes With Amidosulfones. *Advanced Synthesis and Catalysis*, **2017**, 359, 4111-4116	5.6	10
113	Zinc-Air Batteries: Atomic Modulation of Fe-Co-Nitrogen-Carbon Bifunctional Oxygen Electrodes for Rechargeable and Flexible All-Solid-State Zinc-Air Battery (Adv. Energy Mater. 13/2017). *Advanced Energy Materials*, **2017**, 7,	21.8	2
112	The phosphorescence properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization. *Organic Chemistry Frontiers*, **2017**, 4, 2191-2201	5.2	8
111	Anionic ancillary ligands in cyclometalated Ru(II) complex sensitizers improve photovoltaic efficiency of dye-sensitized solar cells: insights from theoretical investigations. *Journal of Materials Chemistry A*, **2017**, 5, 15567-15577	13	29
110	A density functional theory investigation of the stability, aromaticity, and photophysical behavior for the highly conjugated macrocycles containing 4 pyrroles. *Journal of Physical Organic Chemistry*, **2017**, 30, e3617	2.1	3

109	The influence of a dye□TiO2 interface on DSSC performance: a theoretical exploration with a ruthenium dye. *RSC Advances*, **2016**, 6, 81976-81982	3.7	20
108	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. *Physical Chemistry Chemical Physics*, **2016**, 18, 29591-29599	3.6	9
107	New exploration towards dinuclear iridium(II) complexes materials under chlorine-bridged precursor. *RSC Advances*, **2016**, 6, 68960-68963	3.7	3
106	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. *RSC Advances*, **2016**, 6, 104735-104741	3.7	18
105	A series of pure orange-yellow iridium complexes with low efficiency roll-off: A computational study. *Chemical Research in Chinese Universities*, **2016**, 32, 451-454	2.2	8
104	Theoretical investigation on the spectroscopic properties of Zn porphyrin and Zn tetrapyrrin. *Synthetic Metals*, **2016**, 213, 18-24	3.6	8
103	Theoretical study and design of highly efficient platinum(II) complexes bearing tetradentate ligands for OLED. *RSC Advances*, **2016**, 6, 11648-11656	3.7	28
102	Theoretical study on thermal cis-to-trans isomerization of BF2-coordinated azo compounds of the para-substitution with electron donating groups. *Dyes and Pigments*, **2016**, 129, 100-108	4.6	13
101	Theoretical study on fluorescent probes for cyanide based on the indolium functional group. *Organic Electronics*, **2016**, 30, 1-11	3.5	8
100	Theoretical description of dye regeneration on the TiO 2 □dye□electrolyte model. *Computational Materials Science*, **2016**, 111, 239-246	3.2	18
99	Theoretical Studies of Spectroscopic Properties of Several Binding Models of Z907 to TiO2 Surface in Dye-Sensitized Solar Cell. *Science of Advanced Materials*, **2016**, 8, 1719-1727	2.3	2
98	How the substituents in corannulene and sumanene derivatives alter their molecular assemblings and charge transport properties?--A theoretical study with a dimer model. *Journal of Computational Chemistry*, **2016**, 37, 813-24	3.5	12
97	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. *Journal of Materials Chemistry C*, **2016**, 4, 10130-10145	7.1	23
96	Theoretical and experimental study on intramolecular charge-transfer in symmetric bi-1,3,4-oxadiazole derivatives. *Journal of Photochemistry and Photobiology A: Chemistry*, **2015**, 312, 20-27	4.7	24
95	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?. *Organic Electronics*, **2015**, 26, 164-175	3.5	14
94	Theoretical investigation on remote-control photocycloreversion of dithienylethene driven by azobenzene chromophores. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 137, 987-94	4.4	4
93	Theoretical studies of fluorine substituent effect on organic photo-sensitizers in dye sensitized solar cells. *Computational and Theoretical Chemistry*, **2015**, 1067, 119-128	2	4
92	The induced current strengths and aromatic pathways of heteroporphyrins and their antiaromatic derivatives. *International Journal of Quantum Chemistry*, **2015**, 115, 983-988	2.1	5

91	Discovering the intermediate of dye regeneration in dye-sensitized solar cells: Theoretical investigations on the interaction between organic dye with different donors and . *Dyes and Pigments*, **2015**, 120, 74-84	4.6	21
90	Exploring the sensitization properties of thienyl-functionalized tripyrrole Ru(II) complexes on TiO2 (101) surface: a theoretical study. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	3
89	Theoretical research on the effect of regulated π-conjugation on the photophysical properties of Ir(III) complexes. *Physical Chemistry Chemical Physics*, **2015**, 17, 10014-21	3.6	26
88	Theoretical investigation on excited-state cyclization reactions of platinum-sensitized dithienylethene complexes. *Journal of Physical Chemistry A*, **2015**, 119, 2819-28	2.8	10
87	Theoretical studies on the spectroscopic properties of porphyrin derivatives for dye-sensitized solar cell application. *RSC Advances*, **2015**, 5, 33653-33665	3.7	24
86	Polymorphism dependent charge transport property of 9,10-bis((E)-2-(pyrid-2-yl)vinyl)anthracene: a theoretical study. *RSC Advances*, **2015**, 5, 18875-18880	3.7	6
85	Controllable molecular aggregation and fluorescence properties of 1,3,4-oxadiazole derivatives. *Journal of Materials Chemistry C*, **2015**, 3, 11681-11688	7.1	19
84	A relativistic DFT probe of energetics and structural properties of catalytically important macrocyclic diuranium(III) complexes. *Inorganica Chimica Acta*, **2015**, 437, 95-102	2.7	2
83	Theoretical studies of heteroatom-doping in TiO2 to enhance the electron injection in dye-sensitized solar cells. *RSC Advances*, **2015**, 5, 79868-79873	3.7	11
82	Planar amine-based dye features the rigidified O-bridged dithiophene π-spacer: A potential high-efficiency sensitizer for dye-sensitized solar cells application. *Journal of Power Sources*, **2015**, 275, 207-216	8.9	39
81	Tuning electronic structures of uranyl fluorides via increasing equatorial pyridyl number and extending pyridyl conjugation. *Computational and Theoretical Chemistry*, **2015**, 1051, 144-150	2	1
80	Theoretical investigation on a series of novel S,S-dioxide diarylethenes with abnormal photochromic properties and design of new dyads. *New Journal of Chemistry*, **2015**, 39, 1634-1642	3.6	10
79	Theoretical studies of electronic and optical properties of the triphenylamine-based organic dyes with diketopyrrolopyrrole chromophore. *Dyes and Pigments*, **2015**, 113, 87-95	4.6	41
78	Theoretical study on a series of iridium complexes with low efficiency roll-off property. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 134, 406-12	4.4	19
77	Enhancing Electron Injection in Dye-Sensitized Solar Cells by Adopting W6+-Doped TiO2 Nanowires: A Theoretical Study. *European Journal of Inorganic Chemistry*, **2015**, 2015, 5563-5570	2.3	6
76	The impact of molecular stacking interactions on the electronic structure and charge transport properties in distyrylbenzene (DSB-) based D-A complexes: a theoretical study. *RSC Advances*, **2015**, 5, 47681-47691	3.7	10
75	A theoretical investigation on the π-conjugation effect on the structures and spectral properties of tetra pyrrole zinc complexes. *Synthetic Metals*, **2015**, 210, 258-267	3.6	3
74	Quaternary ammonium hydroxide as a metal-free and halogen-free catalyst for the synthesis of cyclic carbonates from epoxides and carbon dioxide. *Catalysis Science and Technology*, **2015**, 5, 2314-2321	5.5	94

73	Molecular design of organic dyes with diketopyrrolopyrrole for dye-sensitized solar cell: A theoretical approach. *International Journal of Quantum Chemistry*, **2014**, 114, 560-567	2.1	15
72	Theoretical study on the electronic structures and properties of diindolocarbazole isomers. *Journal of Physical Organic Chemistry*, **2014**, 27, 973-980	2.1	6
71	What Makes Hydroxamate a Promising Anchoring Group in Dye-Sensitized Solar Cells? Insights from Theoretical Investigation. *Journal of Physical Chemistry Letters*, **2014**, 5, 3992-9	6.4	58
70	New Zn□+ coordination polymers constructed from acylhydrazidate molecules: synthesis and structural characterization. *Dalton Transactions*, **2014**, 43, 15617-27	4.3	15
69	Analysis of ethyl and methyl centralite vibrational spectra for mapping organic gunshot residues. *Analyst, The*, **2014**, 139, 4270-8	5	14
68	Theoretical investigation of the adsorption, IR, and electron injection of hydroxamate anchor at the TiO2 anatase (1 0 1) surface. *RSC Advances*, **2014**, 4, 19690-19693	3.7	23
67	Heterostructured Co3O4/PEI□CNTs composite: fabrication, characterization and CO gas sensors at room temperature. *Journal of Materials Chemistry A*, **2014**, 2, 4558-4565	13	47
66	Theoretical studies on the interaction of ruthenium sensitizers and redox couple in different deprotonation situations. *Journal of Physical Chemistry A*, **2014**, 118, 2244-52	2.8	11
65	Design of D□□A organic dyes with different acceptor and auxiliary acceptor for highly efficient dye-sensitized solar cells: a computational study. *RSC Advances*, **2014**, 4, 50338-50350	3.7	32
64	Accurate simulation of geometry, singlet-singlet and triplet-singlet excitation of cyclometalated iridium(III) complex. *Journal of Molecular Modeling*, **2014**, 20, 2108	2	5
63	Theoretical investigation of triphenylamine-based sensitizers with different □spacers for DSSC. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 118, 1144-51	4.4	42
62	Excited states of a significantly ruffled porphyrin: computational study on structure-induced rapid decay mechanism via intersystem crossing. *Journal of Physical Chemistry A*, **2014**, 118, 4184-94	2.8	14
61	Theoretical study on molecular packing and electronic structure of bi-1,3,4-oxadiazole derivatives. *RSC Advances*, **2014**, 4, 51942-51949	3.7	7
60	Theoretical investigation on the spectroscopy prosperities of four isomers of an encoder molecule FGDTE. *Dyes and Pigments*, **2014**, 107, 108-117	4.6	3
59	Computational study on zinc porphyrin analogs for use in dye-sensitized solar cells. *Journal of Porphyrins and Phthalocyanines*, **2014**, 18, 406-415	1.8	3
58	Theoretical studies on the dihydrogen bonding between shortchain hydrocarbon and magnesium hydride. *Chemical Research in Chinese Universities*, **2014**, 30, 831-836	2.2	
57	Theoretical Studies on Phosphorescent Materials: The Conjugation-Extended PtII Complexes. *Australian Journal of Chemistry*, **2014**, 67, 1522	1.2	1
56	Theoretical investigation and design of high-efficiency dithiafulvenyl-based sensitizers for dye-sensitized solar cells: the impacts of elongating □spacers and rigidifying dithiophene. *Physical Chemistry Chemical Physics*, **2014**, 16, 9458-68	3.6	33

55	Theoretical studies on structural and spectroscopic properties of photoelectrochemical cell ruthenium sensitizers, derivatives of AR20. *International Journal of Quantum Chemistry*, **2013**, 113, 891-901	2.1	5
54	DFT/TDDFT investigation on bis-cyclometalated alkynylgold(III) complex: Comparison of absorption and emission properties. *Science China Chemistry*, **2013**, 56, 641-647	7.9	1
53	Connection style and spectroscopic properties: Theoretical understanding of the interface between N749 and TiO2 in DSSCs. *Dyes and Pigments*, **2013**, 99, 201-208	4.6	17
52	Theoretical analysis on magnetic properties of conjugated organic molecules containing borepin. *Chemical Research in Chinese Universities*, **2013**, 29, 962-968	2.2	3
51	Synthesis, structural characterization and photoluminescence property of three Zn(2+)/Mn(2+)-acylhydrazidate complexes and two acylhydrazide molecules. *Dalton Transactions*, **2013**, 42, 16547-55	4.3	23
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