

# Wei Shen

## List of Publications by Year in descending order

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118  
papers

1,943  
citations

279798

23  
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docs citations

118  
times ranked

2492  
citing authors

#	ARTICLE	IF	CITATIONS
1	Regulating electron density of NiFe-P nanosheets electrocatalysts by a trifle of Ru for high-efficient overall water splitting. <i>Applied Catalysis B: Environmental</i> , 2020, 263, 118324.	20.2	178
2	Highly conductive and metallic cobalt-nickel selenide nanorods supported on Ni foam as an efficient electrocatalyst for alkaline water splitting. <i>Nanoscale</i> , 2019, 11, 7959-7966.	5.6	107
3	Electron-Deficient Pyrimidine Adopted in Porphyrin Sensitizers: A Theoretical Interpretation of $\pi$ -Spacers Leading to Highly Efficient Photo-to-Electric Conversion Performances in Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9166-9179.	3.1	76
4	Strategy to Modulate the Electron-Rich Units in Donor-Acceptor Copolymers for Improvements of Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17266-17278.	3.1	69
5	A single-atom catalyst of cobalt supported on a defective two-dimensional boron nitride material as a promising electrocatalyst for the oxygen reduction reaction: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6900-6907.	2.8	61
6	Gold(I)-Catalyzed Cycloaddition of 1-(1-Alkynyl)cyclopropyl Ketones with Nucleophiles To Yield Substituted Furans: A DFT Study. <i>Organometallics</i> , 2009, 28, 3129-3139.	2.3	55
7	Theoretical Insights into the Phosphorescence Quantum Yields of Cyclometalated ( $C^{sup>\wedge}S^{sup>C^*}$ ) Platinum(II) NHC Complexes: $\pi$ -Conjugation Controls the Radiative and Nonradiative Decay Processes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3462-3471.	3.1	48
8	Theoretical study on the origin of activity for the oxygen reduction reaction of metal-doped two-dimensional boron nitride materials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10240-10246.	2.8	45
9	Room-temperature synthesis of excellent-performance CsPb1-Sn Br3 perovskite quantum dots and application in light emitting diodes. <i>Materials and Design</i> , 2020, 185, 108246.	7.0	38
10	Theoretical investigations on fluorinated and cyano copolymers for improvements of photovoltaic performances. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 311-323.	2.8	35
11	<i>In situ</i> confinement of Pt within three-dimensional $MoO_2$ @porous carbon for efficient hydrogen evolution. <i>Journal of Materials Chemistry A</i> , 2020, 8, 10409-10418.	10.3	35
12	Theoretical analysis on the electronic structures and properties of PPV fused with electron-withdrawing unit: Monomer, oligomer and polymer. <i>Polymer</i> , 2008, 49, 2614-2620.	3.8	34
13	Influence of $\pi$ -bridge conjugation on the electrochemical properties within hole transporting materials for perovskite solar cells. <i>Nanoscale</i> , 2017, 9, 12916-12924.	5.6	34
14	A novel ball-in-ball hollow oxygen-incorporating cobalt sulfide spheres as high-efficient electrocatalyst for oxygen evolution reaction. <i>Chinese Chemical Letters</i> , 2021, 32, 755-760.	9.0	32
15	A density functional theory study on the thermodynamic and dynamic properties of anthraquinone analogue cathode materials for rechargeable lithium ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12480-12489.	2.8	30
16	Theoretical insights into the effect of a conjugated core on the hole transport properties of hole-transporting materials for perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24574-24582.	2.8	29
17	Theoretical analysis of oxygen reduction reaction activity on single metal (Ni, Pd, Pt, Cu, Ag, Au) atom supported on defective two-dimensional boron nitride materials. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18589-18594.	2.8	29
18	Geometries and Electronic Structures of Co-Oligomers and Co-Polymers Based on Tricyclic Nonclassical Thiophene: A Theoretical Study. <i>Macromolecular Theory and Simulations</i> , 2008, 17, 385-392.	1.4	28

#	ARTICLE	IF	CITATIONS
19	Molecular design of donor-acceptor conjugated copolymers based on C-, Si- and N-bridged dithiophene and thienopyrroledione derivatives units for organic solar cells. <i>Journal of Power Sources</i> , 2014, 245, 217-223.	7.8	28
20	The electronic structures and photophysical properties of platinum complexes with C <sup>N</sup> N ligands: the influence of the carborane substituent. <i>Dalton Transactions</i> , 2015, 44, 18130-18137.	3.3	28
21	Regulating the electron density of dual transition metal sulfide heterostructures for highly efficient hydrogen evolution in alkaline electrolytes. <i>Nanoscale</i> , 2019, 11, 14016-14023.	5.6	26
22	Exploring the role of varied-length spacers in charge transfer: a theoretical investigation on pyrimidine-bridged porphyrin dyes. <i>RSC Advances</i> , 2013, 3, 17515.	3.6	25
23	The electronic and structural properties of nonclassical bicyclic thiophene: Monomer, oligomer and polymer. <i>Polymer</i> , 2007, 48, 3912-3918.	3.8	24
24	Exploring photophysical properties of metal-free coumarin sensitizers: an efficient strategy to improve the performance of dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 53927-53938.	3.6	24
25	Exploring the electrochemical properties of hole transporting materials from first-principles calculations: an efficient strategy to improve the performance of perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1235-1241.	2.8	23
26	Theoretical insight into single Rh atoms anchored on N-doped $\hat{I}^3$ -graphyne as an excellent bifunctional electrocatalyst for the OER and ORR: electronic regulation of graphitic nitrogen. <i>Nanoscale</i> , 2021, 13, 5800-5808.	5.6	23
27	Atomic equidistribution enhanced RuIr electrocatalysts for overall water splitting in the whole pH range. <i>Chemical Engineering Journal</i> , 2022, 450, 137909.	12.7	22
28	Mechanistic Insights into the Cu(I)- and Cu(II)-Catalyzed Cyclization of <i>o</i> -Alkynylbenzaldehydes: The Solvent DMF and Oxidation State of Copper Affect the Reaction Mechanism. <i>Journal of Organic Chemistry</i> , 2015, 80, 6553-6563.	3.2	21
29	Molecular Design of Phenanthrenequinone Derivatives as Organic Cathode Materials. <i>ChemSusChem</i> , 2018, 11, 1215-1222.	6.8	21
30	Theoretical design of donor-acceptor conjugated copolymers based on furo-, thieno-, and selenopheno[3,4-c] thiophene-4,6-dione and benzodithiophene units for organic solar cells. <i>Journal of Molecular Modeling</i> , 2013, 19, 4283-4291.	1.8	20
31	A theoretical study on tuning the electronic structures and photophysical properties of newly designed platinum ( $\text{Pt}(\text{L})_2$ ) complexes by adding substituents on functionalized ligands as highly efficient OLED emitters. <i>Dalton Transactions</i> , 2014, 43, 6500-6512.	3.3	20
32	Understanding the Mechanisms of White Light Emission of a Tetradentate Pt Complex in Various Surrounding Environments. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17968-17975.	3.1	20
33	Synergistic fluorescence quenching of quinolone antibiotics by palladium ( $\text{Pd}(\text{L})_2$ ) and sodium dodecyl benzene sulfonate and the analytical application. <i>Analytical Methods</i> , 2014, 6, 4343-4352.	2.7	19
34	Effect of "push-pull" sensitizers with modified conjugation bridges on the performance of p-type dye-sensitized solar cells. <i>RSC Advances</i> , 2015, 5, 64378-64386.	3.6	19
35	The influence of inserted thiophene into the (A'-B)-bridge on photovoltaic performances of dye-sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2017, 191, 121-128.	4.0	19
36	Cyclopentadithiophene bridged organic sensitizers with different auxiliary acceptor for high performance dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2017, 137, 165-173.	3.7	19

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37	Ultrastable Carbon Quantum Dots-Doped MAPbBr <sub>3</sub> Perovskite with Silica Encapsulation. ACS Applied Materials & Interfaces, 2019, 11, 34348-34354.	8.0	19
38	Exploring the Photodeactivation Pathways of Pt[O <sup>N</sup> C <sup>N</sup> ] Complexes: A Theoretical Perspective. ChemPhysChem, 2016, 17, 69-77.	2.1	18
39	Theoretical investigation of dihydroacridine and diphenylsulphone derivatives as thermally activated delayed fluorescence emitters for organic light-emitting diodes. RSC Advances, 2015, 5, 51586-51591.	3.6	17
40	DFT Study on the Sn <sup>II</sup> -Catalyzed Diastereoselective Synthesis of Tetrahydrofuran from D <sup>A</sup> Cyclopropane and Benzaldehyde. European Journal of Organic Chemistry, 2007, 2007, 4855-4866.	2.4	16
41	Theoretical study of the substituent effect controlling the radiative and non-radiative decay processes of platinum(ii) complexes. Physical Chemistry Chemical Physics, 2017, 19, 23532-23540.	2.8	16
42	Influence of Duschinsky and Herzberg-Teller effects on <i>S</i> <sub>1</sub> vibrational resolved absorption spectra of several porphyrin-like compounds. Journal of Chemical Physics, 2014, 141, 124304.	3.0	15
43	Influence of Base Strength on the Proton-Transfer Reaction by Density Functional Theory. European Journal of Organic Chemistry, 2017, 2017, 3947-3956.	2.4	15
44	What accounts for the color purity of tetradentate Pt complexes? A computational analysis. Physical Chemistry Chemical Physics, 2019, 21, 8073-8080.	2.8	15
45	Molecular design and density functional theory investigation of novel low-bandgap benzobisthiadiazole-based systems: from monomer to polymer. Polymer International, 2011, 60, 211-221.	3.1	14
46	DFT study on the Au( <sup>sc</sup> ) <sub>2</sub> -catalyzed cyclization of indole-allenoate: counterion and solvent effects. New Journal of Chemistry, 2018, 42, 15618-15628.	2.8	14
47	Theoretical Strategy To Design Novel n-Type Copolymers Based on Anthracene Diimide and Pyrido[2,3- <i>g</i> ]quinoline Diimide for Organic Solar Cells. Journal of Physical Chemistry A, 2015, 119, 6884-6896.	2.5	13
48	Exploration of phosphorescent platinum(II) complexes functionalized by distinct main-group units to search for highly efficient blue emitters applied in organic light-emitting diodes: A theoretical study. Inorganica Chimica Acta, 2015, 435, 109-116.	2.4	13
49	Theoretical investigation of regeneration mechanism of the metal-free sensitizer in dye sensitized solar cells. Dyes and Pigments, 2016, 124, 156-164.	3.7	13
50	Ir-Bridge modification of thiazole-bridged DPP polymers for high performance near-IR OSCs. Physical Chemistry Chemical Physics, 2018, 20, 1664-1672.	2.8	13
51	Engineering metallic MoS <sub>2</sub> monolayers with responsive hydrogen evolution electrocatalytic activities for enzymatic reaction monitoring. Journal of Materials Chemistry A, 2021, 9, 11056-11063.	10.3	13
52	Molecular design and density functional theory investigation of novel low-bandgap copolymers between quinoid acceptors and aromatic donors. Polymer International, 2011, 60, 1408-1418.	3.1	11
53	Theoretical Insights into the Photo-Deactivation of Emitting Triplet Excited State of (C <sup>N</sup> )Pt(O <sup>O</sup> ) Complexes: Radiative and Nonradiative Decay Processes. Journal of Physical Chemistry A, 2016, 120, 6813-6821.	2.5	11
54	DFT study on the CuBr-catalyzed synthesis of highly substituted furans: effects of solvent DMF, substrate MeOH, trace H <sub>2</sub> O and the metallic valence state of Cu. RSC Advances, 2016, 6, 20294-20305.	3.6	11

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55	Theoretical investigations on enhancing the performance of terminally diketopyrrolopyrrole-based small-molecular donors in organic solar cell applications. <i>Journal of Molecular Modeling</i> , 2016, 22, 15.	1.8	11
56	Effects of base strength on the copper-catalyzed cycloisomerization of propargylic acetates to form indolizines: A DFT study. <i>Tetrahedron</i> , 2017, 73, 6092-6100.	1.9	11
57	How the Connectivity of Methoxy Substituents Influences the Photovoltaic Properties of Dissymmetric Core Materials: A Theoretical Study on FDT. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8804-8813.	3.1	11
58	Phase Regulation of CsPb <sub>2</sub> Br <sub>5</sub> /CsPbBr <sub>3</sub> Perovskite Nanocrystals by Doping with Divalent Cations: Implications for Optoelectronic Devices with Enhanced Stability and Reduced Toxicity. <i>ACS Applied Nano Materials</i> , 2021, 4, 9213-9222.	5.0	11
59	DFT/TDDFT insight into the impact of ring size of the NHC chelating unit of high effective phosphorescent Platinum (II) complexes. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4467.	3.5	10
60	N, S-codoped porous carbon as metal-free electrocatalyst for oxygen reduction reaction. <i>Journal of Solid State Electrochemistry</i> , 2021, 25, 1765-1773.	2.5	10
61	Theoretical investigations of the small molecular acceptor materials based on oligothiophene "naphthalene diimide in organic solar cells. <i>RSC Advances</i> , 2016, 6, 102159-102171.	3.6	9
62	Effects of thiophene substituents on hole-transporting properties of dipolar chromophores for perovskite solar cells. <i>Journal of Materials Science</i> , 2018, 53, 6626-6636.	3.7	8
63	Electronic structures and photophysical properties of phosphorescent platinum (II) complexes with tridentate C <sup>N</sup> *N cyclometalated ligands. <i>Applied Organometallic Chemistry</i> , 2018, 32, e3929.	3.5	8
64	Effect of double bond conjugation on hole mobility of thiophene-based hole transport materials in perovskite solar cells. <i>Materials Chemistry and Physics</i> , 2020, 240, 122058.	4.0	8
65	DFT study on Ru <sup>II</sup> -catalyzed cyclization of terminal alkynals to cycloalkenes. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 679-687.	2.0	7
66	Theoretical investigation of Ni(PMe <sub>3</sub> ) <sub>4</sub> -catalyzed intermolecular hydroacylation of alkynes with benzaldehydes. <i>Transition Metal Chemistry</i> , 2011, 36, 793-799.	1.4	7
67	Theory study on the properties of thiazazole polymer donors for organic solar cells. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 99-105.	1.9	7
68	The DFT study on non-conjugated polymer host materials based on styrene derivatives for phosphorescent polymer light-emitting diodes. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 554-563.	1.9	7
69	A DFT Insight into Hashmi Phenol Synthesis Catalyzed by M <sub>6</sub> @Au <sub>32</sub> (M=Ag, Cu). <i>TJ ETQ</i> 1.1 0.784314 rgB	3.7	7
70	Theoretical Investigation and Design of Highly Efficient Blue Phosphorescent Iridium(III) Complexes Bearing Fluorinated Aromatic Sulfonyl Groups. <i>ChemPhysChem</i> , 2016, 17, 4149-4157.	2.1	7
71	Theoretical study and design of cyclometalated platinum complexes bearing innovatively a highly-rigid terdentate ligand with carboranyl as a chelating unit. <i>RSC Advances</i> , 2016, 6, 78241-78251.	3.6	7
72	Fine tuning phosphorescent properties of platinum complexes via different N-heterocyclic-based C <sup>E</sup> †N <sup>E</sup> †N ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 836-837, 26-33.	1.8	7

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73	Theoretical insight into the photodeactivation pathway of the tetradentate Pt(II) complex: The $\pi$ -conjugation effect. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4220.	3.5	7
74	Understanding and Breaking the Scaling Relations in the Oxygen Reduction Reaction on PdxCu4-x Subnanoclusters Supported by Defective Two-Dimensional Boron Nitride Materials. <i>Journal of Physical Chemistry C</i> , 2020, 124, 19530-19537.	3.1	7
75	Unveiling the Dual Emission Photo-deactivation Mechanism of a Neutral Heteroleptic Iridium (III) Complex. <i>ChemPhysChem</i> , 2018, 19, 2200-2207.	2.1	7
76	Molecular designing and DFT investigation of novel alternating donor-acceptor dibenzo[b,d]thiophen-based systems: from monomer to polymer. <i>Structural Chemistry</i> , 2012, 23, 97-106.	2.0	6
77	The effects of electron-acceptor strength and donor-to-acceptor ratio on the electronic properties of thieno[3,2-b]thiophene-based donor-acceptor copolymers. <i>Molecular Simulation</i> , 2014, 40, 439-448.	2.0	6
78	Theoretical Investigation on Mechanism of the PPh <sub>3</sub> -Catalyzed Isomerization of Allenic Sulfones to 2-Arylsulfonyl 1,3-Dienes: Effects of Additive as the Proton-Shuttle. <i>ChemistrySelect</i> , 2016, 1, 2971-2978.	1.5	6
79	Theoretical study on the reaction mechanism of Pd(OAc) <sub>2</sub> -catalyzed trifluoroethylation: Role of additive CF <sub>3</sub> COOH. <i>Tetrahedron Letters</i> , 2018, 59, 462-468.	1.4	6
80	Revealing the Unique Properties of Platinum(II) Complexes with Bidentate Bis(o-carborane) Ligands. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 99-108.	2.0	6
81	Highly luminescent and stable quasi-2D perovskite quantum dots by introducing large organic cations. <i>Nanoscale Advances</i> , 2021, 3, 5393-5398.	4.6	6
82	Unveiling the mechanisms of organic room-temperature phosphorescence in various surrounding environments: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26813-26821.	2.8	6
83	DFT studies on the mechanism of Pd(II)-catalyzed intermolecular 1,2-diamination of conjugated dienes. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 979-987.	1.9	5
84	Molecular design of copolymers based on polyfluorene derivatives for Bulk-heterojunction-type solar cells. <i>Journal of Materials Science</i> , 2013, 48, 1205-1213.	3.7	5
85	DFT insights into the cycloisomerization of $\beta$ -alkynylfuran catalyzed by planar gold clusters: mechanism and selectivity, as compared to Au-catalysis. <i>RSC Advances</i> , 2016, 6, 22709-22721.	3.6	5
86	Exploring the effect of vibronic contributions on light harvesting efficiency of NKX-2587 derivatives through vibrationally resolved electronic spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 406-414.	3.9	5
87	Electronic structure and luminescence properties of unique complexes: cyclometalated iridium(III) chelated by o-carboranyl-pyridine ligands. <i>New Journal of Chemistry</i> , 2018, 42, 5955-5966.	2.8	5
88	Theoretical Insight into Molecular Orientation for Thermally Activated Delayed Fluorescence Emitters in Vacuum Deposition. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1665-1672.	3.1	5
89	Theoretical investigation on the geometries and electronic properties of thiophene ring-containing compounds: monomer, oligomer and polymer. <i>Molecular Simulation</i> , 2009, 35, 1279-1287.	2.0	4
90	Quantum chemical study on excited states and charge transfer of oxazolo[4,5-b]-pyridine derivatives. <i>Science China Chemistry</i> , 2012, 55, 2186-2196.	8.2	4

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91	Density functional study on the effect of a new ladder-type structure with different substituent groups (R = H, CH <sub>3</sub> , OCH <sub>3</sub> and CN) for donor-acceptor copolymers. RSC Advances, 2014, 4, 36656.	3.6	4
92	Theoretical Insight Into the Role of Triarylboron Substituents in Tetradentate Dianionic Bis(N-heterocyclic carbene) Platinum(II) Chelates – Improving the Performance of Blue Light Emission. European Journal of Inorganic Chemistry, 2015, 2015, 1902-1911.	2.0	4
93	Mechanism and Charge Effect of Cycloisomerization of Alkynylfuran Catalyzed by Subnanometer Gold Clusters: A Theoretical Study. ChemCatChem, 2016, 8, 461-470.	3.7	4
94	Rational design of carbazolyl and aryl phosphine oxide (APO) based ambipolar host materials for blue electrophosphorescence: a density functional theory study. RSC Advances, 2016, 6, 35416-35424.	3.6	4
95	Highly efficient blue-emitting bis-cyclometalated tetravalent platinum (IV) complexes: A theoretical study. Inorganica Chimica Acta, 2020, 501, 119269.	2.4	4
96	The study of intramolecular decay and intermolecular energy transfer for phosphorescent organic light-emitting devices. Physical Chemistry Chemical Physics, 2021, 23, 7495-7503.	2.8	4
97	DFT study of conductive properties of three polymers formed by bicyclic furans. Molecular Simulation, 2010, 36, 836-846.	2.0	3
98	Theoretical Investigations on Naphthodithiophene Diimide-Based Copolymers as Acceptor for All-Polymer Solar Cell Applications. ChemistrySelect, 2016, 1, 1662-1673.	1.5	3
99	Tuning the electronic and photophysical properties of platinum(II) complexes through ancillary ligand modification: a theoretical study. Molecular Simulation, 2016, 42, 1035-1041.	2.0	3
100	Excited state intersystem crossing and the relaxation dynamics of phosphorescent Ir(III) complexes bearing bipyridine-based C <sup>N</sup> ligand. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 346, 225-235.	3.9	3
101	Influence of vibronic contribution on light harvesting efficiency of NKX-2587 derivatives with oligothiophene as $\pi$ -conjugated linker. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 189, 454-462.	3.9	3
102	Theoretical insights into the effect of ligands on platinum(ii) complexes with a bidentate bis(o-carborane) ligand structure. Photochemical and Photobiological Sciences, 2019, 18, 2421-2429.	2.9	3
103	Effects of intramolecular hydrogen bonds on phosphorescence emission: A theoretical perspective. Applied Organometallic Chemistry, 2020, 34, e5527.	3.5	3
104	Meta-Stable Molecular Configuration Enables Thermally Stable and Solution Processable Organic Charge Transporting Materials. Advanced Functional Materials, 2020, 30, 2000729.	14.9	3
105	Molecular designing of organic conductor based upon the model of polypyrrole. Polymer Science - Series A, 2010, 52, 1355-1360.	1.0	2
106	Density functional theory investigation on the electronic structure of furo[3,4-b]pyridine-type heterocyclics: from monomer to polymer. Structural Chemistry, 2010, 21, 1253-1261.	2.0	2
107	A DFT study of the effects of donor-to-acceptor ratio on the electronic properties of copolymers based on tricyclic non-classical thiophene. Molecular Simulation, 2011, 37, 478-487.	2.0	2
108	Theoretical analysis on geometries and electronic structures of antiaromatic pentalene and its N-substituted derivatives: monomer, oligomers and polymer. Journal of Physical Organic Chemistry, 2012, 25, 278-286.	1.9	2

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109	A potential strategy used for controlling the phosphorescence quantum yield of cyclometalated (CE†C*) platinum(II) NHC complexes: The theoretical insight. <i>Organic Electronics</i> , 2018, 57, 367-376.	2.6	2
110	Unveiling the relationship between the phosphorescent quantum yield and structural modification to construct high-performance Pt(II) complex. <i>Inorganica Chimica Acta</i> , 2020, 512, 119861.	2.4	2
111	Uncovering the unusual effect of halogenation on crystal packing in an azzaacee-based electron transporting material. <i>Materials Chemistry and Physics</i> , 2021, 259, 124060.	4.0	2
112	Face-to-face order-packed mode promotes thermally activated delayed fluorescence to achieve stronger aggregation-induced emission. <i>Journal of Science: Advanced Materials and Devices</i> , 2022, 7, 100432.	3.1	2
113	Theoretical Studies on the Reaction Mechanisms of C <sub>3</sub> H <sub>2</sub> (cyclopropenylidene) and O( <sup>3</sup> P) Radicals. <i>Chinese Journal of Chemistry</i> , 2009, 27, 49-55.	4.9	1
114	Theoretical investigations of the electronic structures of carbazole-based triphenylphosphine oxide derivatives, potential bipolar host materials in blue-phosphorescent devices. <i>Journal of Molecular Modeling</i> , 2015, 21, 320.	1.8	1
115	Density Functional Study on A-Units Based on Thieno[3,4-c]pyrrole-4,6-dione for Organic Solar Cells. <i>Journal of Electronic Materials</i> , 2017, 46, 4825-4834.	2.2	1
116	Regulating Interfacial Coupling and Electron Transport for Efficient Electron-Transporting Materials. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10140-10150.	3.1	1
117	The electronic properties of poly( <i>p</i> -phenylenevinylene) derivatives and their monomers and oligomers. <i>Molecular Simulation</i> , 2008, 34, 637-643.	2.0	0
118	Theoretical Investigation of Donor–Acceptor Copolymers Based on C-, Si-, and Ge-Bridged Thieno[3,2-b]dithiophene for Organic Solar Cell Applications. <i>Journal of Electronic Materials</i> , 2016, 45, 5427-5435.	2.2	0