

# Wei Shen

## List of Publications by Year in descending order

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118  
papers

1,943  
citations

279798

23  
h-index

330143

37  
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118  
all docs

118  
docs citations

118  
times ranked

2492  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	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
4	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
5	Engineering metallic MoS <sub>2</sub> monolayers with responsive hydrogen evolution electrocatalytic activities for enzymatic reaction monitoring. <i>Journal of Materials Chemistry A</i> , 2021, 9, 11056-11063.	10.3	13
6	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
7	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
8	The study of intramolecular decay and intermolecular energy transfer for phosphorescent organic light-emitting devices. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7495-7503.	2.8	4
9	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
10	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
11	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
12	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
13	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
14	Room-temperature synthesis of excellent-performance CsPb <sub>1</sub> -Sn Br <sub>3</sub> perovskite quantum dots and application in light emitting diodes. <i>Materials and Design</i> , 2020, 185, 108246.	7.0	38
15	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
16	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
17	Highly efficient blue-emitting of bis-cyclometalated tetravalent platinum (IV) complexes: A theoretical study. <i>Inorganica Chimica Acta</i> , 2020, 501, 119269.	2.4	4
18	Understanding and Breaking the Scaling Relations in the Oxygen Reduction Reaction on Pd <sub>x</sub> Cu <sub>4-x</sub> Subnanoclusters Supported by Defective Two-Dimensional Boron Nitride Materials. <i>Journal of Physical Chemistry C</i> , 2020, 124, 19530-19537.	3.1	7

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19	<i>In situ</i> confinement of Pt within three-dimensional MoO <sub>2</sub> @porous carbon for efficient hydrogen evolution. <i>Journal of Materials Chemistry A</i> , 2020, 8, 10409-10418.	10.3	35
20	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
21	Effects of intramolecular hydrogen bonds on phosphorescence emission: A theoretical perspective. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5527.	3.5	3
22	Meta-Stable Molecular Configuration Enables Thermally Stable and Solution Processable Organic Charge Transporting Materials. <i>Advanced Functional Materials</i> , 2020, 30, 2000729.	14.9	3
23	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
24	Theoretical insights into the effect of ligands on platinum(ii) complexes with a bidentate bis(o-carborane) ligand structure. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 2421-2429.	2.9	3
25	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
26	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
27	Ultrastable Carbon Quantum Dots-Doped MAPbBr <sub>3</sub> Perovskite with Silica Encapsulation. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 34348-34354.	8.0	19
28	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
29	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
30	What accounts for the color purity of tetradentate Pt complexes? A computational analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8073-8080.	2.8	15
31	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
32	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
33	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
34	A potential strategy used for controlling the phosphorescence quantum yield of cyclometalated (C <sup>+</sup> C*) platinum(II) NHC complexes: The theoretical insight. <i>Organic Electronics</i> , 2018, 57, 367-376.	2.6	2
35	Molecular Design of Phenanthrenequinone Derivatives as Organic Cathode Materials. <i>ChemSusChem</i> , 2018, 11, 1215-1222.	6.8	21
36	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

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37	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
38	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
39	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
40	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
41	Influence of vibronic contribution on light harvesting efficiency of NKX-2587 derivatives with oligothiophene as $\pi$ -conjugated linker. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 189, 454-462.	3.9	3
42	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
43	$\pi$ -Bridge modification of thiazole-bridged DPP polymers for high performance near-IR OSCs. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1664-1672.	2.8	13
44	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
45	DFT study on the Au( $\sigma$ -Cp) <sup>-</sup> -catalyzed cyclization of indole-allenoate: counterion and solvent effects. <i>New Journal of Chemistry</i> , 2018, 42, 15618-15628.	2.8	14
46	Unveiling the Dual Emission Photo $\pi$ -Deactivation Mechanism of a Neutral Heteroleptic Iridium (III) Complex. <i>ChemPhysChem</i> , 2018, 19, 2200-2207.	2.1	7
47	The influence of inserted thiophene into the ( $\pi$ -A'- $\pi$ )-bridge on photovoltaic performances of dye-sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2017, 191, 121-128.	4.0	19
48	Fine tuning phosphorescent properties of platinum complexes via different N-heterocyclic-based C $\pi$ N $\pi$ N ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 836-837, 26-33.	1.8	7
49	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
50	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
51	Excited state intersystem crossing and the relaxation dynamics of phosphorescent Ir(III) complexes bearing bipyridine-based C <sup>N</sup> ligand. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 346, 225-235.	3.9	3
52	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
53	Influence of Base Strength on the Proton $\pi$ -Transfer Reaction by Density Functional Theory. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 3947-3956.	2.4	15
54	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

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55	Theoretical study of the substituent effect controlling the radiative and non-radiative decay processes of platinum(II) complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23532-23540.	2.8	16
56	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
57	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
58	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
59	Mechanism and Charge Effect of Cycloisomerization of $\pi$ -alkynylfuran Catalyzed by Subnanometer Gold Clusters: A Theoretical Study. <i>ChemCatChem</i> , 2016, 8, 461-470.	3.7	4
60	A DFT Insight into Hashmi Phenol Synthesis Catalyzed by $M_6@Au_{32}$ (M=Ag, Cu). <i>J. Theor. Comput. Chem.</i> , 2016, 10, 1-10.	3.7	7
61	Exploring the Photodeactivation Pathways of $Pt[O^N^C^N]$ Complexes: A Theoretical Perspective. <i>ChemPhysChem</i> , 2016, 17, 69-77.	2.1	18
62	Rational design of carbazolyl and aryl phosphine oxide (APO) based ambipolar host materials for blue electrophosphorescence: a density functional theory study. <i>RSC Advances</i> , 2016, 6, 35416-35424.	3.6	4
63	Theoretical investigations of the small molecular acceptor materials based on oligothiophene $\pi$ -naphthalene diimide in organic solar cells. <i>RSC Advances</i> , 2016, 6, 102159-102171.	3.6	9
64	Theoretical Investigation on Mechanism of the $PPh_3$ -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
65	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
66	Theoretical Insights into the Photo-Deactivation of Emitting Triplet Excited State of $(C^N)Pt(O^O)$ Complexes: Radiative and Nonradiative Decay Processes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6813-6821.	2.5	11
67	Theoretical Investigations on Naphthodithiophene Diimide-Based Copolymers as Acceptor for All-Polymer Solar Cell Applications. <i>ChemistrySelect</i> , 2016, 1, 1662-1673.	1.5	3
68	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
69	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
70	Tuning the electronic and photophysical properties of platinum(II) complexes through ancillary ligand modification: a theoretical study. <i>Molecular Simulation</i> , 2016, 42, 1035-1041.	2.0	3
71	Theoretical Insights into the Phosphorescence Quantum Yields of Cyclometalated $(C^*Pt^*)$ 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
72	DFT insights into the cycloisomerization of $\pi$ -alkynylfuran catalyzed by planar gold clusters: mechanism and selectivity, as compared to $Au_1$ -catalysis. <i>RSC Advances</i> , 2016, 6, 22709-22721.	3.6	5

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73	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
74	Theoretical investigations on enhancing the performance of terminally diketopyrrolopyrrole-based small-molecular donors in organic solar cell applications. Journal of Molecular Modeling, 2016, 22, 15.	1.8	11
75	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
76	The DFT study on nonconjugated polymer host materials based on styrene derivatives for phosphorescent polymer light-emitting diodes. Journal of Physical Organic Chemistry, 2015, 28, 554-563.	1.9	7
77	Theoretical Strategy To Design Novel n-Type Copolymers Based on Anthracene Diimide and Pyrido[2,3-g]quinoline Diimide for Organic Solar Cells. Journal of Physical Chemistry A, 2015, 119, 6884-6896.	2.5	13
78	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
79	Theoretical investigations of the electronic structures of carbazole-based triphenylphosphine oxide derivatives, potential bipolar host materials in blue-phosphorescent devices. Journal of Molecular Modeling, 2015, 21, 320.	1.8	1
80	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. Journal of Organic Chemistry, 2015, 80, 6553-6563.	3.2	21
81	Effect of "push-pull" sensitizers with modified conjugation bridges on the performance of p-type dye-sensitized solar cells. RSC Advances, 2015, 5, 64378-64386.	3.6	19
82	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
83	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
84	The electronic structures and photophysical properties of platinum complexes with C <sup>N</sup> N ligands: the influence of the carborane substituent. Dalton Transactions, 2015, 44, 18130-18137.	3.3	28
85	Influence of Duschinsky and Herzberg-Teller effects on <i>S</i> <sup>1</sup> <i>S</i> <sub>0</sub> vibrationally resolved absorption spectra of several porphyrin-like compounds. Journal of Chemical Physics, 2014, 141, 124304.	3.0	15
86	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. Molecular Simulation, 2014, 40, 439-448.	2.0	6
87	Theory study on the properties of thiazazole polymer donors for organic solar cells. Journal of Physical Organic Chemistry, 2014, 27, 99-105.	1.9	7
88	Molecular design of donor-acceptor conjugated copolymers based on C-, Si- and N-bridged dithiophene and thienopyrroledione derivatives units for organic solar cells. Journal of Power Sources, 2014, 245, 217-223.	7.8	28
89	Exploring photophysical properties of metal-free coumarin sensitizers: an efficient strategy to improve the performance of dye-sensitized solar cells. RSC Advances, 2014, 4, 53927-53938.	3.6	24
90	A theoretical study on tuning the electronic structures and photophysical properties of newly designed platinum(II) complexes by adding substituents on functionalized ligands as highly efficient OLED emitters. Dalton Transactions, 2014, 43, 6500-6512.	3.3	20

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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 investigations on fluorinated and cyano copolymers for improvements of photovoltaic performances. Physical Chemistry Chemical Physics, 2014, 16, 311-323.	2.8	35
93	Strategy to Modulate the Electron-Rich Units in Donor-Acceptor Copolymers for Improvements of Organic Photovoltaics. Journal of Physical Chemistry C, 2014, 118, 17266-17278.	3.1	69
94	Synergistic fluorescence quenching of quinolone antibiotics by palladium(II) and sodium dodecyl benzene sulfonate and the analytical application. Analytical Methods, 2014, 6, 4343-4352.	2.7	19
95	Exploring the role of varied-length spacers in charge transfer: a theoretical investigation on pyrimidine-bridged porphyrin dyes. RSC Advances, 2013, 3, 17515.	3.6	25
96	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. Journal of Molecular Modeling, 2013, 19, 4283-4291.	1.8	20
97	Molecular design of copolymers based on polyfluorene derivatives for Bulk-heterojunction-type solar cells. Journal of Materials Science, 2013, 48, 1205-1213.	3.7	5
98	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. Journal of Physical Chemistry C, 2012, 116, 9166-9179.	3.1	76
99	Quantum chemical study on excited states and charge transfer of oxazolo[4,5-b]-pyridine derivatives. Science China Chemistry, 2012, 55, 2186-2196.	8.2	4
100	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
101	Molecular designing and DFT investigation of novel alternating donor-acceptor dibenzo[b,d]thiophen-based systems: from monomer to polymer. Structural Chemistry, 2012, 23, 97-106.	2.0	6
102	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
103	Theoretical investigation of Ni(PMe <sub>3</sub> ) <sub>4</sub> -catalyzed intermolecular hydroacylation of alkynes with benzaldehydes. Transition Metal Chemistry, 2011, 36, 793-799.	1.4	7
104	Molecular design and density functional theory investigation of novel low-band-gap benzobisthiadiazole-based systems: from monomer to polymer. Polymer International, 2011, 60, 211-221.	3.1	14
105	Molecular design and density functional theory investigation of novel low-band-gap copolymers between quinoid acceptors and aromatic donors. Polymer International, 2011, 60, 1408-1418.	3.1	11
106	Molecular designing of organic conductor based upon the model of polypyrrole. Polymer Science - Series A, 2010, 52, 1355-1360.	1.0	2
107	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
108	DFT study of conductive properties of three polymers formed by bicyclic furans. Molecular Simulation, 2010, 36, 836-846.	2.0	3

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109	Theoretical Studies on the Reaction Mechanisms of C <sub>3</sub> H <sub>2</sub> (cyclopropenylidene) and O( <sup>3</sup> P) Radicals. Chinese Journal of Chemistry, 2009, 27, 49-55.	4.9	1
110	DFT study on Ru <sup>II</sup> -catalyzed cyclization of terminal alkynals to cycloalkenes. International Journal of Quantum Chemistry, 2009, 109, 679-687.	2.0	7
111	Gold(I)-Catalyzed Cycloaddition of 1-(1-Alkynyl)cyclopropyl Ketones with Nucleophiles To Yield Substituted Furans: A DFT Study. Organometallics, 2009, 28, 3129-3139.	2.3	55
112	Theoretical investigation on the geometries and electronic properties of thiophene ring-containing compounds: monomer, oligomer and polymer. Molecular Simulation, 2009, 35, 1279-1287.	2.0	4
113	DFT studies on the mechanism of Pd(II)-catalyzed intermolecular 1,2-diamination of conjugated dienes. Journal of Physical Organic Chemistry, 2008, 21, 979-987.	1.9	5
114	Geometries and Electronic Structures of Co <sup>0</sup> Oligomers and Co <sup>0</sup> Polymers Based on Tricyclic Nonclassical Thiophene: A Theoretical Study. Macromolecular Theory and Simulations, 2008, 17, 385-392.	1.4	28
115	Theoretical analysis on the electronic structures and properties of PPV fused with electron-withdrawing unit: Monomer, oligomer and polymer. Polymer, 2008, 49, 2614-2620.	3.8	34
116	The electronic properties of poly( <i>p</i> -phenylenevinylene) derivatives and their monomers and oligomers. Molecular Simulation, 2008, 34, 637-643.	2.0	0
117	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
118	The electronic and structural properties of nonclassical bicyclic thiophene: Monomer, oligomer and polymer. Polymer, 2007, 48, 3912-3918.	3.8	24