

# Guochun Yang

## List of Publications by Year in descending order

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5819  
citing authors

#	ARTICLE	IF	CITATIONS
1	Organic Polymorphs: One-Compound-Based Crystals with Molecular-Conformation- and Packing-Dependent Luminescent Properties. <i>Advanced Materials</i> , 2014, 26, 6168-6173.	21.0	262
2	TiC <sub>3</sub> Monolayer with High Specific Capacity for Sodium-Ion Batteries. <i>Journal of the American Chemical Society</i> , 2018, 140, 5962-5968.	13.7	244
3	Highly Efficient Long-Wavelength Thermally Activated Delayed Fluorescence OLEDs Based on Dicyanopyrazino Phenanthrene Derivatives. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 9892-9901.	8.0	168
4	Two-Dimensional PC <sub>6</sub> with Direct Band Gap and Anisotropic Carrier Mobility. <i>Journal of the American Chemical Society</i> , 2019, 141, 1599-1605.	13.7	144
5	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. <i>Physical Review Letters</i> , 2016, 116, 057002.	7.8	132
6	Lithium lanthanum titanate perovskite as an anode for lithium ion batteries. <i>Nature Communications</i> , 2020, 11, 3490.	12.8	121
7	Gold as a 6p-Element in Dense Lithium Aurides. <i>Journal of the American Chemical Society</i> , 2016, 138, 4046-4052.	13.7	101
8	Predicted Pressure-Induced Superconducting Transition in Electride $\text{LiP}$ . <i>Physical Review Letters</i> , 2019, 122, 097002.	7.8	94
9	Theoretical discussions on electron transport properties of perylene bisimide derivatives with different molecular packings and intermolecular interactions. <i>Journal of Materials Chemistry</i> , 2011, 21, 134-143.	6.7	88
10	High performance full color OLEDs based on a class of molecules with dual carrier transport channels and small singlet-triplet splitting. <i>Chemical Communications</i> , 2015, 51, 10632-10635.	4.1	88
11	Theoretical Study on the Electronic Spectrum and the Origin of Remarkably Large Third-Order Nonlinear Optical Properties of Organoimide Derivatives of Hexamolybdates. <i>Journal of Physical Chemistry B</i> , 2006, 110, 23092-23098.	2.6	84
12	Gold with +4 and +6 Oxidation States in AuF <sub>4</sub> and AuF <sub>6</sub> . <i>Journal of the American Chemical Society</i> , 2018, 140, 9545-9550.	13.7	80
13	High-Temperature Ferromagnetism in an Fe <sub>3</sub> P Monolayer with a Large Magnetic Anisotropy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2733-2738.	4.6	79
14	Stable and metallic two-dimensional TaC <sub>2</sub> as an anode material for lithium-ion battery. <i>Journal of Materials Chemistry A</i> , 2017, 5, 18698-18706.	10.3	75
15	Metallic P <sub>3</sub> C monolayer as anode for sodium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 405-411.	10.3	75
16	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. <i>Scientific Reports</i> , 2015, 5, 15433.	3.3	71
17	Nanotube-assembled pine-needle-like CuS as an effective energy booster for sodium-ion storage. <i>Journal of Materials Chemistry A</i> , 2019, 7, 10619-10628.	10.3	70
18	Insight into the role of Li <sub>2</sub> S <sub>2</sub> in Li-S batteries: a first-principles study. <i>Journal of Materials Chemistry A</i> , 2015, 3, 8865-8869.	10.3	68

#	ARTICLE	IF	CITATIONS
19	Vibrational Circular Dichroism Spectroscopy of Chiral Molecules. Topics in Current Chemistry, 2010, 298, 189-236.	4.0	65
20	Probing chiral solute-water hydrogen bonding networks by chirality transfer effects: A vibrational circular dichroism study of glycidol in water. Journal of Chemical Physics, 2009, 130, 164506.	3.0	60
21	Density Functional Theory Study on the First Hyperpolarizabilities of Organoimido Derivatives of Hexamolybdates. Journal of Physical Chemistry B, 2005, 109, 22332-22336.	2.6	59
22	Theoretical Study on the Second-Order Nonlinear Optical Properties of Asymmetric Spirosilabifluorene Derivatives. Journal of Physical Chemistry A, 2006, 110, 4817-4821.	2.5	58
23	Photocatalytic Reduction of Graphene Oxide—TiO <sub>2</sub> Nanocomposites for Improving Resistive—Switching Memory Behaviors. Small, 2018, 14, e1801325.	10.0	58
24	Effect of $\pi$ -Conjugated Length of Bridging Ligand on the Optoelectronic Properties of Platinum(II) Dimers. Inorganic Chemistry, 2008, 47, 2347-2355.	4.0	54
25	A Stable, Magnetic, and Metallic Li <sub>3</sub> O <sub>4</sub> Compound as a Discharge Product in a Li—Air Battery. Journal of Physical Chemistry Letters, 2014, 5, 2516-2521.	4.6	52
26	Accurate identification of layer number for few-layer WS <sub>2</sub> and WSe <sub>2</sub> via spectroscopic study. Nanotechnology, 2018, 29, 124001.	2.6	52
27	Structure and Electronic Properties of Fe <sub>2</sub> SH <sub>3</sub> Compound under High Pressure. Inorganic Chemistry, 2016, 55, 11434-11439.	4.0	50
28	Anisotropic Janus SiP <sub>2</sub> Monolayer as a Photocatalyst for Water Splitting. Journal of Physical Chemistry Letters, 2021, 12, 2464-2470.	4.6	49
29	A controllable and reversible phase transformation between all-inorganic perovskites for white light emitting diodes. Journal of Materials Chemistry C, 2020, 8, 8374-8379.	5.5	48
30	Reversible Redox-Switchable Second-Order Optical Nonlinearity in Polyoxometalate: A Quantum Chemical Study of [PW <sub>11</sub> O <sub>39</sub> (ReN)] <sup>n−</sup> ( <i>n</i> = 3–7). Inorganic Chemistry, 2008, 47, 5245-5252.	4.0	47
31	The influence of the diphenylphosphoryl moiety on the phosphorescent properties of heteroleptic iridium(III) complexes and the OLED performance: a theoretical study. Journal of Materials Chemistry C, 2014, 2, 2859.	5.5	46
32	Dicyanomethylenated Acridone Based Crystals: Torsional Vibration Confinement Induced Emission with Supramolecular Structure Dependent and Stimuli Responsive Characteristics. Journal of Physical Chemistry C, 2016, 120, 587-597.	3.1	45
33	Prediction of Second-Order Optical Nonlinearity of Trisorganotin-Substituted $\beta^2$ -Keggin Polyoxotungstate. Inorganic Chemistry, 2006, 45, 7864-7868.	4.0	44
34	Understanding the role of lithium sulfide clusters in lithium—sulfur batteries. Journal of Materials Chemistry A, 2017, 5, 9293-9298.	10.3	43
35	Pressure-induced stable BeN <sub>4</sub> as a high-energy density material. Journal of Power Sources, 2017, 365, 155-161.	7.8	43
36	FeP <sub>3</sub> monolayer as a high-efficiency catalyst for hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 25665-25671.	10.3	43

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37	Recent Advances and Applications of Inorganic Electrides. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3841-3852.	4.6	43
38	Theoretical Study on Photophysical and Charge Transport Properties of 1,6-Bis(2-hydroxyphenyl)pyridylboron Bis(4-n-butylphenyl)phenyleneamine Compound. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8758-8762.	2.5	41
39	Conformations of Serine in Aqueous Solutions as Revealed by Vibrational Circular Dichroism. <i>ChemPhysChem</i> , 2012, 13, 1272-1281.	2.1	41
40	Conformational Distributions of <i>N</i> -Acetyl-L-cysteine in Aqueous Solutions: A Combined Implicit and Explicit Solvation Treatment of VA and VCD Spectra. <i>ChemPhysChem</i> , 2012, 13, 2310-2321.	2.1	41
41	O <sub>2</sub> Adsorption Associated with Sulfur Vacancies on MoS <sub>2</sub> Microspheres. <i>Inorganic Chemistry</i> , 2019, 58, 2169-2176.	4.0	40
42	IrF <sub>8</sub> Molecular Crystal under High Pressure. <i>Journal of the American Chemical Society</i> , 2019, 141, 5409-5414.	13.7	40
43	Quantum Chemical Study of Structures, Electronic Spectrum, and Nonlinear Optical Properties of Gold~Pentacene Complexes. <i>Organometallics</i> , 2007, 26, 2082-2087.	2.3	38
44	Theoretical Study on Photophysical Properties of Phenolpyridyl Boron Complexes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2739-2744.	2.5	38
45	Pressure-Induced Stable Li <sub>5</sub> P for High-Performance Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21199-21205.	3.1	36
46	A hypervalent and cubically coordinated molecular phase of IF <sub>8</sub> predicted at high pressure. <i>Chemical Science</i> , 2019, 10, 2543-2550.	7.4	36
47	How Do the Different Defect Structures and Element Substitutions Affect the Nonlinear Optical Properties of Lacunary Keggin Polyoxometalates? A DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 4179-4183.	2.0	33
48	Vibrational absorption, vibrational circular dichroism, and theoretical studies of methyl lactate self-aggregation and methyl lactate-methanol intermolecular interactions. <i>Journal of Chemical Physics</i> , 2010, 132, 234513.	3.0	33
49	DFT Studies on second-order nonlinear optical properties of mono (salicylaldiminato) Nickel(II) polyenyl Schiff base metal complexes. <i>Chemical Physics Letters</i> , 2007, 443, 163-168.	2.6	31
50	Computational study on second-order nonlinear optical (NLO) properties of a novel class of two-dimensional $\beta$ - and W-shaped sandwich metallocarborane-containing chromophores. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2380-2387.	1.8	31
51	The effects of self-aggregation on the vibrational circular dichroism and optical rotation measurements of glycidol. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6787.	2.8	30
52	Chiroptical, linear, and second-order nonlinear optical properties of binaphthol derivatives. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 8418.	2.8	30
53	Chirality recognition of the protonated serine dimer and octamer by infrared multiphoton dissociation spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1873-1886.	2.8	30
54	DFT characterization on the mechanism of water splitting catalyzed by single-Ru-substituted polyoxometalates. <i>Dalton Transactions</i> , 2013, 42, 10617.	3.3	30

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55	Computational predictions of two-dimensional anode materials of metal-ion batteries. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1473.	14.6	30
56	Computational Study on Second-Order Nonlinear Response of a Series of Two-Dimensional Carbazole-Cored Chromophores. Journal of Physical Chemistry C, 2008, 112, 7021-7028.	3.1	29
57	Nonmetallic FeH <sub>6</sub> under High Pressure. Journal of Physical Chemistry C, 2018, 122, 12022-12028.	3.1	29
58	An Organic Emitter Displaying Dual Emissions and Efficient Delayed Fluorescence White OLEDs. Advanced Optical Materials, 2019, 7, 1801667.	7.3	28
59	Photophysical properties of azaboradibenzo[6]helicene derivatives. Journal of Materials Chemistry C, 2013, 1, 2354.	5.5	27
60	Theoretical insights into [PMo12O <sub>40</sub> ]3 <sup>-</sup> grafted on single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 9177.	2.8	27
61	Theoretical Study on the Chiroptical Optical Properties of Chiral Fullerene C <sub>60</sub> Derivative. Journal of Physical Chemistry A, 2011, 115, 13356-13363.	2.5	26
62	Hexagonal BC <sub>2</sub> N with Remarkably High Hardness. Journal of Physical Chemistry C, 2018, 122, 6801-6807.	3.1	26
63	Theoretical studies on the electronic structure and spectral properties of versatile diarylethene-containing 1,10-phenanthroline ligands and their rhenium(I) complexes. Journal of Organometallic Chemistry, 2007, 692, 5368-5374.	1.8	25
64	Complementary Resistive Switching Observed in Graphene Oxide-Based Memory Device. IEEE Electron Device Letters, 2018, 39, 488-491.	3.9	25
65	The relationship between intermolecular interactions and charge transport properties of trifluoromethylated polycyclic aromatic hydrocarbons. Organic Electronics, 2014, 15, 1896-1905.	2.6	24
66	Element substitution of kesterite Cu <sub>2</sub> ZnSnS <sub>4</sub> for efficient counter electrode of dye-sensitized solar cells. Scientific Reports, 2018, 8, 8714.	3.3	24
67	Predication of second-order optical nonlinearity of [(Bu <sub>2</sub> tIm)AuX] (X=halogen) using time-dependent density-functional theory combined with sum-over-states method. Journal of Chemical Physics, 2005, 123, 134302.	3.0	23
68	Theoretical Study on the Optoelectronic Properties of Electron-Withdrawing Substituted Diethynylfluorenyl Gold(I) Complexes. Journal of Physical Chemistry A, 2006, 110, 13036-13044.	2.5	23
69	Chiroptical, linear, and second-order nonlinear optical properties of tetrathiafulvalenylallene: a multifunctional molecular material. Journal of Materials Chemistry C, 2013, 1, 1399.	5.5	23
70	Adsorption Energy Optimization of Co <sub>3</sub> O <sub>4</sub> through Rapid Surface Sulfurization for Efficient Counter Electrode in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2017, 121, 12524-12530.	3.1	23
71	Phase diagram, stability and electronic properties of an Fe-P system under high pressure: a first principles study. RSC Advances, 2017, 7, 15986-15991.	3.6	23
72	Pressure-induced hydride superconductors above 200 K. Matter and Radiation at Extremes, 2021, 6, .	3.9	23

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73	TD-DFT investigation on the low-lying excited states of spiro-bithiophene. Chemical Physics Letters, 2006, 429, 180-184.	2.6	22
74	Theoretical Study on a Novel Series of Fullerene-Containing Organometallics $\text{Fe}(\text{C}_5\text{X}_5)_2$ (X = CH, N). Theoretical Chemistry Accounts, 2011, 128, 257-264.	2.5	22
75	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. Journal of Physical Chemistry C, 2018, 122, 12448-12453.	3.1	22
76	Boron kagome-layer induced intrinsic superconductivity in a $\text{MnB}_2\text{C}_3$ monolayer with a high critical temperature. Physical Review B, 2020, 102, .	3.2	22
77	Superconducting ternary hydrides under high pressure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	22
78	Enhanced Electroluminescence from ZnO Quantum Dot Light-Emitting Diodes via Introducing $\text{Al}_2\text{O}_3$ Retarding Layer and Ag@ZnO Hybrid Nanodots. Advanced Optical Materials, 2017, 5, 1700493.	7.3	21
79	Determination of the absolute configurations of bicyclo[3.1.0]hexane derivatives via electronic circular dichroism, optical rotation dispersion and vibrational circular dichroism spectroscopy and density functional theory calculations. Organic and Biomolecular Chemistry, 2010, 8, 3777.	2.8	20
80	Charge transport and electronic properties of N-heteroquinones: quadruple weak hydrogen bonds and strong $\pi$ - $\pi$ stacking interactions. Theoretical Chemistry Accounts, 2011, 128, 257-264.	1.4	20
81	Isomer dependent molecular packing and carrier mobility of <i>N</i> -phenylcarbazole-phenanthro[9,10- <i>cd</i> ]imidazole based materials as hosts for efficient electrophosphorescence devices. Journal of Materials Chemistry C, 2019, 7, 13486-13492.	5.5	20
82	Quantum chemical study of redox-switchable second-order optical nonlinearity in Keggin-type organoimido derivative $[\text{PW}_{11}\text{O}_{39}(\text{ReNC}_6\text{H}_5)]^{4-}$ ( $n=4$ ). Theoretical Chemistry Accounts, 2009, 122, 265-273.	1.4	19
83	Quantum chemical study of structures, electronic spectrum, and nonlinear optical properties of polynuclear lithium compounds. Computational and Theoretical Chemistry, 2011, 966, 14-19.	2.5	19
84	Enhancement of Exciton Emission from Multilayer $\text{MoS}_2$ at High Temperatures: Intervalley Transfer versus Interlayer Decoupling. Small, 2017, 13, 1700157.	10.0	19
85	Calculations of two-photon absorption cross-sections of stilbene and bis (styryl) benzene derivatives by means of TDDFT-SOS method. Computational and Theoretical Chemistry, 2005, 726, 61-65.	1.5	18
86	Superconducting boron allotropes. Physical Review B, 2020, 101, .	3.2	18
87	Achieving high conductivity p-type $\text{Ga}_2\text{O}_3$ through Al-N and In-N co-doping. Chemical Physics Letters, 2020, 746, 137308.	2.6	18
88	Anisotropic and High-Mobility $\text{C}_3\text{S}$ Monolayer as a Photocatalyst for Water Splitting. Journal of Physical Chemistry Letters, 2021, 12, 8320-8327.	4.6	18
89	Hyperpolarizabilities of para-nitroaniline and bis[4-(dimethylamino)phenyl] squaraine: The effects of functional/basis set based on TDDFT-SOS method. Computational and Theoretical Chemistry, 2006, 773, 9-14.	1.5	17
90	Determination of the Absolute Configuration of Pentacoordinate Chiral Phosphorus Compounds in Solution by Using Vibrational Circular Dichroism Spectroscopy and Density Functional Theory. Chemistry - A European Journal, 2010, 16, 2518-2527.	3.3	17

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91	Diastereomers of the pentacoordinate chiral phosphorus compounds in solution: absolute configurations and predominant conformations. Dalton Transactions, 2010, 39, 6953.	3.3	17
92	Synthesis and characterizations of novel spindle-like terphenyl-type chromophores for non-linear optical materials. Tetrahedron, 2011, 67, 4110-4117.	1.9	17
93	Silicon Framework-Based Lithium Silicides at High Pressures. ACS Applied Materials & Interfaces, 2016, 8, 16761-16767.	8.0	17
94	Pressure-Induced Stable Beryllium Peroxide. Inorganic Chemistry, 2017, 56, 5233-5238.	4.0	17
95	Exploring the Limits of Transition-Metal Fluorination at High Pressures. Angewandte Chemie - International Edition, 2020, 59, 9155-9162.	13.8	17
96	Theoretical investigation of structures, electronic spectra and nonlinear optical properties of gold-pentacene (Au <sub>2</sub> C <sub>22</sub> H <sub>14</sub> ) complexes. Journal of Organometallic Chemistry, 2009, 694, 1266-1272.	1.8	16
97	Redox-switching second-order nonlinear optical responses of N <sup>N</sup> N ruthenium complexes. Computational and Theoretical Chemistry, 2012, 979, 112-118.	2.5	16
98	Theoretical studies of the effect of electron-withdrawing dicyanovinyl group on the electronic and charge-transport properties of fluorene-thiophene oligomers. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	16
99	Theoretical Study on the Rectifying Performance of Organoimido Derivatives of Hexamolybdates. ChemPhysChem, 2013, 14, 610-617.	2.1	16
100	Fluorescent photoswitching of a naphthopyran-benzimidazole dyad with high-degree fluorescent modulation within poly(methyl methacrylate) matrices. Optical Materials, 2013, 35, 1504-1512.	3.6	16
101	Ten-fold coordinated polymorph and metallization of TiO <sub>2</sub> under high pressure. RSC Advances, 2015, 5, 54253-54257.	3.6	16
102	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. Physical Review B, 2021, 103, .	3.2	16
103	SiCP <sub>4</sub> Monolayer with a Direct Band Gap and High Carrier Mobility for Photocatalytic Water Splitting. Journal of Physical Chemistry Letters, 2022, 13, 190-197.	4.6	16
104	DFT/FF study on electronic structure and second-order NLO property of dinuclear gold complex [Au(SeC <sub>2</sub> B <sub>10</sub> H <sub>11</sub> )(PPh <sub>3</sub> )] <sub>2</sub> . Synthetic Metals, 2005, 152, 273-276.	3.9	15
105	Theoretical predication of third-order optical nonlinearities of [Al <sub>4</sub> MAI <sub>4</sub> ] <sup>n+</sup> (n = 0, 2, M = Ti, V and) Tj ETQq1 1,0,784314 rgBT /Ove	1.4	15
106	Nonplanar Donor-Acceptor Chiral Molecules with Large Second-Order Optical Nonlinearities: 1,1,4,4-Tetracyanobuta-1,3-diene Derivatives. Journal of Physical Chemistry A, 2014, 118, 1094-1102.	2.5	15
107	Theoretical study on the second-order nonlinear optical properties of nonconjugated D-π-A chromophores. International Journal of Quantum Chemistry, 2009, 109, 1553-1559.	2.0	14
108	Theoretical study on dithieno[3,2-b:2',3'-d]phosphole derivatives: high-efficiency blue-emitting materials with ambipolar semiconductor behavior. Theoretical Chemistry Accounts, 2010, 127, 419-427.	1.4	14



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109	Photophysical properties of quinoxaline-fused [7]carbohelicene derivatives. RSC Advances, 2015, 5, 72907-72915.	3.6	14
110	Understanding the photophysical properties of chiral dinuclear $\text{Re}(\text{Cp}^*)_2$ complexes and the role of $\text{Re}(\text{Cp}^*)_2$ in their complexes. Dalton Transactions, 2016, 45, 7285-7293.	3.3	14
111	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. Physical Review B, 2019, 100, .	3.2	14
112	Unveiling the Role of Oxygen Vacancy in $\text{Li}_{2-x}\text{MnO}_3$ upon Delithiation. Journal of Physical Chemistry C, 2019, 123, 23403-23409.	3.1	14
113	Anisotropic $\text{PC}_{6-x}\text{N}$ Monolayer with Wide Band Gap and Ultrahigh Carrier Mobility. Journal of Physical Chemistry C, 2020, 124, 4330-4337.	3.1	14
114	Pressure-induced superconductivity in Li-Te electrides. Physical Review B, 2021, 104, .	3.2	14
115	Triphenylamine-based pH chemosensor: Synthesis, crystal structure, photophysical properties and computational studies. Synthetic Metals, 2009, 159, 2497-2501.	3.9	13
116	Determination of the absolute configurations of synthetic daunorubicin analogues using vibrational circular dichroism spectroscopy and density functional theory. Chirality, 2010, 22, 734-743.	2.6	13
117	Theoretical study on the charge transport property of $\text{Pt}(\text{CNtBu})_2(\text{CN})_2$ nanowires induced by $\text{Pt}^{\delta+}\text{Pt}^{\delta-}$ interactions. Dalton Transactions, 2012, 41, 7272.	3.3	13
118	High-temperature driven inter-valley carrier transfer and significant fluorescence enhancement in multilayer $\text{WS}_2$ . Nanoscale Horizons, 2018, 3, 598-605.	8.0	13
119	Pressure-induced new chemistry. Chinese Physics B, 2019, 28, 106106.	1.4	13
120	Exploring the origin of electrochemical performance of Cr-doped $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ . Physical Chemistry Chemical Physics, 2020, 22, 3831-3838.	2.8	13
121	Janus MoPC Monolayer with Superior Electrocatalytic Performance for the Hydrogen Evolution Reaction. ACS Applied Materials & Interfaces, 2022, 14, 7836-7844.	8.0	13
122	Disproportionation of $\text{SO}_2$ at High Pressure and Temperature. Physical Review Letters, 2022, 128, 106001.	7.8	13
123	Charge transport and luminescent properties of $\text{C}_6\text{F}_5\text{Cu}(\text{py})$ and their relationships with cuprophilic interactions: a density functional theory investigation. Theoretical Chemistry Accounts, 2010, 127, 735-742.	1.4	12
124	Effects of the substituting groups and proton abstraction on the nonlinear optical properties of heteroleptic bis-tridentate $\text{Ru}(\text{II})$ complexes. Journal of Organometallic Chemistry, 2011, 696, 3384-3391.	1.8	12
125	TDDFT studies on the structures and ECD spectra of chiral bisarylimidos bearing different lengths of o-alkoxy chain-substituted polyoxomolybdates. Journal of Molecular Graphics and Modelling, 2012, 35, 49-56.	2.4	12
126	Structural and electronic properties of alkali metal peroxides at high pressures. RSC Advances, 2015, 5, 104337-104342.	3.6	12



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127	Photophysical Properties of Chiral Tetraphenylethylene Derivatives with the Fixed Propeller-Like Conformation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5032-5039.	3.1	12
128	Theoretical Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Polyfluoroarylcyanation of Alkynes: Origin of Selectivity for C≡CN Bond Activation. <i>Organometallics</i> , 2018, 37, 2594-2601.	2.3	12
129	Theoretical study on group III elements and F co-doped ZnO. <i>Journal of Alloys and Compounds</i> , 2020, 819, 153012.	5.5	12
130	Design and synthesis of clathrate $\text{LaB}_8$ with superconductivity. <i>Physical Review B</i> , 2021, 104, .	3.2	12
131	Assignment of the absolute configuration of dinuclear zirconium complexes containing two homochiral N atoms using TDDFT calculations of ECD. <i>Chemical Physics Letters</i> , 2011, 502, 266-270.	2.6	11
132	TDDFT studies on chiral organophosphonate substituted divacant Keggin-type polyoxotungstate: diplex multistep-redox-triggered chiroptical and NLO switch. <i>Dalton Transactions</i> , 2012, 41, 10097.	3.3	11
133	Prediction of the Xe-He binary phase diagram at high pressures. <i>Chemical Physics Letters</i> , 2015, 640, 115-118.	2.6	11
134	Synthesis, crystal structures and DNA-binding properties of Cd(II), Cu(II) and Ni(II) complexes with 2-(2-pyridyl)benzothiazole. <i>Synthetic Metals</i> , 2015, 200, 1-6.	3.9	11
135	IrN <sub>4</sub> and IrN <sub>7</sub> as potential high-energy-density materials. <i>Journal of Chemical Physics</i> , 2021, 154, 054706.	3.0	11
136	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4203-4210.	4.6	11
137	Highly Photoluminescent Monolayer MoS <sub>2</sub> and WS <sub>2</sub> Achieved via Superacid Assisted Vacancy RepARATION and Doping Strategy. <i>Laser and Photonics Reviews</i> , 2021, 15, 2100104.	8.7	11
138	BC <sub>6</sub> P Monolayer: Isostructural and Isoelectronic Analogues of Graphene with Desirable Properties for K-Ion Batteries. <i>Chemistry of Materials</i> , 2021, 33, 9262-9269.	6.7	11
139	Theoretical study on the second-order nonlinear optical properties and reorganization energy of silafluorenes and spirobisilafluorenes derivatives. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 249-256.	1.4	10
140	Density Functional Theory Investigation on the Second-Order Nonlinear Optical Properties of Chlorobenzyl- $\alpha$ -Carborane Derivatives. <i>Chinese Journal of Chemistry</i> , 2012, 30, 2349-2355.	4.9	10
141	Theoretical study on the photophysical properties of chiral mononuclear and dinuclear zinc complexes. <i>RSC Advances</i> , 2013, 3, 2241-2247.	3.6	10
142	Understanding photophysical properties of chiral conjugated corrals for organic photovoltaics. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3495-3502.	5.5	10
143	Wide Band Gap P <sub>3</sub> S Monolayer with Anisotropic and Ultrahigh Carrier Mobility. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8481-8488.	4.6	10
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