Guochun Yang

List of Publications by Year
in descending order

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215	5,475	81839	123376
papers	citations	39 h-index	61 g-index

218	218	218	5819
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Organic Polymorphs: Oneâ€Compoundâ€Based Crystals with Molecularâ€Conformationâ€•and Packingâ€Dependent Luminescent Properties. Advanced Materials, 2014, 26, 6168-6173.	11.1	262
2	TiC₃ Monolayer with High Specific Capacity for Sodium-Ion Batteries. Journal of the American Chemical Society, 2018, 140, 5962-5968.	6.6	244
3	Highly Efficient Long-Wavelength Thermally Activated Delayed Fluorescence OLEDs Based on Dicyanopyrazino Phenanthrene Derivatives. ACS Applied Materials & Interfaces, 2017, 9, 9892-9901.	4.0	168
4	Two-Dimensional PC₆ with Direct Band Gap and Anisotropic Carrier Mobility. Journal of the American Chemical Society, 2019, 141, 1599-1605.	6.6	144
5	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. Physical Review Letters, 2016, 116, 057002.	2.9	132
6	Lithium lanthanum titanate perovskite as an anode for lithium ion batteries. Nature Communications, 2020, 11, 3490.	5.8	121
7	Gold as a 6p-Element in Dense Lithium Aurides. Journal of the American Chemical Society, 2016, 138, 4046-4052.	6.6	101
8	Predicted Pressure-Induced Superconducting Transition in Electride <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Li</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="normal">P</mml:mi></mml:mrow></mml:math>. Physical Review Letters, 2019, 122, 097002.	2.9	94
9	Theoretical discussions on electron transport properties of perylene bisimide derivatives with different molecular packings and intermolecular interactions. Journal of Materials Chemistry, 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 singletâ€“triplet splitting. Chemical Communications, 2015, 51, 10632-10635.	2.2	88
11	Theoretical Study on the Electronic Spectrum and the Origin of Remarkably Large Third-Order Nonlinear Optical Properties of Organoimide Derivatives of Hexamolybdates. Journal of Physical Chemistry B, 2006, 110, 23092-23098.	1.2	84
12	Gold with +4 and +6 Oxidation States in AuF₄ and AuF₆. Journal of the American Chemical Society, 2018, 140, 9545-9550.	6.6	80
13	High-Temperature Ferromagnetism in an Fe₃P Monolayer with a Large Magnetic Anisotropy. Journal of Physical Chemistry Letters, 2019, 10, 2733-2738.	2.1	79
14	Stable and metallic two-dimensional TaC₂as an anode material for lithium-ion battery. Journal of Materials Chemistry A, 2017, 5, 18698-18706.	5.2	75
15	Metallic P₃C monolayer as anode for sodium-ion batteries. Journal of Materials Chemistry A, 2019, 7, 405-411.	5.2	75
16	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	1.6	71
17	Nanotube-assembled pine-needle-like CuS as an effective energy booster for sodium-ion storage. Journal of Materials Chemistry A, 2019, 7, 10619-10628.	5.2	70
18	Insight into the role of Li₂S₂ in Liâ€“S batteries: a first-principles study. Journal of Materials Chemistry A, 2015, 3, 8865-8869.	5.2	68

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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.	1.2	60
21	Density Functional Theory Study on the First Hyperpolarizabilities of Organoimido Derivatives of Hexamolybdates. Journal of Physical Chemistry B, 2005, 109, 22332-22336.	1.2	59
22	Theoretical Study on the Second-Order Nonlinear Optical Properties of Asymmetric Spirosilabifluorene Derivatives. Journal of Physical Chemistry A, 2006, 110, 4817-4821.	1.1	58
23	Photocatalytic Reduction of Graphene Oxideâ€“TiO₂ Nanocomposites for Improving Resistiveâ€Switching Memory Behaviors. Small, 2018, 14, e1801325.	5.2	58
24	Effect of Ï€-Conjugated Length of Bridging Ligand on the Optoelectronic Properties of Platinum(II) Dimers. Inorganic Chemistry, 2008, 47, 2347-2355.	1.9	54
25	A Stable, Magnetic, and Metallic Li3O4Compound as a Discharge Product in a Liâ€“Air Battery. Journal of Physical Chemistry Letters, 2014, 5, 2516-2521.	2.1	52
26	Accurate identification of layer number for few-layer WS₂and WSe₂via spectroscopic study. Nanotechnology, 2018, 29, 124001.	1.3	52
27	Structure and Electronic Properties of Fe₂SH₃ Compound under High Pressure. Inorganic Chemistry, 2016, 55, 11434-11439.	1.9	50
28	Anisotropic Janus SiP₂ Monolayer as a Photocatalyst for Water Splitting. Journal of Physical Chemistry Letters, 2021, 12, 2464-2470.	2.1	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.	2.7	48
30	Reversible Redox-Switchable Second-Order Optical Nonlinearity in Polyoxometalate: A Quantum Chemical Study of [PW₁₁O₃₉(ReN)]^{nâ^’} (n = 3â^’7). Inorganic Chemistry, 2008, 47, 5245-5252.	1.9	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.	2.7	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.	1.5	45
33	Prediction of Second-Order Optical Nonlinearity of Trisorganotin-Substituted Î²-Keggin Polyoxotungstate. Inorganic Chemistry, 2006, 45, 7864-7868.	1.9	44
34	Understanding the role of lithium sulfide clusters in lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2017, 5, 9293-9298.	5.2	43
35	Pressure-induced stable BeN 4 as a high-energy density material. Journal of Power Sources, 2017, 365, 155-161.	4.0	43
36	FeP₃ monolayer as a high-efficiency catalyst for hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 25665-25671.	5.2	43

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37	Recent Advances and Applications of Inorganic Electrides. Journal of Physical Chemistry Letters, 2020, 11, 3841-3852.	2.1	43
38	Theoretical Study on Photophysical and Charge Transport Properties of 1,6-Bis(2-hydroxyphenol)pyridylboron Bis(4-n-butylphenyl)phenyleneamine Compound. Journal of Physical Chemistry A, 2006, 110, 8758-8762.	1.1	41
39	Conformations of Serine in Aqueous Solutions as Revealed by Vibrational Circular Dichroism. ChemPhysChem, 2012, 13, 1272-1281.	1.0	41
40	Conformational Distributions of Nâ€Acetylâ€<scp>L</scp>â€cysteine in Aqueous Solutions: A Combined Implicit and Explicit Solvation Treatment of VA and VCD Spectra. ChemPhysChem, 2012, 13, 2310-2321.	1.0	41
41	O₂ Adsorption Associated with Sulfur Vacancies on MoS₂ Microspheres. Inorganic Chemistry, 2019, 58, 2169-2176.	1.9	40
42	IrF₈ Molecular Crystal under High Pressure. Journal of the American Chemical Society, 2019, 141, 5409-5414.	6.6	40
43	Quantum Chemical Study of Structures, Electronic Spectrum, and Nonlinear Optical Properties of Goldâ"Pentacene Complexes. Organometallics, 2007, 26, 2082-2087.	1.1	38
44	Theoretical Study on Photophysical Properties of Phenolpyridyl Boron Complexes. Journal of Physical Chemistry A, 2007, 111, 2739-2744.	1.1	38
45	Pressure-Induced Stable Li₅P for High-Performance Lithium-Ion Batteries. Journal of Physical Chemistry C, 2017, 121, 21199-21205.	1.5	36
46	A hypervalent and cubically coordinated molecular phase of IF₈predicted at high pressure. Chemical Science, 2019, 10, 2543-2550.	3.7	36
47	How Do the Different Defect Structures and Element Substitutions Affect the Nonlinear Optical Properties of Lacunary Keggin Polyoxometalates? A DFT Study. European Journal of Inorganic Chemistry, 2006, 2006, 4179-4183.	1.0	33
48	Vibrational absorption, vibrational circular dichroism, and theoretical studies of methyl lactate self-aggregation and methyl lactate-methanol intermolecular interactions. Journal of Chemical Physics, 2010, 132, 234513.	1.2	33
49	DFT Studies on second-order nonlinear optical properties of mono (salicylaldiminato) Nickel(II) polyenyl Schiff base metal complexes. Chemical Physics Letters, 2007, 443, 163-168.	1.2	31
50	Computational study on second-order nonlinear optical (NLO) properties of a novel class of two-dimensional Î›- and W-shaped sandwich metallocarborane-containing chromophores. Journal of Organometallic Chemistry, 2011, 696, 2380-2387.	0.8	31
51	The effects of self-aggregation on the vibrational circular dichroism and optical rotation measurements of glycidol. Physical Chemistry Chemical Physics, 2008, 10, 6787.	1.3	30
52	Chiroptical, linear, and second-order nonlinear optical properties of binaphthol derivatives. Organic and Biomolecular Chemistry, 2012, 10, 8418.	1.5	30
53	Chirality recognition of the protonated serine dimer and octamer by infrared multiphoton dissociation spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 1873-1886.	1.3	30
54	DFT characterization on the mechanism of water splitting catalyzed by single-Ru-substituted polyoxometalates. Dalton Transactions, 2013, 42, 10617.	1.6	30

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55	Computational predictions of twoâ€dimensional anode materials of metalâ€ion batteries. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1473.	6.2	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.	1.5	29
57	Nonmetallic FeH₆ under High Pressure. Journal of Physical Chemistry C, 2018, 122, 12022-12028.	1.5	29
58	An Organic Emitter Displaying Dual Emissions and Efficient Delayed Fluorescence White OLEDs. Advanced Optical Materials, 2019, 7, 1801667.	3.6	28
59	Photophysical properties of azaboradibenzo[6]helicene derivatives. Journal of Materials Chemistry C, 2013, 1, 2354.	2.7	27
60	Theoretical insights into [PMo12O40]3â^' grafted on single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 9177.	1.3	27
61	Theoretical Study on the Chiroptical Optical Properties of Chiral Fullerene C₆₀Derivative. Journal of Physical Chemistry A, 2011, 115, 13356-13363.	1.1	26
62	Hexagonal BC₂N with Remarkably High Hardness. Journal of Physical Chemistry C, 2018, 122, 6801-6807.	1.5	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.	0.8	25
64	Complementary Resistive Switching Observed in Graphene Oxide-Based Memory Device. IEEE Electron Device Letters, 2018, 39, 488-491.	2.2	25
65	The relationship between intermolecular interactions and charge transport properties of trifluoromethylated polycyclic aromatic hydrocarbons. Organic Electronics, 2014, 15, 1896-1905.	1.4	24
66	Element substitution of kesterite Cu2ZnSnS4 for efficient counter electrode of dye-sensitized solar cells. Scientific Reports, 2018, 8, 8714.	1.6	24
67	Predication of second-order optical nonlinearity of [(Bu2tIm)AuX] (X=halogen) using time-dependent density-functional theory combined with sum-over-states method. Journal of Chemical Physics, 2005, 123, 134302.	1.2	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.	1.1	23
69	Chiroptical, linear, and second-order nonlinear optical properties of tetrathiafulvalenylallene: a multifunctional molecular material. Journal of Materials Chemistry C, 2013, 1, 1399.	2.7	23
70	Adsorption Energy Optimization of Co₃O₄ through Rapid Surface Sulfurization for Efficient Counter Electrode in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2017, 121, 12524-12530.	1.5	23
71	Phase diagram, stability and electronic properties of an Feâ€“P system under high pressure: a first principles study. RSC Advances, 2017, 7, 15986-15991.	1.7	23
72	Pressure-induced hydride superconductors above 200 K. Matter and Radiation at Extremes, 2021, 6, .	1.5	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.	1.2	22
74	Theoretical Study on a Novel Series of Fullerene-Containing Organometallics Fe(Î·5-C55X5)2 (X = CH, N,) Tj ETQq0 0 0 rgBT /Overlock 10 8086-8092.	1.1	22
75	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. Journal of Physical Chemistry C, 2018, 122, 12448-12453.	1.5	22
76	Boron kagome-layer induced intrinsic superconductivity in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MnB</mml:mi><mml:mn>3</mml:mn></mml:msub></mml monolayer with a high critical temperature. Physical Review B, 2020, 102, .	1.1	22
77	Superconducting ternary hydrides under high pressure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	22
78	Enhanced Electroluminescence from ZnO Quantum Dot Lightâ€Emitting Diodes via Introducing Al₂O₃ Retarding Layer and Ag@ZnO Hybrid Nanodots. Advanced Optical Materials, 2017, 5, 1700493.	3.6	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.	1.5	20
80	Charge transport and electronic properties of N-heteroquinones: quadruple weak hydrogen bonds and strong Ï€â€“Ï€ stacking interactions. Theoretical Chemistry Accounts, 2011, 128, 257-264.	0.5	20
81	Isomer dependent molecular packing and carrier mobility of N-phenylcarbazoleâ€“phenanthro[9,10-d]imidazole based materials as hosts for efficient electrophosphorescence devices. Journal of Materials Chemistry C, 2019, 7, 13486-13492.	2.7	20
82	Quantum chemical study of redox-switchable second-order optical nonlinearity in Keggin-type organoimido derivative [PW11O39(ReNC6H5)] nâ¯ (nÂ=Â2â€“4). Theoretical Chemistry Accounts, 2009, 122, 265-273.	0.5	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.	1.1	19
84	Enhancement of Exciton Emission from Multilayer MoS₂ at High Temperatures: Intervalley Transfer versus Interlayer Decoupling. Small, 2017, 13, 1700157.	5.2	19
85	Calculations of two-photon absorption cross-sections of stibene 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, .	1.1	18
87	Achieving high conductivity p-type Ga2O3 through Al-N and In-N co-doping. Chemical Physics Letters, 2020, 746, 137308.	1.2	18
88	Anisotropic and High-Mobility C₃S Monolayer as a Photocatalyst for Water Splitting. Journal of Physical Chemistry Letters, 2021, 12, 8320-8327.	2.1	18
89	Hyperpolarizabilities of para-nitroaniline and bis[4-(dimethylamino)phenyl] squaraine: The effects of functional/basis set based on TDDFTâ€“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.	1.7	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.	1.6	17
92	Synthesis and characterizations of novel spindle-like terphenyl-type chromophores for non-linear optical materials. Tetrahedron, 2011, 67, 4110-4117.	1.0	17
93	Silicon Framework-Based Lithium Silicides at High Pressures. ACS Applied Materials & Interfaces, 2016, 8, 16761-16767.	4.0	17
94	Pressure-Induced Stable Beryllium Peroxide. Inorganic Chemistry, 2017, 56, 5233-5238.	1.9	17
95	Exploring the Limits of Transitionâ€Metal Fluorination at High Pressures. Angewandte Chemie - International Edition, 2020, 59, 9155-9162.	7.2	17
96	Theoretical investigation of structures, electronic spectra and nonlinear optical properties of gold-pentacene (Au2C22H14) complexes. Journal of Organometallic Chemistry, 2009, 694, 1266-1272.	0.8	16
97	Redox-switching second-order nonlinear optical responses of N^N^N ruthenium complexes. Computational and Theoretical Chemistry, 2012, 979, 112-118.	1.1	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.	0.5	16
99	Theoretical Study on the Rectifying Performance of Organoimido Derivatives of Hexamolybdates. ChemPhysChem, 2013, 14, 610-617.	1.0	16
100	Fluorescent photoswitching of a naphthopyranâ€“benzimidazole dyad with high-degree fluorescent modulation within poly(methyl methacrylate) matrices. Optical Materials, 2013, 35, 1504-1512.	1.7	16
101	Ten-fold coordinated polymorph and metallization of TiO₂under high pressure. RSC Advances, 2015, 5, 54253-54257.	1.7	16
102	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. Physical Review B, 2021, 103, .	1.1	16
103	SiCP₄ Monolayer with a Direct Band Gap and High Carrier Mobility for Photocatalytic Water Splitting. Journal of Physical Chemistry Letters, 2022, 13, 190-197.	2.1	16
104	DFT/FF study on electronic structure and second-order NLO property of dinuclear gold complex [Au(SeC2B10H11)(PPh3)]2. Synthetic Metals, 2005, 152, 273-276.	2.1	15
105	Theoretical predication of third-order optical nonlinearities of [Al4MAl4] nâ^' (nÂ= 0â€“2, M = Ti, V and) Tj ETQq1 1 0.784314 rgBT /O	0.5	15
106	Nonplanar Donorâ€“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.	1.1	15
107	Theoretical study on the secondâ€order nonlinear optical properties of nonconjugated Dâ€Ïâ€A chromophores. International Journal of Quantum Chemistry, 2009, 109, 1553-1559.	1.0	14
108	Theoretical study on dithieno[3,2-b:2â€²,3â€²-d]phosphole derivatives: high-efficiency blue-emitting materials with ambipolar semiconductor behavior. Theoretical Chemistry Accounts, 2010, 127, 419-427.	0.5	14

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109	Photophysical properties of quinoxaline-fused [7]carbohelicene derivatives. RSC Advances, 2015, 5, 72907-72915.	1.7	14
110	Understanding the photophysical properties of chiral dinuclear Re(<scp>i</scp>) complexes and the role of Re(<scp>i</scp>) in their complexes. Dalton Transactions, 2016, 45, 7285-7293.	1.6	14
111	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. Physical Review B, 2019, 100, .	1.1	14
112	Unveiling the Role of Oxygen Vacancy in Li₂MnO₃ upon Delithiation. Journal of Physical Chemistry C, 2019, 123, 23403-23409.	1.5	14
113	Anisotropic PC₆N Monolayer with Wide Band Gap and Ultrahigh Carrier Mobility. Journal of Physical Chemistry C, 2020, 124, 4330-4337.	1.5	14
114	Pressure-induced superconductivity in Li-Te electrides. Physical Review B, 2021, 104, .	1.1	14
115	Triphenylamine-based pH chemosensor: Synthesis, crystal structure, photophysical properties and computational studies. Synthetic Metals, 2009, 159, 2497-2501.	2.1	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.	1.3	13
117	Theoretical study on the charge transport property of Pt(CNtBu)2(CN)2 nanowires induced by Ptâ‹¯Pt interactions. Dalton Transactions, 2012, 41, 7272.	1.6	13
118	High-temperature driven inter-valley carrier transfer and significant fluorescence enhancement in multilayer WS₂. Nanoscale Horizons, 2018, 3, 598-605.	4.1	13
119	Pressure-induced new chemistry. Chinese Physics B, 2019, 28, 106106.	0.7	13
120	Exploring the origin of electrochemical performance of Cr-doped LiNi0.5Mn1.5O4. Physical Chemistry Chemical Physics, 2020, 22, 3831-3838.	1.3	13
121	Janus MoPC Monolayer with Superior Electrocatalytic Performance for the Hydrogen Evolution Reaction. ACS Applied Materials & Interfaces, 2022, 14, 7836-7844.	4.0	13
122	Disproportionation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> at High Pressure and Temperature. Physical Review Letters, 2022, 128, 106001.	2.9	13
123	Charge transport and luminescent properties of C6F5Cu(py) and their relationships with cuprophilic interactions: a density functional theory investigation. Theoretical Chemistry Accounts, 2010, 127, 735-742.	0.5	12
124	Effects of the substituting groups and proton abstraction on the nonlinear optical properties of heteroleptic bis-tridentate Ru(II) complexes. Journal of Organometallic Chemistry, 2011, 696, 3384-3391.	0.8	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.	1.3	12
126	Structural and electronic properties of alkali metal peroxides at high pressures. RSC Advances, 2015, 5, 104337-104342.	1.7	12

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127	Photophysical Properties of Chiral Tetraphenylethylene Derivatives with the Fixed Propeller-Like Conformation. Journal of Physical Chemistry C, 2018, 122, 5032-5039.	1.5	12
128	Theoretical Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Polyfluoroarylcyanation of Alkynes: Origin of Selectivity for Câ€“CN Bond Activation. Organometallics, 2018, 37, 2594-2601.	1.1	12
129	Theoretical study on group III elements and F co-doped ZnO. Journal of Alloys and Compounds, 2020, 819, 153012.	2.8	12
130	Design and synthesis of clathrate <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaB</mml:mi><mml:mn>8</mml:mn></mml:msub></mm with superconductivity. Physical Review B, 2021, 104, .	1.1	12
131	Assignment of the absolute configuration of dinuclear zirconium complexes containing two homochiral N atoms using TDDFT calculations of ECD. Chemical Physics Letters, 2011, 502, 266-270.	1.2	11
132	TDDFT studies on chiral organophosphonate substituted divacant Keggin-type polyoxotungstate: diplex multistep-redox-triggered chiroptical and NLO switch. Dalton Transactions, 2012, 41, 10097.	1.6	11
133	Prediction of the Xeâ€“He binary phase diagram at high pressures. Chemical Physics Letters, 2015, 640, 115-118.	1.2	11
134	Synthesis, crystal structures and DNA-binding properties of Cd(II), Cu(II) and Ni(II) complexes with 2-(2-pyridyl)benzothiazole. Synthetic Metals, 2015, 200, 1-6.	2.1	11
135	IrN4 and IrN7 as potential high-energy-density materials. Journal of Chemical Physics, 2021, 154, 054706.	1.2	11
136	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 4203-4210.	2.1	11
137	Highly Photoluminescent Monolayer MoS₂ and WS₂ Achieved via Superacid Assisted Vacancy Reparation and Doping Strategy. Laser and Photonics Reviews, 2021, 15, 2100104.	4.4	11
138	BC₆P Monolayer: Isostructural and Isoelectronic Analogues of Graphene with Desirable Properties for K-Ion Batteries. Chemistry of Materials, 2021, 33, 9262-9269.	3.2	11
139	Theoretical study on the second-order nonlinear optical properties and reorganization energy of silafluorenes and spirobisilafluorenes derivatives. Theoretical Chemistry Accounts, 2011, 128, 249-256.	0.5	10
140	Density Functional Theory Investigation on the Secondâ€Order Nonlinear Optical Properties of Chlorobenzylâ€oâ€Carborane Derivatives. Chinese Journal of Chemistry, 2012, 30, 2349-2355.	2.6	10
141	Theoretical study on the photophysical properties of chiral mononuclear and dinuclear zinc complexes. RSC Advances, 2013, 3, 2241-2247.	1.7	10
142	Understanding photophysical properties of chiral conjugated corrals for organic photovoltaics. Journal of Materials Chemistry C, 2017, 5, 3495-3502.	2.7	10
143	Wide Band Gap P₃S Monolayer with Anisotropic and Ultrahigh Carrier Mobility. Journal of Physical Chemistry Letters, 2021, 12, 8481-8488.	2.1	10
144	Strainâ€Induced Magnetism in MSi₂N₄ (M = V, Cr): A Firstâ€Principles Study. Annalen Der Physik, 2021, 533, 2100273.	0.9	10

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145	Janus Mo₂P₃ Monolayer as an Electrocatalyst for Hydrogen Evolution. ACS Applied Materials & Interfaces, 2021, 13, 57422-57429.	4.0	10
146	A superconducting boron allotrope featuring anticlinal pentapyramids. Journal of Materials Chemistry C, 2022, 10, 672-679.	2.7	10
147	Bonding-unsaturation-dependent superconductivity in P-rich sulfides. Matter and Radiation at Extremes, 2022, 7, .	1.5	10
148	Quantum chemistry studies on the Ruâ€“M interactions and the 31P NMR in [Ru(CO)3(Ph2Ppy)2(MCl2)] (M=Zn, Cd, Hg). Journal of Organometallic Chemistry, 2006, 691, 1927-1933.	0.8	9
149	Theoretical investigation on two-dimensional molecule-based second-order nonlinear optical materials of the disubstituted o-carborane derivatives. Computational and Theoretical Chemistry, 2012, 992, 142-149.	1.1	9
150	Theoretical study on photophysical properties of novel bis(BF₂)â€2,2â€²â€bidipyrrins dyes: Effect of variation in monomer structure. International Journal of Quantum Chemistry, 2012, 112, 440-452.	1.0	9
151	Achieving high hydrogen evolution reaction activity of a Mo₂C monolayer. Physical Chemistry Chemical Physics, 2020, 22, 26189-26199.	1.3	9
152	Fabrication of Alkali Metal Boride: Honeycombâ€Like Structured NaB 4 with High Hardness and Excellent Electrical Conductivity. Advanced Functional Materials, 0, , 2110872.	7.8	9
153	THEORETICAL STUDY ON THE SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF C,B-SUBSTITUTED CARBORANE CONJUGATED DERIVATIVES. Journal of Theoretical and Computational Chemistry, 2012, 11, 1121-1133.	1.8	8
154	Structural and Superconducting Properties of Tungsten Hydrides Under High Pressure. Frontiers in Physics, 2018, 6, .	1.0	8
155	Achieving high transparent Î²-Ga2O3 through AlGa-InGa-VO. Journal of Alloys and Compounds, 2019, 792, 405-410.	2.8	8
156	The photophysical properties of cycloparaphenylene-based compounds with figure-eight configurations. New Journal of Chemistry, 2020, 44, 12185-12193.	1.4	8
157	Pressure-induced Naâ€“Au compounds with novel structural units and unique charge transfer. Physical Chemistry Chemical Physics, 2021, 23, 6455-6461.	1.3	8
158	Pressure-induced yttrium oxides with unconventional stoichiometries and novel properties. Physical Review Materials, 2021, 5, .	0.9	8
159	Superconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LaP</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> with graphenelike phosphorus layers. Physical Review B, 2022, 105, .	1.1	8
160	Superconducting Li10Se electride under pressure. Journal of Chemical Physics, 2022, 156, .	1.2	8
161	Theoretical studies on one- and two-photon absorption properties of rubrene and its derivatives. Synthetic Metals, 2006, 156, 1218-1224.	2.1	7
162	Theoretical study on the electronic structures and optical properties of oxadisilole-substituted acenes. Chemical Physics Letters, 2008, 466, 37-43.	1.2	7

#	Article	IF	Citations
163	Cooperative enhancement of two-photon absorption cross sections in three-branched oligofluorene with boron center. Computational and Theoretical Chemistry, 2008, 855, 69-76.	1.5	7
164	A theoretical study of ambipolar organic transport material: 1,4-Bis(pentafluorobenzyl)[60]-fullerene. Chemical Physics Letters, 2011, 506, 255-259.	1.2	7
165	Theoretical investigations on electronic spectra and the redox-switchable second-order nonlinear optical responses of rhodium(I)-9,10-phenanthrenediimine complexes. Journal of Molecular Graphics and Modelling, 2012, 33, 19-25.	1.3	7
166	Chiral macrocyclic imine nickel(II) coordination complexes with diverse photophysical properties. Dyes and Pigments, 2017, 140, 70-78.	2.0	7
167	Unveiling photophysical properties of phenanthro[9,10-d]imidazole derivatives for organic light-emitting diodes. Organic Electronics, 2017, 50, 220-227.	1.4	7
168	Mixedâ€valence Compounds: AuO₂ and AuS. ChemPhysChem, 2018, 19, 2989-2994.	1.0	7
169	Prediction of novel boronâ€“carbon based clathrates. Physical Chemistry Chemical Physics, 2022, 24, 16884-16890.	1.3	7
170	Density functional study of magnetic exchange of dinuclear manganese complexes with the heteropolymolyanion: [MnII 2(X n+Mo9O33)2]2(nâ^'10)â^' (X = PV, AsV, SeVI). Science in China Series B: Chemistry, 2008, 51, 1174-1181.	0.8	6
171	The effect of multiple weak interactions on the charge transport ability in polymorphs. Synthetic Metals, 2011, 161, 1073-1078.	2.1	6
172	Computational study of chiral molecules with high intrinsic hyperpolarizabilities. Molecular Physics, 2012, 110, 333-341.	0.8	6
173	Secondâ€order nonlinear optical responses switching of Nâ^§Nâ^§N ruthenium carboxylate complexes with protonâ€electron transfer. International Journal of Quantum Chemistry, 2012, 112, 779-788.	1.0	6
174	Tetragonal Structure BC₄ as a Superhard Material. Journal of Physical Chemistry C, 2017, 121, 10119-10123.	1.5	6
175	Unveiling the Photophysical Properties of Boron Heptaaryldipyrromethene Derivatives. ChemPhysChem, 2018, 19, 2751-2757.	1.0	6
176	Unraveling the synergetic mechanism of physisorption and chemisorption in laser-irradiated monolayer WS2. Nano Research, 2021, 14, 4274-4280.	5.8	6
177	Theoretical study on characteristics of structure and vibrational frequency of spiro-linked complex Zn(PyIm)2 (PyIm = 2(2â€²-pyridine)-imidazole) in excited state. Chemical Physics Letters, 2006, 418, 302-306.	1.2	5
178	THEORETICAL INVESTIGATION ON SECOND-ORDER NONLINEAR OPTICAL PROPERTIES AND REDOX-SWITCHING OF PHENYL NITRONYL-NITROXIDE RADICAL DERIVATIVES. Journal of Theoretical and Computational Chemistry, 2012, 11, 1075-1088.	1.8	5
179	The effect of intermolecular interactions on the charge transport properties of thiazole/thiophene-based oligomers with trifluoromethylphenyl. Journal of Molecular Graphics and Modelling, 2014, 51, 79-85.	1.3	5
180	Electron transport via phenylâ€“perfluorophenyl interaction in crystals of fluorine-substituted dibenzalacetones. RSC Advances, 2014, 4, 50188-50194.	1.7	5

#	Article	IF	Citations
181	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. RSC Advances, 2015, 5, 104426-104432.	1.7	5
182	Structural transitions and electronic properties of sodium superoxide at high pressures. RSC Advances, 2016, 6, 67910-67915.	1.7	5
183	Theoretical study on the photophysical properties of boron-fused double helicenes. RSC Advances, 2017, 7, 56543-56549.	1.7	5
184	Pressure-stabilized graphene-like P layer in superconducting LaP₂. Physical Chemistry Chemical Physics, 2022, 24, 6469-6475.	1.3	5
185	Theoretical study on thiophene-based double helicenes with intrinsic large second-order nonlinear optical response. RSC Advances, 2016, 6, 84705-84711.	1.7	4
186	Memory Devices: Photocatalytic Reduction of Graphene Oxide-TiO2 Nanocomposites for Improving Resistive-Switching Memory Behaviors (Small 29/2018). Small, 2018, 14, 1870136.	5.2	4
187	Unconventional stable stoichiometry of vanadium peroxide. Physical Chemistry Chemical Physics, 2020, 22, 11460-11466.	1.3	4
188	Pressure-stabilized hexafluorides of first-row transition metals. Physical Chemistry Chemical Physics, 2022, 24, 1736-1742.	1.3	4
189	DFT Study on Second-order Nonlinear Optical Properties of a Series of Three-dimensional Cobalt(II) Metal Complexes. Acta Physico-chimica Sinica, 2006, 22, 836-839.	0.6	3
190	The modulation of electronic and optical properties of OXD-X through introduction of the electron-withdrawing groups: A DFT study. Journal of Molecular Graphics and Modelling, 2010, 28, 427-434.	1.3	3
191	Determination of the charge transport abilities of polymorphs [C6F5Cu]2(4,4â€²-bipy) with different interactions: a density functional theoretical investigation. Theoretical Chemistry Accounts, 2011, 129, 45-51.	0.5	3
192	Pressure-induced reappearance of superconductivity in the oC24 phase of lithium. Solid State Communications, 2016, 225, 7-11.	0.9	3
193	Nickel Hydrides under High Pressure. Journal of Physical Chemistry C, 2019, 123, 24243-24247.	1.5	3
194	Theoretical considerations of superconducting HfBH2 and HfB2H under high pressure. Journal of Applied Physics, 2021, 130, 153904.	1.1	3
195	The metallic C6S monolayer with high specific capacity for K-ion batteries. Materials Today Chemistry, 2022, 25, 100951.	1.7	3
196	Theoretical Study on One- and Two-Photon Absorption Properties of PPV Derivative with Electron-Donor Phenylanthracene as Pendent Group. Chinese Journal of Chemistry, 2007, 25, 465-471.	2.6	2
197	Photophysical properties of chiral covalent organic cages. Computational and Theoretical Chemistry, 2017, 1120, 1-7.	1.1	2
198	Structural and electronic properties of tungsten oxides under high pressures. Journal of Physics Condensed Matter, 2020, 32, 085403.	0.7	2

#	Article	IF	Citations
199	Tailoring p-type conductivity of aluminum nitride via transition metal and fluorine doping. Journal of Alloys and Compounds, 2021, 862, 158017.	2.8	2
200	Superconducting ScP4 with a novel phosphorus framework. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	1.1	2
201	Au with sp³ Hybridization in Li₅AuP₂. Journal of Physical Chemistry Letters, 2022, 13, 236-242.	2.1	2
202	THE INVESTIGATION ON ELECTRONIC STRUCTURE AND SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF IIâ€“VI SEMICONDUCTOR CLUSTERS BY TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. Journal of Theoretical and Computational Chemistry, 2007, 06, 585-594.	1.8	1
203	Theoretical Investigation on Electronic Transition of Tris(8â€quinolinolate) Aluminum Grafted on Poly(pâ€phenylenevinylene) Units with the Localizedâ€densityâ€matrix Method. Chinese Journal of Chemistry, 2009, 27, 1891-1896.	2.6	1
204	The influence of Mâ€¦M attraction on nonlinear optical properties of (XMPH₃)₂ (X = F, Cl; and M = Au, Ag and Cu): A theoretical study. International Journal of Quantum Chemistry, 2010, 110, 865-873.	1.0	1
205	Theoretical study on the second-order nonlinear optical properties of gold (III) alkyl complexes. Synthetic Metals, 2009, 159, 2406-2409.	2.1	1
206	Electronic structure and second-order nonlinear optical property of chiral peropyrenes. Journal of Molecular Modeling, 2019, 25, 220.	0.8	1
207	Exploring the Limits of Transitionâ€Metal Fluorination at High Pressures. Angewandte Chemie, 2020, 132, 9240-9247.	1.6	1
208	Prediction of new thermodynamically stable ZnN2O3 at high pressure. Physical Chemistry Chemical Physics, 2020, 22, 10941-10948.	1.3	1
209	A Semiconducting Cationic Squareâ€Grid Network with Fe III Centers Displaying Unusual Dynamic Behavior. European Journal of Inorganic Chemistry, 2020, 2020, 1255-1259.	1.0	1
210	Semiconducting MnB₅ monolayer as a potential photovoltaic material. Journal of Physics Condensed Matter, 2021, 33, 175702.	0.7	1
211	A new MoCN monolayer containing stable cyano structural units as a high-efficiency catalyst for the hydrogen evolution reaction. Nanoscale, 2022, , .	2.8	1
212	Theoretical study on photophysical properties of Pt(II) triarylborons with a 2,2-bpy core derivatives. Journal of Molecular Graphics and Modelling, 2013, 44, 311-317.	1.3	0
213	Mixed-valence Compounds: AuO2 and AuS. ChemPhysChem, 2018, 19, 2971-2971.	1.0	0
214	Understanding photophysical properties of iridium complexes with N-(5-phenyl-1,3,4-oxadiazol-2-yl)-diphenylphosphinic amide as the ancillary ligand. New Journal of Chemistry, 2019, 43, 16975-16980.	1.4	0
215	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ba</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> phase featuring v-shape <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> unit at high pressure. Physical Review Research, 2022, 4, .	1.3	0