Guochun Yang

List of Publications by Year
in descending order

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215 papers	5,475 citations	81900 39 h-index	123424 61 g-index
218 all docs	218 docs citations	218 times ranked	5819 citing authors

#	Article	IF	Citations
1	Superconducting ternary hydrides under high pressure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	22
2	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 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, .	3.2	8
3	Pressure-stabilized hexafluorides of first-row transition metals. Physical Chemistry Chemical Physics, 2022, 24, 1736-1742.	2.8	4
4	A new MoCN monolayer containing stable cyano structural units as a high-efficiency catalyst for the hydrogen evolution reaction. Nanoscale, 2022, , .	5.6	1
5	A superconducting boron allotrope featuring anticlinal pentapyramids. Journal of Materials Chemistry C, 2022, 10, 672-679.	5.5	10
6	Janus MoPC Monolayer with Superior Electrocatalytic Performance for the Hydrogen Evolution Reaction. ACS Applied Materials & Interfaces, 2022, 14, 7836-7844.	8.0	13
7	Pressure-stabilized graphene-like P layer in superconducting LaP₂. Physical Chemistry Chemical Physics, 2022, 24, 6469-6475.	2.8	5
8	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.	7.8	13
9	Superconducting ScP4 with a novel phosphorus framework. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	2.3	2
10	SiCP₄ 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
11	Au with sp³ Hybridization in Li₅AuP₂. Journal of Physical Chemistry Letters, 2022, 13, 236-242.	4.6	2
12	Semiconducting <mml:math 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, .	3.6	0
13	Superconducting Li10Se electride under pressure. Journal of Chemical Physics, 2022, 156, .	3.0	8
14	Prediction of novel boronâ€“carbon based clathrates. Physical Chemistry Chemical Physics, 2022, 24, 16884-16890.	2.8	7
15	The metallic C6S monolayer with high specific capacity for K-ion batteries. Materials Today Chemistry, 2022, 25, 100951.	3.5	3
16	Bonding-unsaturation-dependent superconductivity in P-rich sulfides. Matter and Radiation at Extremes, 2022, 7, .	3.9	10
17	Tailoring p-type conductivity of aluminum nitride via transition metal and fluorine doping. Journal of Alloys and Compounds, 2021, 862, 158017.	5.5	2
18	Pressure-induced Naâ€“Au compounds with novel structural units and unique charge transfer. Physical Chemistry Chemical Physics, 2021, 23, 6455-6461.	2.8	8

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19	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
20	IrN4 and IrN7 as potential high-energy-density materials. Journal of Chemical Physics, 2021, 154, 054706.	3.0	11
21	Anisotropic Janus SiP₂ Monolayer as a Photocatalyst for Water Splitting. Journal of Physical Chemistry Letters, 2021, 12, 2464-2470.	4.6	49
22	Semiconducting MnB₅ monolayer as a potential photovoltaic material. Journal of Physics Condensed Matter, 2021, 33, 175702.	1.8	1
23	Pressure-induced yttrium oxides with unconventional stoichiometries and novel properties. Physical Review Materials, 2021, 5, .	2.4	8
24	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 4203-4210.	4.6	11
25	Anisotropic and High-Mobility C₃S Monolayer as a Photocatalyst for Water Splitting. Journal of Physical Chemistry Letters, 2021, 12, 8320-8327.	4.6	18
26	Unraveling the synergetic mechanism of physisorption and chemisorption in laser-irradiated monolayer WS2. Nano Research, 2021, 14, 4274-4280.	10.4	6
27	Wide Band Gap P₃S Monolayer with Anisotropic and Ultrahigh Carrier Mobility. Journal of Physical Chemistry Letters, 2021, 12, 8481-8488.	4.6	10
28	Strainâ€Induced Magnetism in MSi₂N₄ (M = V, Cr): A Firstâ€Principles Study. Annalen Der Physik, 2021, 533, 2100273.	2.4	10
29	Pressure-induced superconductivity in Li-Te electrides. Physical Review B, 2021, 104, .	3.2	14
30	Pressure-induced hydride superconductors above 200 K. Matter and Radiation at Extremes, 2021, 6, .	3.9	23
31	Theoretical considerations of superconducting HfBH2 and HfB2H under high pressure. Journal of Applied Physics, 2021, 130, 153904.	2.5	3
32	Janus Mo₂P₃ Monolayer as an Electrocatalyst for Hydrogen Evolution. ACS Applied Materials & Interfaces, 2021, 13, 57422-57429.	8.0	10
33	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></m with superconductivity. Physical Review B, 2021, 104, .	3.2	12
34	Highly Photoluminescent Monolayer MoS₂ and WS₂ Achieved via Superacid Assisted Vacancy Reparation and Doping Strategy. Laser and Photonics Reviews, 2021, 15, 2100104.	8.7	11
35	BC₆P Monolayer: Isostructural and Isoelectronic Analogues of Graphene with Desirable Properties for K-Ion Batteries. Chemistry of Materials, 2021, 33, 9262-9269.	6.7	11
36	Structural and electronic properties of tungsten oxides under high pressures. Journal of Physics Condensed Matter, 2020, 32, 085403.	1.8	2

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37	Theoretical study on group III elements and F co-doped ZnO. Journal of Alloys and Compounds, 2020, 819, 153012.	5.5	12
38	Lithium lanthanum titanate perovskite as an anode for lithium ion batteries. Nature Communications, 2020, 11, 3490.	12.8	121
39	Achieving high hydrogen evolution reaction activity of a Mo₂C monolayer. Physical Chemistry Chemical Physics, 2020, 22, 26189-26199.	2.8	9
40	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:math> monolayer with a high critical temperature. Physical Review B, 2020, 102, .	3.2	23
41	Superconducting boron allotropes. Physical Review B, 2020, 101, .	3.2	18
42	Unconventional stable stoichiometry of vanadium peroxide. Physical Chemistry Chemical Physics, 2020, 22, 11460-11466.	2.8	4
43	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
44	Computational predictions of twoâ€dimensional anode materials of metalâ€ion batteries. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1473.	14.6	30
45	Exploring the Limits of Transitionâ€Metal Fluorination at High Pressures. Angewandte Chemie - International Edition, 2020, 59, 9155-9162.	13.8	17
46	Exploring the Limits of Transitionâ€Metal Fluorination at High Pressures. Angewandte Chemie, 2020, 132, 9240-9247.	2.0	1
47	Achieving high conductivity p-type Ga2O3 through Al-N and In-N co-doping. Chemical Physics Letters, 2020, 746, 137308.	2.6	18
48	The photophysical properties of cycloparaphenylene-based compounds with figure-eight configurations. New Journal of Chemistry, 2020, 44, 12185-12193.	2.8	8
49	Anisotropic PC₆N Monolayer with Wide Band Gap and Ultrahigh Carrier Mobility. Journal of Physical Chemistry C, 2020, 124, 4330-4337.	3.1	14
50	Exploring the origin of electrochemical performance of Cr-doped LiNi0.5Mn1.5O4. Physical Chemistry Chemical Physics, 2020, 22, 3831-3838.	2.8	13
51	Prediction of new thermodynamically stable ZnN2O3 at high pressure. Physical Chemistry Chemical Physics, 2020, 22, 10941-10948.	2.8	1
52	A Semiconducting Cationic Squareâ€Grid Network with Fe III Centers Displaying Unusual Dynamic Behavior. European Journal of Inorganic Chemistry, 2020, 2020, 1255-1259.	2.0	1
53	Recent Advances and Applications of Inorganic Electrides. Journal of Physical Chemistry Letters, 2020, 11, 3841-3852.	4.6	43
54	Electronic structure and second-order nonlinear optical property of chiral peropyrenes. Journal of Molecular Modeling, 2019, 25, 220.	1.8	1

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55	Pressure-induced new chemistry. Chinese Physics B, 2019, 28, 106106.	1.4	13
56	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. Physical Review B, 2019, 100, .	3.2	14
57	O₂ Adsorption Associated with Sulfur Vacancies on MoS₂ Microspheres. Inorganic Chemistry, 2019, 58, 2169-2176.	4.0	40
58	Nickel Hydrides under High Pressure. Journal of Physical Chemistry C, 2019, 123, 24243-24247.	3.1	3
59	Unveiling the Role of Oxygen Vacancy in Li₂MnO₃ upon Delithiation. Journal of Physical Chemistry C, 2019, 123, 23403-23409.	3.1	14
60	Metallic P₃C monolayer as anode for sodium-ion batteries. Journal of Materials Chemistry A, 2019, 7, 405-411.	10.3	75
61	A hypervalent and cubically coordinated molecular phase of IF₈predicted at high pressure. Chemical Science, 2019, 10, 2543-2550.	7.4	36
62	High-Temperature Ferromagnetism in an Fe₃P Monolayer with a Large Magnetic Anisotropy. Journal of Physical Chemistry Letters, 2019, 10, 2733-2738.	4.6	79
63	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></mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="normal">P</mml:mi></mml:mrow></mml:math>. Physical Review Letters, 2019, 122, 097002.	7.8	94
64	Nanotube-assembled pine-needle-like CuS as an effective energy booster for sodium-ion storage. Journal of Materials Chemistry A, 2019, 7, 10619-10628.	10.3	70
65	IrF₈ Molecular Crystal under High Pressure. Journal of the American Chemical Society, 2019, 141, 5409-5414.	13.7	40
66	An Organic Emitter Displaying Dual Emissions and Efficient Delayed Fluorescence White OLEDs. Advanced Optical Materials, 2019, 7, 1801667.	7.3	28
67	Achieving high transparent Î²-Ga2O3 through AlGa-InGa-VO. Journal of Alloys and Compounds, 2019, 792, 405-410.	5.5	8
68	FeP₃ monolayer as a high-efficiency catalyst for hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 25665-25671.	10.3	43
69	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.	5.5	20
70	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.	2.8	0
71	Two-Dimensional PC₆ with Direct Band Gap and Anisotropic Carrier Mobility. Journal of the American Chemical Society, 2019, 141, 1599-1605.	13.7	144
72	Hexagonal BC₂N with Remarkably High Hardness. Journal of Physical Chemistry C, 2018, 122, 6801-6807.	3.1	26

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73	Complementary Resistive Switching Observed in Graphene Oxide-Based Memory Device. IEEE Electron Device Letters, 2018, 39, 488-491.	3.9	25
74	Photophysical Properties of Chiral Tetraphenylethylene Derivatives with the Fixed Propeller-Like Conformation. Journal of Physical Chemistry C, 2018, 122, 5032-5039.	3.1	12
75	TiC₃ Monolayer with High Specific Capacity for Sodium-Ion Batteries. Journal of the American Chemical Society, 2018, 140, 5962-5968.	13.7	244
76	Accurate identification of layer number for few-layer WS₂and WSe₂via spectroscopic study. Nanotechnology, 2018, 29, 124001.	2.6	52
77	Mixed-valence Compounds: AuO2 and AuS. ChemPhysChem, 2018, 19, 2971-2971.	2.1	0
78	Structural and Superconducting Properties of Tungsten Hydrides Under High Pressure. Frontiers in Physics, 2018, 6, .	2.1	8
79	Memory Devices: Photocatalytic Reduction of Graphene Oxide-TiO2 Nanocomposites for Improving Resistive-Switching Memory Behaviors (Small 29/2018). Small, 2018, 14, 1870136.	10.0	4
80	Mixedâ€valence Compounds: AuO₂ and AuS. ChemPhysChem, 2018, 19, 2989-2994.	2.1	7
81	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. Journal of Physical Chemistry C, 2018, 122, 12448-12453.	3.1	22
82	High-temperature driven inter-valley carrier transfer and significant fluorescence enhancement in multilayer WS₂. Nanoscale Horizons, 2018, 3, 598-605.	8.0	13
83	Photocatalytic Reduction of Graphene Oxideâ€“TiO₂ Nanocomposites for Improving Resistiveâ€Switching Memory Behaviors. Small, 2018, 14, e1801325.	10.0	58
84	Gold with +4 and +6 Oxidation States in AuF₄ and AuF₆. Journal of the American Chemical Society, 2018, 140, 9545-9550.	13.7	80
85	Unveiling the Photophysical Properties of Boron Heptaaryldipyrromethene Derivatives. ChemPhysChem, 2018, 19, 2751-2757.	2.1	6
86	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.	2.3	12
87	Nonmetallic FeH₆ under High Pressure. Journal of Physical Chemistry C, 2018, 122, 12022-12028.	3.1	29
88	Element substitution of kesterite Cu2ZnSnS4 for efficient counter electrode of dye-sensitized solar cells. Scientific Reports, 2018, 8, 8714.	3.3	24
89	Chiral macrocyclic imine nickel(II) coordination complexes with diverse photophysical properties. Dyes and Pigments, 2017, 140, 70-78.	3.7	7
90	Understanding photophysical properties of chiral conjugated corrals for organic photovoltaics. Journal of Materials Chemistry C, 2017, 5, 3495-3502.	5.5	10

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91	Enhancement of Exciton Emission from Multilayer MoS₂ at High Temperatures: Intervalley Transfer versus Interlayer Decoupling. Small, 2017, 13, 1700157.	10.0	19
92	Highly Efficient Long-Wavelength Thermally Activated Delayed Fluorescence OLEDs Based on Dicyanopyrazino Phenanthrene Derivatives. ACS Applied Materials & Interfaces, 2017, 9, 9892-9901.	8.0	168
93	Pressure-Induced Stable Beryllium Peroxide. Inorganic Chemistry, 2017, 56, 5233-5238.	4.0	17
94	Understanding the role of lithium sulfide clusters in lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2017, 5, 9293-9298.	10.3	43
95	Tetragonal Structure BC₄ as a Superhard Material. Journal of Physical Chemistry C, 2017, 121, 10119-10123.	3.1	6
96	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.	3.1	23
97	Phase diagram, stability and electronic properties of an Feâ€“P system under high pressure: a first principles study. RSC Advances, 2017, 7, 15986-15991.	3.6	23
98	Photophysical properties of chiral covalent organic cages. Computational and Theoretical Chemistry, 2017, 1120, 1-7.	2.5	2
99	Pressure-induced stable BeN 4 as a high-energy density material. Journal of Power Sources, 2017, 365, 155-161.	7.8	43
100	Pressure-Induced Stable Li₅P for High-Performance Lithium-Ion Batteries. Journal of Physical Chemistry C, 2017, 121, 21199-21205.	3.1	36
101	Stable and metallic two-dimensional TaC₂as an anode material for lithium-ion battery. Journal of Materials Chemistry A, 2017, 5, 18698-18706.	10.3	75
102	Unveiling photophysical properties of phenanthro[9,10-d]imidazole derivatives for organic light-emitting diodes. Organic Electronics, 2017, 50, 220-227.	2.6	7
103	Theoretical study on the photophysical properties of boron-fused double helicenes. RSC Advances, 2017, 7, 56543-56549.	3.6	5
104	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.	7.3	21
105	Structural transitions and electronic properties of sodium superoxide at high pressures. RSC Advances, 2016, 6, 67910-67915.	3.6	5
106	Theoretical study on thiophene-based double helicenes with intrinsic large second-order nonlinear optical response. RSC Advances, 2016, 6, 84705-84711.	3.6	4
107	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. Physical Review Letters, 2016, 116, 057002.	7.8	132
108	Structure and Electronic Properties of Fe₂SH₃ Compound under High Pressure. Inorganic Chemistry, 2016, 55, 11434-11439.	4.0	50

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109	Silicon Framework-Based Lithium Silicides at High Pressures. ACS Applied Materials & Interfaces, 2016, 8, 16761-16767.	8.0	17
110	Pressure-induced reappearance of superconductivity in the oC24 phase of lithium. Solid State Communications, 2016, 225, 7-11.	1.9	3
111	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.	3.3	14
112	Gold as a 6p-Element in Dense Lithium Aurides. Journal of the American Chemical Society, 2016, 138, 4046-4052.	13.7	101
113	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
114	Prediction of the Xeâ€“He binary phase diagram at high pressures. Chemical Physics Letters, 2015, 640, 115-118.	2.6	11
115	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	3.3	71
116	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.	4.1	88
117	Structural and electronic properties of alkali metal peroxides at high pressures. RSC Advances, 2015, 5, 104337-104342.	3.6	12
118	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.	3.9	11
119	Ten-fold coordinated polymorph and metallization of TiO₂under high pressure. RSC Advances, 2015, 5, 54253-54257.	3.6	16
120	Insight into the role of Li₂S₂ in Liâ€“S batteries: a first-principles study. Journal of Materials Chemistry A, 2015, 3, 8865-8869.	10.3	68
121	Photophysical properties of quinoxaline-fused [7]carbohelicene derivatives. RSC Advances, 2015, 5, 72907-72915.	3.6	14
122	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. RSC Advances, 2015, 5, 104426-104432.	3.6	5
123	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.	2.4	5
124	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.	2.5	15
125	Electron transport via phenylâ€“perfluorophenyl interaction in crystals of fluorine-substituted dibenzalacetones. RSC Advances, 2014, 4, 50188-50194.	3.6	5
126	Organic Polymorphs: Oneâ€Compoundâ€Based Crystals with Molecularâ€Conformationâ€•and Packingâ€Dependent Luminescent Properties. Advanced Materials, 2014, 26, 6168-6173.	21.0	262

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127	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
128	A Stable, Magnetic, and Metallic Li3O4Compound as a Discharge Product in a Liâ€“Air Battery. Journal of Physical Chemistry Letters, 2014, 5, 2516-2521.	4.6	52
129	The relationship between intermolecular interactions and charge transport properties of trifluoromethylated polycyclic aromatic hydrocarbons. Organic Electronics, 2014, 15, 1896-1905.	2.6	24
130	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.	2.4	0
131	Chirality recognition of the protonated serine dimer and octamer by infrared multiphoton dissociation spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 1873-1886.	2.8	30
132	Theoretical study on the photophysical properties of chiral mononuclear and dinuclear zinc complexes. RSC Advances, 2013, 3, 2241-2247.	3.6	10
133	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
134	Photophysical properties of azaboradibenzo[6]helicene derivatives. Journal of Materials Chemistry C, 2013, 1, 2354.	5.5	27
135	Theoretical insights into [PMo12O40]3â^' grafted on single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 9177.	2.8	27
136	Theoretical Study on the Rectifying Performance of Organoimido Derivatives of Hexamolybdates. ChemPhysChem, 2013, 14, 610-617.	2.1	16
137	Fluorescent photoswitching of a naphthopyranâ€“benzimidazole dyad with high-degree fluorescent modulation within poly(methyl methacrylate) matrices. Optical Materials, 2013, 35, 1504-1512.	3.6	16
138	DFT characterization on the mechanism of water splitting catalyzed by single-Ru-substituted polyoxometalates. Dalton Transactions, 2013, 42, 10617.	3.3	30
139	Density Functional Theory Investigation on the Secondâ€Order Nonlinear Optical Properties of Chlorobenzylâ€oâ€Carborane Derivatives. Chinese Journal of Chemistry, 2012, 30, 2349-2355.	4.9	10
140	Theoretical study on the charge transport property of Pt(CNtBu)2(CN)2 nanowires induced by Ptâ‹¯Pt interactions. Dalton Transactions, 2012, 41, 7272.	3.3	13
141	TDDFT studies on chiral organophosphonate substituted divacant Keggin-type polyoxotungstate: diplex multistep-redox-triggered chiroptical and NLO switch. Dalton Transactions, 2012, 41, 10097.	3.3	11
142	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
143	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
144	Redox-switching second-order nonlinear optical responses of N^N^N ruthenium complexes. Computational and Theoretical Chemistry, 2012, 979, 112-118.	2.5	16

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145	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.	2.5	9
146	Chiroptical, linear, and second-order nonlinear optical properties of binaphthol derivatives. Organic and Biomolecular Chemistry, 2012, 10, 8418.	2.8	30
147	Computational study of chiral molecules with high intrinsic hyperpolarizabilities. Molecular Physics, 2012, 110, 333-341.	1.7	6
148	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.	2.0	9
149	Secondâ€order nonlinear optical responses switching of Nâˆ§Nâˆ§N ruthenium carboxylate complexes with protonâ€electron transfer. International Journal of Quantum Chemistry, 2012, 112, 779-788.	2.0	6
150	Conformations of Serine in Aqueous Solutions as Revealed by Vibrational Circular Dichroism. ChemPhysChem, 2012, 13, 1272-1281.	2.1	41
151	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.	2.1	41
152	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
153	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.	2.4	7
154	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
155	Theoretical Study on the Chiroptical Optical Properties of Chiral Fullerene C₆₀Derivative. Journal of Physical Chemistry A, 2011, 115, 13356-13363.	2.5	26
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