Rongjian Sa

List of Publications by Year
in descending order

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146 papers	4,768 citations	134610 34 h-index	129628 63 g-index
147 all docs	147 docs citations	147 times ranked	5799 citing authors

#	Article	IF	Citations
1	TM3 (TMÂ=ÂV, Fe, Mo, W) single-cluster catalyst confined on porous BN for electrocatalytic nitrogen reduction. Journal of Materials Science and Technology, 2022, 108, 46-53.	5.6	19
2	A DFT study of the stability and optoelectronic properties of all-inorganic lead-free halide perovskites. Journal of Physics and Chemistry of Solids, 2022, 161, 110413.	1.9	11
3	The effect of the A-site cation on the stability and physical properties of vacancy-ordered double perovskites A2PtI6 (A = Tl, K, Rb, and Cs). Journal of Solid State Chemistry, 2022, 305, 122714.	1.4	5
4	First-principles calculations to investigate the electronic and optical properties of Cu2ZnSnS4 with Ag and Se codoping. Chemical Physics, 2022, 554, 111418.	0.9	6
5	First-principles study of the structural, electronic and optical properties of Zn1-Hg Se (x = 0, 0.25,) Tj ETQq1 1 0.784314 rgBT /Overlo	1.3	3
6	Microenvironments Enabled by Covalent Organic Framework Linkages for Modulating Active Metal Species in Photocatalytic CO₂ Reduction. Advanced Functional Materials, 2022, 32, .	7.8	59
7	Interconnected N-doped MXene spherical shells for highly efficient capacitive deionization. Environmental Science: Nano, 2022, 9, 204-213.	2.2	12
8	The mechanical and optoelectronic properties of (Cu1-Ag)2ZnSnSe4 solid solutions: A theoretical study. Materials Chemistry and Physics, 2022, 279, 125757.	2.0	4
9	Bandgap engineering and optoelectronic properties of all-inorganic lead-free Pd-based double perovskites. Arabian Journal of Chemistry, 2022, 15, 103785.	2.3	5
10	Revealing the influence of B-site doping on the physical properties of CsPbI3: A DFT investigation. Journal of Solid State Chemistry, 2022, 309, 122956.	1.4	11
11	Adsorption Behavior of Environmental Gas Molecules on Pristine and Defective MoSi₂N₄: Possible Application as Highly Sensitive and Reusable Gas Sensors. ACS Omega, 2022, 7, 8706-8716.	1.6	20
12	Photoelectron Transfer Mediated by the Interfacial Electron Effects for Boosting Visible-Light-Driven CO₂ Reduction. ACS Catalysis, 2022, 12, 3550-3557.	5.5	83
13	High-Throughput computational screening of Single-atom embedded in defective BN nanotube for electrocatalytic nitrogen fixation. Applied Surface Science, 2022, 591, 153130.	3.1	13
14	Accelerating water oxidation kinetics via synergistic in-layer modification and interlayer reconstruction over hetero-epitaxial Fe-Mn-O nanosheets. Chemical Engineering Journal, 2022, 441, 136122.	6.6	10
15	Two Cocrystal Polymorphs of Palmatine Chloride with Racemic Hesperetin. Crystal Growth and Design, 2022, 22, 1073-1082.	1.4	14
16	Bandgap engineering of Na1-Ag SbS2 alloys for photovoltaic applications. Materials Research Bulletin, 2022, 152, 111862.	2.7	6
17	Effect of rare-earth doping on adsorption of carbon atom on ferrum surface and in ferrum subsurface: A first-principles study. Journal of Rare Earths, 2021, 39, 1144-1150.	2.5	6
18	The effects of cation and halide anion on the electronic and optical properties of Ti-based double perovskite: A first-principles calculations. Journal of Physics and Chemistry of Solids, 2021, 150, 109852.	1.9	9

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19	First-principles calculations of structural, electronic, and optical properties of double perovskites Cs2Sn1-B I6 (BÂ=ÂSi, Ge; xÂ=Â0, 0.25, 0.50, 0.75, 1). Chemical Physics, 2021, 542, 111075.	0.9	11
20	First-principles study of the stability, electronic and optical properties of CdTe under hydrostatic pressure. Chemical Physics Letters, 2021, 764, 138272.	1.2	11
21	Defective Fe₃GeTe₂ monolayer as a promising electrocatalyst for spontaneous nitrogen reduction reaction. Journal of Materials Chemistry A, 2021, 9, 6945-6954.	5.2	18
22	Metalâ€“Organic Framework-Derived CuS Nanocages for Selective CO ₂ Electroreduction to Formate. CCS Chemistry, 2021, 3, 199-207.	4.6	23
23	High-throughput screening of transition metal single-atom catalyst anchored on Janus MoSSe basal plane for hydrogen evolution reaction. International Journal of Hydrogen Energy, 2021, 46, 10337-10345.	3.8	30
24	The mechanical, electronic and optical properties of BiPX4 (Xâ€¯=â€¯S, Se): a theoretical study. Materials Today Communications, 2021, 26, 102062.	0.9	0
25	Theoretical screening of group IIIA-VIIA elements doping to promote hydrogen evolution of MoS2 basal plane. Applied Surface Science, 2021, 542, 148535.	3.1	31
26	(Li,Na)SbS2 as a promising solar absorber material: A theoretical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119389.	2.0	6
27	Stable and high efficiency mixed-cation lead-based halide perovskite: A theoretical study. Physica B: Condensed Matter, 2021, 610, 412938.	1.3	1
28	First-principles study of the stability, mechanical, electronic and optical properties of Cd0.75Hg0.25Se. Chemical Physics, 2021, 546, 111164.	0.9	3
29	Theoretical study of mixed-halide influence on the stability and electronic properties of CsCd(Cl/Br)3. Computational and Theoretical Chemistry, 2021, 1200, 113251.	1.1	2
30	Pressure-induced band gap tuning in Cs2TiBr6: A theoretical study. Journal of Solid State Chemistry, 2021, 300, 122244.	1.4	3
31	Enhancing the hydrogen evolution reaction by non-precious transition metal (Non-metal) atom doping in defective MoSi2N4 monolayer. Applied Surface Science, 2021, 563, 150388.	3.1	49
32	Efficient electrochemical CO2 reduction on C2N monolayer supported transition metals trimer catalysts: A DFT study. Applied Surface Science, 2021, 564, 150331.	3.1	24
33	A promising all-inorganic double perovskite Rb2TiBr6 for photovoltaic applications: Insight from first-principles calculations. Journal of Solid State Chemistry, 2021, 303, 122473.	1.4	10
34	Engineering interfacial coupling between Mo2C nanosheets and Co@NC polyhedron for boosting electrocatalytic water splitting and zinc-air batteries. Applied Catalysis B: Environmental, 2021, 296, 120360.	10.8	79
35	Exploring the electronic and optical properties of vacancy-ordered double perovskites Cs2PtX6 (X =) Tj ETQq1 1 0.784314 rgBT /Over	1.4	10
36	Electronic and Optical Properties of Organicâ€“Inorganic MASn1â^'xGexI3 Perovskites: A First-Principles Study. Journal of Cluster Science, 2020, 31, 1103-1109.	1.7	8

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37	Ionicâ€Liquidâ€Modified Clickâ€Based Porous Organic Polymers for Controlling Capture and Catalytic Conversion of CO₂. ChemSusChem, 2020, 13, 180-187.	3.6	65
38	Exploring electronic and optical properties of Ge-based perovskites under strain: Insights from the first-principles calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 118013.	2.0	12
39	Theoretical screening of efficient single-atom catalysts for nitrogen fixation based on a defective BN monolayer. Nanoscale, 2020, 12, 1541-1550.	2.8	95
40	Insight into the Improved Phase Stability of CsPbI3 from First-Principles Calculations. ACS Omega, 2020, 5, 893-896.	1.6	34
41	Three-in-One: Opened Charge-transfer channel, positively shifted oxidation potential, and enhanced visible light response of g-C3N4 photocatalyst through K and S Co-doping. International Journal of Hydrogen Energy, 2020, 45, 4534-4544.	3.8	46
42	Theoretical study of structural stability, electronic and optical properties of MA1âˆ’x Cs x PbI3 for photovoltaic applications. Applied Physics Express, 2020, 13, 011007.	1.1	3
43	Indirect-to-direct band gap transition and optical properties of metal alloys of Cs₂Te_{1âˆ’x}Ti_xI₆: a theoretical study. RSC Advances, 2020, 10, 36734-36740.	1.7	12
44	Theoretical study of Zr doping on the stability, mechanical, electronic and optical properties of Cs2TiI6. Optical Materials, 2020, 110, 110497.	1.7	23
45	A first-principles study on the optoelectronic properties of mixed-halide double perovskites Cs₂TiI_{6âˆ’x}Br_x. New Journal of Chemistry, 2020, 44, 13613-13618.	1.4	29
46	Accelerated design of photovoltaic Ruddlesdenâ€“Popper perovskite Ca6Sn4S14âˆ’xOx using machine learning. APL Materials, 2020, 8, .	2.2	9
47	Carbon Dioxide Conversion Upgraded by Hostâ€guest Cooperation between Nitrogenâ€Rich Covalent Organic Framework and Imidazoliumâ€Based Ionic Polymer. ChemSusChem, 2020, 13, 6050-6050.	3.6	5
48	Carbon Dioxide Conversion Upgraded by Hostâ€guest Cooperation between Nitrogenâ€Rich Covalent Organic Framework and Imidazoliumâ€Based Ionic Polymer. ChemSusChem, 2020, 13, 6323-6329.	3.6	48
49	The effect of organic cation doping on the stability and optoelectronic properties of Î±-CsPbI3. Journal of Solid State Chemistry, 2020, 290, 121577.	1.4	5
50	Metalloporphyrin-based covalent organic frameworks composed of the electron donor-acceptor dyads for visible-light-driven selective CO2 reduction. Science China Chemistry, 2020, 63, 1289-1294.	4.2	73
51	MOF-aided topotactic transformation into nitrogen-doped porous Mo₂C mesocrystals for upgrading the pH-universal hydrogen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 20429-20435.	5.2	24
52	Recent Advances on Metalloporphyrinâ€Based Materials for Visibleâ€Lightâ€Driven CO₂ Reduction. ChemSusChem, 2020, 13, 6124-6140.	3.6	49
53	Enhancing hydrogen evolution of MoS2 basal planes by combining single-boron catalyst and compressive strain. Frontiers of Physics, 2020, 15, 1.	2.4	20
54	First-principles study of the structural stability, electronic and optical properties of CH3-F NH3GeI3 (xÂ=Â0, 1, 2, 3) halide perovskites. Chemical Physics Letters, 2020, 761, 138020.	1.2	1

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55	Crystalline Hydrogenâ€Bonded Organic Chains Achieving Ultralong Phosphorescence via Tripletâ€“Triplet Energy Transfer. Advanced Optical Materials, 2020, 8, 2000281.	3.6	15
56	A non-carbon catalyst support upgrades the intrinsic activity of ruthenium for hydrogen evolution electrocatalysis via strong interfacial electronic effects. Nano Energy, 2020, 75, 104981.	8.2	39
57	Breaking the limitation of sodium-ion storage for nanostructured carbon anode by engineering desolvation barrier with neat electrolytes. Nano Energy, 2020, 74, 104895.	8.2	49
58	A first-principle study of the structural, mechanical, electronic and optical properties of vacancy-ordered double perovskite Cs2TeX6 (XÂ=ÂCl, Br, I). Chemical Physics Letters, 2020, 754, 137538.	1.2	40
59	Robust ruthenium diphosphide nanoparticles for pH-universal hydrogen evolution reaction with platinum-like activity. Applied Catalysis B: Environmental, 2020, 274, 119092.	10.8	69
60	Adsorption behavior of CO, CO2, H2, H2O, NO, and O2 on pristine and defective 2D monolayer ferromagnetic Fe3GeTe2. Applied Surface Science, 2020, 527, 146894.	3.1	20
61	Integrating single Ni sites into biomimetic networks of covalent organic frameworks for selective photoreduction of CO₂. Chemical Science, 2020, 11, 6915-6922.	3.7	78
62	Covalent Organic Framework Hosting Metalloporphyrinâ€Based Carbon Dots for Visibleâ€Lightâ€Driven Selective CO₂Reduction. Advanced Functional Materials, 2020, 30, 2002654.	7.8	125
63	Mechanistic study of visible light-driven CdS or g-C3N4-catalyzed C H direct trifluoromethylation of (hetero)arenes using CF3SO2Na as the trifluoromethyl source. Journal of Catalysis, 2020, 389, 533-543.	3.1	21
64	Effect of rubidium incorporation on the structural, electronic and properties of MAPbI3. Chemical Physics Letters, 2020, 743, 137179.	1.2	2
65	Mixed-Cation Mixed-Metal Halide Perovskites for Photovoltaic Applications: A Theoretical Study. ACS Omega, 2020, 5, 4347-4351.	1.6	13
66	The electrochemical overall water splitting promoted by MoS2 in coupled nickelâ€“iron (oxy)hydride/molybdenum sulfide/graphene composite. Chemical Engineering Journal, 2020, 397, 125454.	6.6	32
67	Stable lead-free perovskite solar cells: A first-principles investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118493.	2.0	7
68	The effect of divalent europium doping on stability and electronic properties of CH₃NH₃PbI₃: a theoretical investigation. Applied Physics Express, 2020, 13, 101001.	1.1	2
69	First-principles insight into the structural, mechanical, electronic and optical properties of Be3X2 (X) Tj ETQq1 1 0.784314 rgBT /Over	1.9	3
70	Understanding structure-function relationships in HZSM-5 zeolite catalysts for photocatalytic oxidation of isopropyl alcohol. Journal of Catalysis, 2019, 377, 322-331.	3.1	21
71	First-principles insights of electronic and optical properties of Zn-doped CH3NH3PbI3 for photovoltaic applications. Applied Physics Express, 2019, 12, 082011.	1.1	6
72	Tuning electronic and optical properties of CsPbI3 by applying strain: A first-principles theoretical study. Chemical Physics Letters, 2019, 732, 136642.	1.2	40

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73	2,4,6â€Tri(4â€pyridyl)â€1,3,5â€triazine: Photoinduced Charge Separation and Photochromism in the Crystalline State. Chemistry - A European Journal, 2019, 25, 13972-13976.	1.7	30
74	Formation of Cu_{3,4}(TCA), making the TCA complex a highly selective probe for Cu²⁺ detection: a TDDFT study. Journal of Materials Chemistry C, 2019, 7, 2443-2456.	2.7	12
75	First-principles insight on the electronic and optical properties of Ge-based inorganic perovskites. Applied Physics Express, 2019, 12, 071007.	1.1	9
76	Photoâ€Induced Chloride Atom Transfer Radical Addition and Aminocarbonylation Reactions. Asian Journal of Organic Chemistry, 2019, 8, 1513-1518.	1.3	13
77	A comparative study of structural, electronic and optical properties based on metal-doped methylammonium lead halidesviafirst-principles calculations. New Journal of Chemistry, 2019, 43, 9453-9457.	1.4	6
78	Assigning the Absolute Configurations of Chiral Primary Amines Based on Experimental and DFT-Calculated 19F Nuclear Magnetic Resonance. Frontiers in Chemistry, 2019, 7, 318.	1.8	4
79	Photovoltaic Performance of Lead-Less Hybrid Perovskites from Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 12638-12646.	1.5	39
80	Experimental and theoretical study for CO₂ activation and chemical fixation with epoxides. RSC Advances, 2019, 9, 13122-13127.	1.7	10
81	A Covalent Organic Framework Bearing Single Ni Sites as a Synergistic Photocatalyst for Selective Photoreduction of CO₂ to CO. Journal of the American Chemical Society, 2019, 141, 7615-7621.	6.6	525
82	Thermochromic Behavior of Azobenzeneâ€based Coordination Polymer with Reversible Breathing Process. ChemistrySelect, 2019, 4, 3222-3227.	0.7	2
83	TCA self-assembled fluorescence probe for Cu (II) ion based on the unique configuration of extra nuclear electrons of metal ions: A TDDFT study. Computational and Theoretical Chemistry, 2019, 1157, 1-10.	1.1	0
84	Photoresponsive triazole-based donorâ€“acceptor molecules: color change and heat/air-stable diradicals. Journal of Materials Chemistry C, 2019, 7, 3100-3104.	2.7	25
85	Computational exploration of substrate and ligand effects in nickel-catalyzed Câ€“Si bond carboxylation with CO2. Organic Chemistry Frontiers, 2019, 6, 3629-3635.	2.3	10
86	An Ultraâ€Robust and Crystalline Redeemable Hydrogenâ€Bonded Organic Framework for Synergistic Chemoâ€Photodynamic Therapy. Angewandte Chemie - International Edition, 2018, 57, 7691-7696.	7.2	303
87	Fluorescent Metalâ€“Organic Framework (MOF) as a Highly Sensitive and Quickly Responsive Chemical Sensor for the Detection of Antibiotics in Simulated Wastewater. Inorganic Chemistry, 2018, 57, 1060-1065.	1.9	270
88	Synergistic Effect of Doping and Compositing on Photocatalytic Efficiency: A Case Study of La₂Ti₂O₇. ACS Applied Materials & Interfaces, 2018, 10, 39327-39335.	4.0	17
89	Novel Salt Cocrystal of Chrysin with Berberine: Preparation, Characterization, and Oral Bioavailability. Crystal Growth and Design, 2018, 18, 4724-4730.	1.4	39
90	A promising lead-free fluoride carbonate SHG material designed from a theoretical perspective. Dalton Transactions, 2017, 46, 2635-2642.	1.6	15

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91	Screening novel candidates for mid-IR nonlinear optical materials from I₃â€“Vâ€“VI₄compounds. Journal of Materials Chemistry C, 2017, 5, 1963-1972.	2.7	32
92	A comprehensive understanding of water photooxidation on Ag₃PO₄ surfaces. RSC Advances, 2017, 7, 23994-24003.	1.7	13
93	Theoretical perspectives on the structure, electronic, and optical properties of titanosilicates Li₂M₄[(TiO)Si₄O₁₂] (M = K⁺,) Tj ETQq1 1 0.784314 rgBT /Overlock 1	3.3	0
94	Computation-predicted, stable, and inexpensive single-atom nanocatalyst Pt@Mo₂C â€“ an important advanced material for H₂ production. Journal of Materials Chemistry A, 2017, 5, 14658-14672.	5.2	34
95	Second-order nonlinear optical switching with a record-high contrast for a photochromic and thermochromic bistable crystal. Chemical Science, 2017, 8, 7751-7757.	3.7	104
96	Improved thermoelectric power factor and conversion efficiency of perovskite barium stannate. RSC Advances, 2017, 7, 32703-32709.	1.7	34
97	A highly stable and white-light-emitting Eu(<scp>iii</scp>) MOF. Dalton Transactions, 2016, 45, 18661-18667.	1.6	25
98	Interfacial electronic structure and charge transfer of hybrid graphene quantum dot and graphitic carbon nitride nanocomposites: insights into high efficiency for photocatalytic solar water splitting. Physical Chemistry Chemical Physics, 2016, 18, 1050-1058.	1.3	57
99	Highly stable and sensitive LnMOF ratiometric thermometers constructed with mixed ligands. Dalton Transactions, 2015, 44, 3067-3074.	1.6	85
100	A topological pattern for understanding the structures of boranes and borane analog compounds. Structural Chemistry, 2015, 26, 353-364.	1.0	7
101	NLO Properties of Unidirectional Lengthening [Pt3(CO)3(Î¼2-CO)3] n 2â^' Clusters: A TDDFT Study. Journal of Cluster Science, 2015, 26, 1511-1526.	1.7	0
102	Neolignans with a Rare 2-Oxaspiro[4.5]deca-6,9-dien-8-one Motif from the Stem Bark of Cinnamomum subavenium. Journal of Natural Products, 2015, 78, 1740-1744.	1.5	32
103	Exploring Second-Order Nonlinear Optical Properties and Switching Ability of a Series of Dithienylethene-Containing, Cyclometalated Platinum Complexes: A Theoretical Investigation. Journal of Physical Chemistry A, 2015, 119, 8174-8181.	1.1	12
104	Structure, elastic and piezoelectric properties of A 3 BO 7 (A = Ga, Al; B = P, As) compounds: A DFT study. Computational Materials Science, 2015, 106, 1-4.	1.4	8
105	A novel Pd3O9@Î±-Al2O3 catalyst under a hydroxylated effect: high activity in the CO oxidation reaction. Physical Chemistry Chemical Physics, 2015, 17, 32140-32148.	1.3	5
106	The electronic, optical and ferroelectric properties of BiFeO3 during polarization reversal: A first principle study. Journal of Alloys and Compounds, 2015, 623, 393-400.	2.8	23
107	Mechanism of enhanced photocatalytic activities on N-doped La 2 Ti 2 O 7 : An insight from density-functional calculations. International Journal of Hydrogen Energy, 2015, 40, 980-989.	3.8	27
108	Molecular orbital closed loops analysis of the third-order NLO response of polyanion [M8O26]4â^' (MÂ=ÂCr, Mo, W): a TDDFT study. Structural Chemistry, 2014, 25, 539-549.	1.0	10

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109	Three Cd(II) coordination polymers assembled by flexible 2,2â€²-azodibenzoic acid and N-donor auxiliary ligand: Structural diversities and luminescent properties. Inorganic Chemistry Communication, 2014, 40, 194-199.	1.8	17
110	Receding mechanism of NLO response of polyanion [M8O26]4â^' (M = Cr, Mo, W) and the closed loops theory analysis. New Journal of Chemistry, 2014, 38, 2619-2628.	1.4	3
111	Evaluation of Interactions between Urokinase Plasminogen and Inhibitors Using Molecular Dynamic Simulation and Free-Energy Calculation. Journal of Physical Chemistry A, 2014, 118, 9113-9119.	1.1	13
112	A white-light-emitting LnMOF with color properties improved via Eu3+ doping: an alternative approach to a rational design for solid-state lighting. Chemical Communications, 2014, 50, 1820.	2.2	68
113	Diterpenoids with Immunosuppressive Activities from Cinnamomum cassia. Journal of Natural Products, 2014, 77, 1948-1954.	1.5	41
114	A facile method for synthesis of N-doped TiO2 nanooctahedra, nanoparticles, and nanospheres and enhanced photocatalytic activity. Applied Surface Science, 2013, 273, 278-286.	3.1	44
115	Ab initio study of elasticity, piezoelectricity, and nonlinear optical performance in monoclinic NaAsSe2. Journal of Alloys and Compounds, 2013, 568, 16-20.	2.8	25
116	Micranthanone A, a New Diterpene with an Unprecedented Carbon Skeleton from Rhododendron micranthum. Organic Letters, 2013, 15, 3094-3097.	2.4	45
117	Closed loops theory on the third-order nonlinear optical property ofÎ±- andÎ²- isomers of [M8O26]4â^': a TDDFT study. Molecular Physics, 2013, 111, 3081-3086.	0.8	2
118	Strain-induced improvements on linear and nonlinear optical properties of SrB4O7 crystal. AIP Advances, 2012, 2, 032170.	0.6	15
119	A topological pattern for the understanding of the stability and aromaticity of closo-boranes: constructing closo-borane from nido-boranes. Structural Chemistry, 2012, 23, 1797-1800.	1.0	6
120	A discussion on the electronic structure of arachno-borane B4H10. Structural Chemistry, 2012, 23, 841-845.	1.0	6
121	Doping and temperature dependence of thermoelectric properties of AgGaTe2: First principles investigations. Chemical Physics Letters, 2012, 537, 62-64.	1.2	25
122	Mechanism Insights into Second-Order Nonlinear Optical Responses of Anionic Metal Clusters. Journal of Cluster Science, 2011, 22, 365-380.	1.7	4
123	(Hyper)polarizabilities and optical absorption spectra of MSi12 clusters (M=Scâ€“Zn): A theoretical study. Chemical Physics Letters, 2010, 490, 132-137.	1.2	23
124	Nitroguanidineâ€Fused Bicyclic Guanidinium Salts: A Family of Highâ€Density Energetic Materials. Chemistry - A European Journal, 2010, 16, 8522-8529.	1.7	48
125	Mixed-metal effects on ultra-incompressible metal diborides: Density functional computations. Chemical Physics Letters, 2010, 494, 31-36.	1.2	12
126	Modulating the electronic structures and optical absorption spectra of BeO nanotubes by uniaxial strain. Applied Physics Letters, 2010, 97, 051901.	1.5	9

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127	Bis[3-(5-nitroimino-1,2,4-triazolate)]-Based Energetic Salts: Synthesis and Promising Properties of a New Family of High-Density Insensitive Materials. Journal of the American Chemical Society, 2010, 132, 11904-11905.	6.6	273
128	Magnetic properties of nonmetal atoms absorbed MoS2 monolayers. Applied Physics Letters, 2010, 96, .	1.5	199
129	Theoretical studies on the bonding of Cd2+ to adenine and thymine: Tautomeric equilibrium and metalation in base pairing. Chemical Physics Letters, 2009, 467, 387-392.	1.2	13
130	Solvent effect on quadratic hyperpolarizability of 4-(dimethylamino-4â€²-stilbazole)tungsten pentacarbonyl: A revisit of mechanism for second-order response. Chemical Physics Letters, 2009, 471, 229-233.	1.2	12
131	Dipole polarizabilities of trimetallic nitride endohedral fullerenes M3N@C2n (M=Sc and Y; 2n=68â€“98). Chemical Physics Letters, 2009, 475, 73-77.	1.2	8
132	Stabilities of 3d transition-metal doped Si14 clusters. Chemical Physics Letters, 2009, 483, 30-34.	1.2	38
133	Second-order nonlinear optical properties of transition metal clusters [MoS4Cu4X2Py2] (M = Mo, W;) Tj ETQq1 1 0.784314 rgBT /Ov	1.3	10
134	Two cobalt(II) coordination polymers [Co2(H2O)4(Hbidc)2]n and [Co(Hbidc)]n (Hbidc =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 Td (CrystEngComm, 2009, 11, 1054.	1.3	53
135	Mononuclear, trinuclear, and hetero-trinuclear supramolecular complexes containing a new tri-sulfonate ligand and cobalt(II)/copper(II)-(1,10-phenanthroline)2 building blocks. Journal of Solid State Chemistry, 2008, 181, 539-551.	1.4	4
136	Size-dependence of stability and optical properties of lead sulfide clusters. Chemical Physics Letters, 2008, 457, 163-168.	1.2	19
137	Direct Metalâ^'Metal Interaction Contributions to Quadratic Hyperpolarizability: A Study on Dirhenium Complexes. Journal of Physical Chemistry A, 2008, 112, 4965-4972.	1.1	20
138	The effect of ligands on the first hyperpolarizabilities of rich d electron molecular system: iridium clusters, a TDDFT study. Molecular Physics, 2008, 106, 2537-2544.	0.8	8
139	Solvent and Intermolecular Effects on First Hyperpolarizabilities of Organometallic Tungstenâ^'Carbonyl Complexes, A TDDFT Study. Journal of Physical Chemistry A, 2007, 111, 7925-7932.	1.1	19
140	Substituting effect on first hyperpolarizability of R-terminated polysilaacetylene oligomers. Computational and Theoretical Chemistry, 2007, 823, 28-33.	1.5	3
141	Carbocationâ€“Ï€ interaction with Carâ€“Parrinello molecular dynamics: Ab initio molecular dynamics investigation of complex of methyl cation with benzene. Chemical Physics Letters, 2007, 435, 24-28.	1.2	12
142	How Does Ammonium Dynamically Interact with Benzene in Aqueous Media? A First Principle Study Using the Carâ^'Parrinello Molecular Dynamics Method. Journal of Physical Chemistry B, 2006, 110, 5094-5098.	1.2	31
143	Large hyperpolarizabilities of trinuclear transition metal clusters [MAg2X4(C5H5NS)(PPh3)2]Â·CH2Cl2(M = Mo, W; X = S, Se): a DFT study. New Journal of Chemistry, 2005, 29, 362-365.	1.4	12
144	A theoretical study on the second-order nonlinear optical susceptibilities of lithium formate monohydrate crystal, HCOOLiÂ·H2O. Optical Materials, 2003, 22, 353-359.	1.7	5

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145	Theoretical studies of nonlinear optical crystals in metal cluster compounds. Journal of Crystal Growth, 2002, 237-239, 663-667.	0.7	8
146	Density functional theory studies on the potential energy surface and hyperpolarizability of polyamidoamide dendrimer. Chemical Physics Letters, 2002, 363, 343-348.	1.2	19