Guochun Yang

List of Publications by Citations

203	3,969	34	51
papers	citations	h-index	g-index
218	4,771	4.9	5.76
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
203	Organic polymorphs: one-compound-based crystals with molecular-conformation- and packing-dependent luminescent properties. *Advanced Materials*, **2014**, 26, 6168-73	24	224
202	TiC Monolayer with High Specific Capacity for Sodium-Ion Batteries. *Journal of the American Chemical Society*, **2018**, 140, 5962-5968	16.4	152
201	Highly Efficient Long-Wavelength Thermally Activated Delayed Fluorescence OLEDs Based on Dicyanopyrazino Phenanthrene Derivatives. *ACS Applied Materials & Interfaces*, **2017**, 9, 9892-9901	9.5	128
200	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. *Physical Review Letters*, **2016**, 116, 057002	7.4	104
199	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		83
198	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, 23092-8	3.4	81
197	High performance full color OLEDs based on a class of molecules with dual carrier transport channels and small singlet-triplet splitting. *Chemical Communications*, **2015**, 51, 10632-5	5.8	79
196	Two-Dimensional PC with Direct Band Gap and Anisotropic Carrier Mobility. *Journal of the American Chemical Society*, **2019**, 141, 1599-1605	16.4	76
195	Gold as a 6p-Element in Dense Lithium Aurides. *Journal of the American Chemical Society*, **2016**, 138, 4046-52	14	70
194	Insight into the role of Li2S2 in Li–S batteries: a first-principles study. *Journal of Materials Chemistry A*, **2015**, 3, 8865-8869	13	57
193	Vibrational circular dichroism spectroscopy of chiral molecules. *Topics in Current Chemistry*, **2011**, 298, 189-236		57
192	Density functional theory study on the first hyperpolarizabilities of organoimido derivatives of hexamolybdates. *Journal of Physical Chemistry B*, **2005**, 109, 22332-6	3.4	57
191	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. *Scientific Reports*, **2015**, 5, 15433	4.9	56
190	Theoretical study on the second-order nonlinear optical properties of asymmetric spirosilabifluorene derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 4817-21	2.8	55
189	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	3.9	53
188	Predicted Pressure-Induced Superconducting Transition in Electride Li_{6}P. *Physical Review Letters*, **2019**, 122, 097002	7.4	51
187	High-Temperature Ferromagnetism in an FeP Monolayer with a Large Magnetic Anisotropy. *Journal of Physical Chemistry Letters*, **2019**, 10, 2733-2738	6.4	50

186	Gold with +4 and +6 Oxidation States in AuF and AuF. *Journal of the American Chemical Society*, **2018**, 140, 9545-9550	16.4	50
185	Stable and metallic two-dimensional TaC2 as an anode material for lithium-ion battery. *Journal of Materials Chemistry A*, **2017**, 5, 18698-18706	13	50
184	Lithium lanthanum titanate perovskite as an anode for lithium ion batteries. *Nature Communications*, **2020**, 11, 3490	17.4	50
183	Metallic P3C monolayer as anode for sodium-ion batteries. *Journal of Materials Chemistry A*, **2019**, 7, 405-411	13	49
182	A Stable, Magnetic, and Metallic Li3O4 Compound as a Discharge Product in a Li-Air Battery. *Journal of Physical Chemistry Letters*, **2014**, 5, 2516-21	6.4	48
181	Effect of pi-conjugated length of bridging ligand on the optoelectronic properties of platinum(II) dimers. *Inorganic Chemistry*, **2008**, 47, 2347-55	5.1	48
180	Photocatalytic Reduction of Graphene Oxide-TiO Nanocomposites for Improving Resistive-Switching Memory Behaviors. *Small*, **2018**, 14, e1801325	11	45
179	Reversible redox-switchable second-order optical nonlinearity in polyoxometalate: a quantum chemical study of [PW11O39(ReN)]n- (n = 3-7). *Inorganic Chemistry*, **2008**, 47, 5245-52	5.1	43
178	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	7.1	42
177	Prediction of second-order optical nonlinearity of trisorganotin-substituted beta-Keggin polyoxotungstate. *Inorganic Chemistry*, **2006**, 45, 7864-8	5.1	42
176	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	3.8	40
175	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, 8758-62	2.8	40
174	Nanotube-assembled pine-needle-like CuS as an effective energy booster for sodium-ion storage. *Journal of Materials Chemistry A*, **2019**, 7, 10619-10628	13	39
173	Conformational distributions of N-acetyl-L-cysteine in aqueous solutions: a combined implicit and explicit solvation treatment of VA and VCD spectra. *ChemPhysChem*, **2012**, 13, 2310-21	3.2	38
172	Structure and Electronic Properties of FeSH Compound under High Pressure. *Inorganic Chemistry*, **2016**, 55, 11434-11439	5.1	35
171	Theoretical study on photophysical properties of phenolpyridyl boron complexes. *Journal of Physical Chemistry A*, **2007**, 111, 2739-44	2.8	35
170	Understanding the role of lithium sulfide clusters in lithium–sulfur batteries. *Journal of Materials Chemistry A*, **2017**, 5, 9293-9298	13	34
169	Accurate identification of layer number for few-layer WS and WSe via spectroscopic study. *Nanotechnology*, **2018**, 29, 124001	3.4	33

168	Quantum Chemical Study of Structures, Electronic Spectrum, and Nonlinear Optical Properties of Gold(I) Pentacene Complexes. *Organometallics*, **2007**, 26, 2082-2087	3.8	33
167	Conformations of serine in aqueous solutions as revealed by vibrational circular dichroism. *ChemPhysChem*, **2012**, 13, 1272-81	3.2	30
166	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	2.3	30
165	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	3.9	29
164	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	3.8	29
163	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	2.5	29
162	Computational study on second-order nonlinear optical (NLO) properties of a novel class of two-dimensional □and W-shaped sandwich metallocarborane-containing chromophores. *Journal of Organometallic Chemistry*, **2011**, 696, 2380-2387	2.3	28
161	The effects of self-aggregation on the vibrational circular dichroism and optical rotation measurements of glycidol. *Physical Chemistry Chemical Physics*, **2008**, 10, 6787-95	3.6	28
160	IrF Molecular Crystal under High Pressure. *Journal of the American Chemical Society*, **2019**, 141, 5409-5414	16.4	27
159	A controllable and reversible phase transformation between all-inorganic perovskites for white light emitting diodes. *Journal of Materials Chemistry C*, **2020**, 8, 8374-8379	7.1	27
158	Pressure-Induced Stable Li5P for High-Performance Lithium-Ion Batteries. *Journal of Physical Chemistry C*, **2017**, 121, 21199-21205	3.8	27
157	Chiroptical, linear, and second-order nonlinear optical properties of binaphthol derivatives. *Organic and Biomolecular Chemistry*, **2012**, 10, 8418-25	3.9	27
156	Chirality recognition of the protonated serine dimer and octamer by infrared multiphoton dissociation spectroscopy. *Physical Chemistry Chemical Physics*, **2013**, 15, 1873-86	3.6	26
155	Theoretical study on the chiroptical optical properties of chiral fullerene C60 derivative. *Journal of Physical Chemistry A*, **2011**, 115, 13356-63	2.8	26
154	O Adsorption Associated with Sulfur Vacancies on MoS Microspheres. *Inorganic Chemistry*, **2019**, 58, 2169-2176	4.8	25
153	DFT characterization on the mechanism of water splitting catalyzed by single-Ru-substituted polyoxometalates. *Dalton Transactions*, **2013**, 42, 10617-25	4.3	25
152	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	2.3	24
151	FeP3 monolayer as a high-efficiency catalyst for hydrogen evolution reaction. *Journal of Materials Chemistry A*, **2019**, 7, 25665-25671	13	24

150	Theoretical insights into [PMo12O40](3-) grafted on single-walled carbon nanotubes. *Physical Chemistry Chemical Physics*, **2013**, 15, 9177-85	3.6	23
149	Photophysical properties of azaboradibenzo[6]helicene derivatives. *Journal of Materials Chemistry C*, **2013**, 1, 2354	7.1	22
148	Pressure-induced stable BeN 4 as a high-energy density material. *Journal of Power Sources*, **2017**, 365, 155-161	8.9	22
147	Predication of second-order optical nonlinearity of [(Bu2t Im)AuX] (X=halogen) using time-dependent density-functional theory combined with sum-over-states method. *Journal of Chemical Physics*, **2005**, 123, 134302	3.9	22
146	Nonmetallic FeH6 under High Pressure. *Journal of Physical Chemistry C*, **2018**, 122, 12022-12028	3.8	21
145	Theoretical study on a novel series of fullerene-containing organometallics Fe(eta5-C55X5)2 (X = CH, N, B) and their large third-order nonlinear optical properties. *Journal of Physical Chemistry A*, **2008**, 112, 8086-92	2.8	21
144	Theoretical study on the optoelectronic properties of electron-withdrawing substituted diethynylfluorenyl gold(I) complexes. *Journal of Physical Chemistry A*, **2006**, 110, 13036-44	2.8	21
143	TD-DFT investigation on the low-lying excited states of spiro-bithiophene. *Chemical Physics Letters*, **2006**, 429, 180-184	2.5	21
142	A hypervalent and cubically coordinated molecular phase of IF predicted at high pressure. *Chemical Science*, **2019**, 10, 2543-2550	9.4	20
141	The relationship between intermolecular interactions and charge transport properties of trifluoromethylated polycyclic aromatic hydrocarbons. *Organic Electronics*, **2014**, 15, 1896-1905	3.5	20
140	Chiroptical, linear, and second-order nonlinear optical properties of tetrathiafulvalenylallene: a multifunctional molecular material. *Journal of Materials Chemistry C*, **2013**, 1, 1399	7.1	20
139	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, 3777-83	3.9	20
138	Complementary Resistive Switching Observed in Graphene Oxide-Based Memory Device. *IEEE Electron Device Letters*, **2018**, 39, 488-491	4.4	19
137	Charge transport and electronic properties of N-heteroquinones: quadruple weak hydrogen bonds and strong π-stacking interactions. *Theoretical Chemistry Accounts*, **2011**, 128, 257-264	1.9	19
136	Phase diagram, stability and electronic properties of an FeP system under high pressure: a first principles study. *RSC Advances*, **2017**, 7, 15986-15991	3.7	18
135	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		18
134	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	3.8	17
133	Quantum chemical study of structures, electronic spectrum, and nonlinear optical properties of polynuclear lithium compounds. *Computational and Theoretical Chemistry*, **2011**, 966, 14-19	2	17

132	Enhancement of Exciton Emission from Multilayer MoS at High Temperatures: Intervalley Transfer versus Interlayer Decoupling. *Small*, **2017**, 13, 1700157	11	16
131	An Organic Emitter Displaying Dual Emissions and Efficient Delayed Fluorescence White OLEDs. *Advanced Optical Materials*, **2019**, 7, 1801667	8.1	16
130	Recent Advances and Applications of Inorganic Electrides. *Journal of Physical Chemistry Letters*, **2020**, 11, 3841-3852	6.4	16
129	Enhanced Electroluminescence from ZnO Quantum Dot Light-Emitting Diodes via Introducing Al2O3 Retarding Layer and Ag@ZnO Hybrid Nanodots. *Advanced Optical Materials*, **2017**, 5, 1700493	8.1	16
128	Redox-switching second-order nonlinear optical responses of N^N^N ruthenium complexes. *Computational and Theoretical Chemistry*, **2012**, 979, 112-118	2	16
127	Fluorescent photoswitching of a naphthopyran–benzimidazole dyad with high-degree fluorescent modulation within poly(methyl methacrylate) matrices. *Optical Materials*, **2013**, 35, 1504-1512	3.3	16
126	Quantum chemical study of redox-switchable second-order optical nonlinearity in Keggin-type organoimido derivative [PW11O39(ReNC6H5)]n (n = 2, 4). *Theoretical Chemistry Accounts*, **2009**, 122, 265-273	1.9	16
125	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		16
124	Anisotropic Janus SiP Monolayer as a Photocatalyst for Water Splitting. *Journal of Physical Chemistry Letters*, **2021**, 12, 2464-2470	6.4	16
123	Pressure-Induced Stable Beryllium Peroxide. *Inorganic Chemistry*, **2017**, 56, 5233-5238	5.1	15
122	Hexagonal BC2N with Remarkably High Hardness. *Journal of Physical Chemistry C*, **2018**, 122, 6801-6807	3.8	15
121	Element substitution of kesterite CuZnSnS for efficient counter electrode of dye-sensitized solar cells. *Scientific Reports*, **2018**, 8, 8714	4.9	15
120	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	1.9	15
119	Theoretical study on the rectifying performance of organoimido derivatives of hexamolybdates. *ChemPhysChem*, **2013**, 14, 610-7	3.2	15
118	Diastereomers of the pentacoordinate chiral phosphorus compounds in solution: absolute configurations and predominant conformations. *Dalton Transactions*, **2010**, 39, 6953-9	4.3	15
117	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, 2518-27	4.8	15
116	Theoretical predication of third-order optical nonlinearities of [Al4MAl4]n (n = 0, 2, M = Ti, V and Cr) clusters. *Theoretical Chemistry Accounts*, **2008**, 119, 329-333	1.9	15
115	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. *Journal of Physical Chemistry C*, **2018**, 122, 12448-12453	3.8	15

114	Isomer dependent molecular packing and carrier mobility of N-phenylcarbazole/phenanthro[9,10-d]imidazole based materials as hosts for efficient electrophosphorescence devices. *Journal of Materials Chemistry C*, **2019**, 7, 13486-13492	7.1	14
113	Triphenylamine-based pH chemosensor: Synthesis, crystal structure, photophysical properties and computational studies. *Synthetic Metals*, **2009**, 159, 2497-2501	3.6	13
112	Photophysical properties of quinoxaline-fused [7]carbohelicene derivatives. *RSC Advances*, **2015**, 5, 72907-72915	3.7	12
111	Understanding the photophysical properties of chiral dinuclear Re(i) complexes and the role of Re(i) in their complexes. *Dalton Transactions*, **2016**, 45, 7285-93	4.3	12
110	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	2.3	12
109	Theoretical study on the second-order nonlinear optical properties of nonconjugated D-π-A chromophores. *International Journal of Quantum Chemistry*, **2009**, 109, 1553-1559	2.1	12
108	Theoretical investigation of structures, electronic spectra and nonlinear optical properties of gold-pentacene (Au2C22H14) complexes. *Journal of Organometallic Chemistry*, **2009**, 694, 1266-1272	2.3	12
107	Synthesis and characterizations of novel spindle-like terphenyl-type chromophores for non-linear optical materials. *Tetrahedron*, **2011**, 67, 4110-4117	2.4	12
106	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	3.6	12
105	Ten-fold coordinated polymorph and metallization of TiO2 under high pressure. *RSC Advances*, **2015**, 5, 54253-54257	3.7	11
104	Photophysical Properties of Chiral Tetraphenylethylene Derivatives with the Fixed Propeller-Like Conformation. *Journal of Physical Chemistry C*, **2018**, 122, 5032-5039	3.8	11
103	Silicon Framework-Based Lithium Silicides at High Pressures. *ACS Applied Materials & Interfaces* , **2016**, 8, 16761-7	9.5	11
102	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, 1094-102	2.8	11
101	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	2.8	11
100	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	3.6	11
99	Theoretical study on the charge transport property of Pt(CN(t)Bu)2(CN)2 nanowires induced by Pt⋯Pt interactions. *Dalton Transactions*, **2012**, 41, 7272-7	4.3	11
98	TDDFT studies on chiral organophosphonate substituted divacant Keggin-type polyoxotungstate: diplex multistep-redox-triggered chiroptical and NLO switch. *Dalton Transactions*, **2012**, 41, 10097-104	4.3	11
97	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	2.5	11

96	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	1.9	11
95	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	1.9	11
94	Determination of the absolute configurations of synthetic daunorubicin analogues using vibrational circular dichroism spectroscopy and density functional theory. *Chirality*, **2010**, 22, 734-43	2.1	11
93	High-temperature driven inter-valley carrier transfer and significant fluorescence enhancement in multilayer WS. *Nanoscale Horizons*, **2018**, 3, 598-605	10.8	11
92	Theoretical Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Polyfluoroarylcyanation of Alkynes: Origin of Selectivity for C□CN Bond Activation. *Organometallics*, **2018**, 37, 2594-2601	3.8	10
91	Pressure-induced new chemistry. *Chinese Physics B*, **2019**, 28, 106106	1.2	10
90	Theoretical study on the photophysical properties of chiral mononuclear and dinuclear zinc complexes. *RSC Advances*, **2013**, 3, 2241-2247	3.7	10
89	Structural and electronic properties of alkali metal peroxides at high pressures. *RSC Advances*, **2015**, 5, 104337-104342	3.7	10
88	Understanding photophysical properties of chiral conjugated corrals for organic photovoltaics. *Journal of Materials Chemistry C*, **2017**, 5, 3495-3502	7.1	9
87	Computational predictions of two-dimensional anode materials of metal-ion batteries. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1473	7.9	9
86	Exploring the Limits of Transition-Metal Fluorination at High Pressures. *Angewandte Chemie - International Edition*, **2020**, 59, 9155-9162	16.4	9
85	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	9
84	Theoretical study on photophysical properties of novel bis(BF2)-2,2?-bidipyrrins dyes: Effect of variation in monomer structure. *International Journal of Quantum Chemistry*, **2012**, 112, 440-452	2.1	9
83	Superconducting boron allotropes. *Physical Review B*, **2020**, 101,	3.3	8
82	Exploring the origin of electrochemical performance of Cr-doped LiNiMnO. *Physical Chemistry Chemical Physics*, **2020**, 22, 3831-3838	3.6	8
81	Density Functional Theory Investigation on the Second-Order Nonlinear Optical Properties of Chlorobenzyl-o-Carborane Derivatives. *Chinese Journal of Chemistry*, **2012**, 30, 2349-2355	4.9	8
80	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
79	Theoretical study on the second-order nonlinear optical properties and reorganization energy of silafluorenes and spirobisilafluorenes derivatives. *Theoretical Chemistry Accounts*, **2011**, 128, 249-256	1.9	8

78	Quantum chemistry studies on the Ru 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	2.3	8
77	Anisotropic and High-Mobility CS Monolayer as a Photocatalyst for Water Splitting. *Journal of Physical Chemistry Letters*, **2021**, 12, 8320-8327	6.4	8
76	Chiral macrocyclic imine nickel(II) coordination complexes with diverse photophysical properties. *Dyes and Pigments*, **2017**, 140, 70-78	4.6	7
75	Achieving high conductivity p-type Ga2O3 through Al-N and In-N co-doping. *Chemical Physics Letters* , **2020**, 746, 137308	2.5	7
74	Anisotropic PC6N Monolayer with Wide Band Gap and Ultrahigh Carrier Mobility. *Journal of Physical Chemistry C*, **2020**, 124, 4330-4337	3.8	7
73	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. *Physical Review B*, **2019**, 100,	3.3	7
72	Prediction of the Xe He binary phase diagram at high pressures. *Chemical Physics Letters*, **2015**, 640, 115-118	2.5	7
71	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	2.8	7
70	Theoretical studies on one- and two-photon absorption properties of rubrene and its derivatives. *Synthetic Metals*, **2006**, 156, 1218-1224	3.6	7
69	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. *Physical Review B*, **2021**, 103,	3.3	7
68	Unveiling the Role of Oxygen Vacancy in Li2MnO3 upon Delithiation. *Journal of Physical Chemistry C* , **2019**, 123, 23403-23409	3.8	6
67	Unveiling the Photophysical Properties of Boron Heptaaryldipyrromethene Derivatives. *ChemPhysChem*, **2018**, 19, 2751-2757	3.2	6
66	Computational study of chiral molecules with high intrinsic hyperpolarizabilities. *Molecular Physics*, **2012**, 110, 333-341	1.7	6
65	Second-order nonlinear optical responses switching of N?N?N ruthenium carboxylate complexes with proton-electron transfer. *International Journal of Quantum Chemistry*, **2012**, 112, 779-788	2.1	6
64	A theoretical study of ambipolar organic transport material: 1,4-Bis(pentafluorobenzyl)[60]-fullerene. *Chemical Physics Letters*, **2011**, 506, 255-259	2.5	6
63	Density functional study of magnetic exchange of dinuclear manganese complexes with the heteropolymolyanion: [MnII 2(Xn+Mo9O33)2]2(n10)[X = PV, AsV, SeVI). *Science in China Series B: Chemistry*, **2008**, 51, 1174-1181		6
62	Cooperative enhancement of two-photon absorption cross sections in three-branched oligofluorene with boron center. *Computational and Theoretical Chemistry*, **2008**, 855, 69-76		6
61	Boron kagome-layer induced intrinsic superconductivity in a MnB3 monolayer with a high critical temperature. *Physical Review B*, **2020**, 102,	3.3	6

60	Tetragonal Structure BC4 as a Superhard Material. *Journal of Physical Chemistry C*, **2017**, 121, 10119-10123	3.8	5
59	Electron transport via phenyl⋯perfluorophenyl interaction in crystals of fluorine-substituted dibenzalacetones. *RSC Advances*, **2014**, 4, 50188-50194	3.7	5
58	Unveiling photophysical properties of phenanthro[9,10-d]imidazole derivatives for organic light-emitting diodes. *Organic Electronics*, **2017**, 50, 220-227	3.5	5
57	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
56	The effect of multiple weak interactions on the charge transport ability in polymorphs. *Synthetic Metals*, **2011**, 161, 1073-1078	3.6	5
55	Theoretical study on the electronic structures and optical properties of oxadisilole-substituted acenes. *Chemical Physics Letters*, **2008**, 466, 37-43	2.5	5
54	Theoretical study on characteristics of structure and vibrational frequency of spiro-linked complex Zn(PyIm)2 (PyIm = 2(2?-pyridine)-imidazole) in excited state. *Chemical Physics Letters*, **2006**, 418, 302-306	2.5	5
53	Theoretical study on group III elements and F co-doped ZnO. *Journal of Alloys and Compounds*, **2020**, 819, 153012	5.7	5
52	Structural and Superconducting Properties of Tungsten Hydrides Under High Pressure. *Frontiers in Physics*, **2018**, 6,	3.9	5
51	Mixed-valence Compounds: AuO and AuS. *ChemPhysChem*, **2018**, 19, 2989-2994	3.2	5
50	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. *RSC Advances*, **2015**, 5, 104426-104432	3.7	4
49	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	2.8	4
48	Superconducting ternary hydrides under high pressure. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	4
47	Achieving high hydrogen evolution reaction activity of a MoC monolayer. *Physical Chemistry Chemical Physics*, **2020**, 22, 26189-26199	3.6	4
46	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. *Journal of Physical Chemistry Letters*, **2021**, 12, 4203-4210	6.4	4
45	Wide Band Gap PS Monolayer with Anisotropic and Ultrahigh Carrier Mobility. *Journal of Physical Chemistry Letters*, **2021**, 12, 8481-8488	6.4	4
44	Nickel Hydrides under High Pressure. *Journal of Physical Chemistry C*, **2019**, 123, 24243-24247	3.8	3
43	Achieving high transparent □Ga2O3 through AlGa-InGa-VO. *Journal of Alloys and Compounds*, **2019**, 792, 405-410	5.7	3

42	The photophysical properties of cycloparaphenylene-based compounds with figure-eight configurations. *New Journal of Chemistry*, **2020**, 44, 12185-12193	3.6	3
41	Determination of the charge transport abilities of polymorphs [C6F5Cu]2(4,4?-bipy) with different interactions: a density functional theoretical investigation. *Theoretical Chemistry Accounts*, **2011**, 129, 45-51	1.9	3
40	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, 427-34	2.8	3
39	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		3
38	Strain-Induced Magnetism in MSi2N4 (M = V, Cr): A First-Principles Study. *Annalen Der Physik*, **2021**, 533, 2100273	2.6	3
37	IrN and IrN as potential high-energy-density materials. *Journal of Chemical Physics*, **2021**, 154, 054706	3.9	3
36	Memory Devices: Photocatalytic Reduction of Graphene Oxide□TiO2 Nanocomposites for Improving Resistive-Switching Memory Behaviors (Small 29/2018). *Small*, **2018**, 14, 1870136	11	3
35	Photophysical properties of chiral covalent organic cages. *Computational and Theoretical Chemistry*, **2017**, 1120, 1-7	2	2
34	Theoretical study on thiophene-based double helicenes with intrinsic large second-order nonlinear optical response. *RSC Advances*, **2016**, 6, 84705-84711	3.7	2
33	Pressure-induced reappearance of superconductivity in the oC24 phase of lithium. *Solid State Communications*, **2016**, 225, 7-11	1.6	2
32	Theoretical study on the photophysical properties of boron-fused double helicenes. *RSC Advances*, **2017**, 7, 56543-56549	3.7	2
31	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	4.9	2
30	Fabrication of Alkali Metal Boride: Honeycomb-Like Structured NaB4 with High Hardness and Excellent Electrical Conductivity. *Advanced Functional Materials*,2110872	15.6	2
29	Superconducting LaP2H2 with graphenelike phosphorus layers. *Physical Review B*, **2022**, 105,	3.3	2
28	Pressure-induced hydride superconductors above 200 K. *Matter and Radiation at Extremes*, **2021**, 6, 068201	4.7	2
27	Structural and electronic properties of tungsten oxides under high pressures. *Journal of Physics Condensed Matter*, **2020**, 32, 085403	1.8	2
26	Pressure-induced yttrium oxides with unconventional stoichiometries and novel properties. *Physical Review Materials*, **2021**, 5,	3.2	2
25	Structural transitions and electronic properties of sodium superoxide at high pressures. *RSC Advances*, **2016**, 6, 67910-67915	3.7	2

24	SiCP Monolayer with a Direct Band Gap and High Carrier Mobility for Photocatalytic Water Splitting.. *Journal of Physical Chemistry Letters*, **2021**, 190-197	6.4	2
23	Unconventional stable stoichiometry of vanadium peroxide. *Physical Chemistry Chemical Physics*, **2020**, 22, 11460-11466	3.6	1
22	Prediction of new thermodynamically stable ZnNO at high pressure. *Physical Chemistry Chemical Physics*, **2020**, 22, 10941-10948	3.6	1
21	A Semiconducting Cationic Square-Grid Network with FeIII Centers Displaying Unusual Dynamic Behavior. *European Journal of Inorganic Chemistry*, **2020**, 2020, 1255-1259	2.3	1
20	Electronic structure and second-order nonlinear optical property of chiral peropyrenes. *Journal of Molecular Modeling*, **2019**, 25, 220	2	1
19	Theoretical Investigation on Electronic Transition of Tris(8-quinolinolate) Aluminum Grafted on Poly(p-phenylenevinylene) Units with the Localized-density-matrix Method. *Chinese Journal of Chemistry*, **2009**, 27, 1891-1896	4.9	1
18	The influence of MM 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*, **2009**, 110, NA-NA	2.1	1
17	Theoretical study on the second-order nonlinear optical properties of gold (III) alkyl complexes. *Synthetic Metals*, **2009**, 159, 2406-2409	3.6	1
16	THE INVESTIGATION ON ELECTRONIC STRUCTURE AND SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF IIVI SEMICONDUCTOR CLUSTERS BY TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. *Journal of Theoretical and Computational Chemistry*, **2007**, 06, 585-594	1.8	1
15	A superconducting boron allotrope featuring anticlinal pentapyramids. *Journal of Materials Chemistry C*, **2022**, 10, 672-679	7.1	1
14	Theoretical considerations of superconducting HfBH2 and HfB2H under high pressure. *Journal of Applied Physics*, **2021**, 130, 153904	2.5	1
13	BC6P Monolayer: Isostructural and Isoelectronic Analogues of Graphene with Desirable Properties for K-Ion Batteries. *Chemistry of Materials*,	9.6	1
12	Pressure-induced Na-Au compounds with novel structural units and unique charge transfer. *Physical Chemistry Chemical Physics*, **2021**, 23, 6455-6461	3.6	1
11	Unraveling the synergetic mechanism of physisorption and chemisorption in laser-irradiated monolayer WS2. *Nano Research*, **2021**, 14, 4274	10	1
10	Superconducting ScP4 with a novel phosphorus framework. *Applied Physics A: Materials Science and Processing*, **2022**, 128, 1	2.6	1
9	Janus MoP Monolayer as an Electrocatalyst for Hydrogen Evolution. *ACS Applied Materials & Interfaces*, **2021**, 13, 57422-57429	9.5	0
8	Highly Photoluminescent Monolayer MoS2 and WS2 Achieved via Superacid Assisted Vacancy Reparation and Doping Strategy. *Laser and Photonics Reviews*, **2021**, 15, 2100104	8.3	0
7	Tailoring p-type conductivity of aluminum nitride via transition metal and fluorine doping. *Journal of Alloys and Compounds*, **2021**, 862, 158017	5.7	0

6	Disproportionation of SO_{2} at High Pressure and Temperature.. *Physical Review Letters*, **2022**, 128, 106001	7.4	0
5	Au with sp Hybridization in LiAuP.. *Journal of Physical Chemistry Letters*, **2021**, 236-242	6.4	0
4	Exploring the Limits of Transition-Metal Fluorination at High Pressures. *Angewandte Chemie*, **2020**, 132, 9240-9247	3.6	
3	Theoretical study on photophysical properties of Pt(II) triarylborons with a 2,2-bpy core derivatives. *Journal of Molecular Graphics and Modelling*, **2013**, 44, 311-7	2.8	
2	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	3.6	
1	Mixed-valence Compounds: AuO2 and AuS. *ChemPhysChem*, **2018**, 19, 2971-2971	3.2	