Zhongmin Su

List of Publications by Year
in descending order

1,247 papers	51,132 citations	2101 100 h-index	5394 164 g-index
1275 all docs	1275 docs citations	1275 times ranked	30719 citing authors

#	Article	IF	Citations
1	Highly Stable Crystalline Catalysts Based on a Microporous Metalâ˜'Organic Framework and Polyoxometalates. Journal of the American Chemical Society, 2009, 131, 1883-1888.	13.7	876
2	Recent advances in porous polyoxometalate-based metalâ€"organic framework materials. Chemical Society Reviews, 2014, 43, 4615-4632.	38.1	845
3	Ultrastable Polymolybdate-Based Metalâ€"Organic Frameworks as Highly Active Electrocatalysts for Hydrogen Generation from Water. Journal of the American Chemical Society, 2015, 137, 7169-7177.	13.7	584
4	Chiral 3D Architectures with Helical Channels Constructed from Polyoxometalate Clusters and Copperâ€"Amino Acid Complexes. Angewandte Chemie - International Edition, 2006, 45, 904-908.	13.8	564
5	Zeolitic imidazolate framework-8 as efficient pH-sensitive drug delivery vehicle. Dalton Transactions, 2012, 41, 6906.	3.3	544
6	Efficient and tunable white-light emission of metalâ€"organic frameworks by iridium-complex encapsulation. Nature Communications, 2013, 4, 2717.	12.8	501
7	Metal Nuclearity Modulated Four-, Six-, and Eight-Connected Entangled Frameworks Based on Mono-, Bi-, and Trimetallic Cores as Nodes. Chemistry - A European Journal, 2006, 12, 2680-2691.	3.3	479
8	Interlocked and Interdigitated Architectures from Self-Assembly of Long Flexible Ligands and Cadmium Salts. Angewandte Chemie - International Edition, 2004, 43, 5036-5040.	13.8	441
9	Effect of Imidazole Arrangements on Proton-Conductivity in Metalâ€"Organic Frameworks. Journal of the American Chemical Society, 2017, 139, 6183-6189.	13.7	436
10	Entangled Coordination Networks with Inherent Features of Polycatenation, Polythreading, and Polyknotting. Angewandte Chemie - International Edition, 2005, 44, 5824-5827.	13.8	416
11	Polyoxometalate-Based Cobaltâ€"Phosphate Molecular Catalysts for Visible Light-Driven Water Oxidation. Journal of the American Chemical Society, 2014, 136, 5359-5366.	13.7	414
12	A Sodalite-Type Porous Metalâ˜'Organic Framework with Polyoxometalate Templates: Adsorption and Decomposition of Dimethyl Methylphosphonate. Journal of the American Chemical Society, 2011, 133, 4178-4181.	13.7	405
13	Chiral Nanoporous Metalâ€Organic Frameworks with High Porosity as Materials for Drug Delivery. Advanced Materials, 2011, 23, 5629-5632.	21.0	378
14	Self-Assembly of Nanometer-Scale [Cu24I10L12]14+ Cages and Ball-Shaped Keggin Clusters into a (4,12)-Connected 3D Framework with Photoluminescent and Electrochemical Properties. Angewandte Chemie - International Edition, 2006, 45, 7411-7414.	13.8	375
15	Density functional theory characterization and design of high-performance diarylamine-fluorenedyes with different Ï€ spacers for dye-sensitized solar cells. Journal of Materials Chemistry, 2012, 22, 568-576.	6.7	355
16	Colorimetric Detection of Pb²⁺ Using Glutathione Functionalized Gold Nanoparticles. ACS Applied Materials & Interfaces, 2010, 2, 1466-1470.	8.0	340
17	An Exceptional 54-Fold Interpenetrated Coordination Polymer with 10³-srs Network Topology. Journal of the American Chemical Society, 2011, 133, 11406-11409.	13.7	328
18	Syntheses and Characterization of Six Coordination Polymers of Zinc(II) and Cobalt(II) with 1,3,5-Benzenetricarboxylate Anion and Bis(imidazole) Ligands. Inorganic Chemistry, 2007, 46, 3027-3037.	4.0	310

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19	N-rich zeolite-like metalâ€“organic framework with sodalite topology: high CO2 uptake, selective gas adsorption and efficient drug delivery. Chemical Science, 2012, 3, 2114.	7.4	277
20	A Fluorescent Sensor for Highly Selective Detection of Nitroaromatic Explosives Based on a 2D, Extremely Stable, Metalâ€“Organic Framework. Chemistry - A European Journal, 2014, 20, 3589-3594.	3.3	271
21	Polyoxometalates in dye-sensitized solar cells. Chemical Society Reviews, 2019, 48, 260-284.	38.1	261
22	Quantum Mechanical Design and Structure of the Li@B₁₀H₁₄Basket with a Remarkably Enhanced Electro-Optical Response. Journal of the American Chemical Society, 2009, 131, 11833-11840.	13.7	260
23	Self-Assembly and Photocatalytic Properties of Polyoxoniobates: {Nb₂₄O₇₂}, {Nb₃₂O₉₆}, and {K₁₂Nb₉₆O₂₈₈} Clusters. Journal of the American Chemical Society, 2012, 134, 14004-14010.	13.7	241
24	Tailored Synthesis of Octopusâ€type Janus Nanoparticles for Synergistic Activelyâ€Targeted and Chemoâ€Photothermal Therapy. Angewandte Chemie - International Edition, 2016, 55, 2118-2121.	13.8	236
25	Highly efficient visible-light-driven CO₂ reduction to formate by a new anthracene-based zirconium MOF via dual catalytic routes. Journal of Materials Chemistry A, 2016, 4, 2657-2662.	10.3	231
26	A Bridge between Pillared-Layer and Helical Structures: A Series of Three-Dimensional Pillared Coordination Polymers with Multiform Helical Chains. Chemistry - A European Journal, 2006, 12, 6528-6541.	3.3	230
27	A Series of Three-Dimensional Lanthanide Coordination Polymers with Rutile and Unprecedented Rutile-Related Topologies. Inorganic Chemistry, 2005, 44, 7122-7129.	4.0	229
28	Assembly of the Highest Connectivity Wells-Dawson Polyoxometalate Coordination Polymer: the Use of Organic Ligand Flexibility. Inorganic Chemistry, 2008, 47, 3274-3283.	4.0	225
29	Chiral polyoxometalate-based materials: From design syntheses to functional applications. Coordination Chemistry Reviews, 2013, 257, 702-717.	18.8	217
30	Self-Assembly of Polyoxometalate-Based Metal Organic Frameworks Based on Octamolybdates and Copper-Organic Units: from Cu^{II}, Cu^{I,II} to Cu^I via Changing Organic Amine. Inorganic Chemistry, 2008, 47, 8179-8187.	4.0	214
31	An unprecedented eight-connected self-penetrating network based on pentanuclear zinc cluster building blocks. Chemical Communications, 2005, , 4789.	4.1	207
32	Solvatochromic Behavior of Chiral Mesoporous Metalâ€“Organic Frameworks and Their Applications for Sensing Small Molecules and Separating Cationic Dyes. Chemistry - A European Journal, 2013, 19, 3639-3645.	3.3	202
33	DFT Study on Sulfur-Doped g-C₃N₄ Nanosheets as a Photocatalyst for CO₂ Reduction Reaction. Journal of Physical Chemistry C, 2018, 122, 7712-7719.	3.1	200
34	How to design proper Ï€-spacer order of the D-Ï€-A dyes for DSSCs? A density functional response. Dyes and Pigments, 2012, 95, 313-321.	3.7	199
35	Stable Luminescent Metalâ€“Organic Frameworks as Dual-Functional Materials To Encapsulate Ln³⁺ Ions for White-Light Emission and To Detect Nitroaromatic Explosives. Inorganic Chemistry, 2015, 54, 3290-3296.	4.0	196
36	Tuning the Dimensionality of the Coordination Polymer Based on Polyoxometalate by Changing the Spacer Length of Ligands. Crystal Growth and Design, 2008, 8, 3717-3724.	3.0	193

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37	Structures and Luminescent Properties of Seven Coordination Polymers of Zinc(II) and Cadmium(II) with 3,3â€²,4,4â€²-Benzophenone Tetracarboxylate Anion and Bis(imidazole). Crystal Growth and Design, 2008, 8, 675-684.	3.0	191
38	Assemblies of Copper Bis(triazole) Coordination Polymers Using the Same Keggin Polyoxometalate Template. Inorganic Chemistry, 2009, 48, 100-110.	4.0	188
39	Unusual parallel and inclined interlocking modes in polyrotaxane-like metalâ€“organic frameworks. Chemical Communications, 2008, , 2233.	4.1	186
40	Polyoxometalate-based materials for sustainable and clean energy conversion and storage. EnergyChem, 2019, 1, 100021.	19.1	183
41	Bottomâ€Up Synthesis of Porous Coordination Frameworks: Apical Substitution of a Pentanuclear Tetrahedral Precursor. Angewandte Chemie - International Edition, 2009, 48, 5291-5295.	13.8	182
42	Thermally Induced Reversible Phase Transformations Accompanied by Emission Switching Between Different Colors of Two Aromaticâ€Amine Compounds. Advanced Materials, 2009, 21, 3165-3169.	21.0	181
43	Role of Excess Electrons in Nonlinear Optical Response. Journal of Physical Chemistry Letters, 2015, 6, 612-619.	4.6	181
44	Chiral Polyoxometalate-Induced Enantiomerically 3D Architectures:â€‰ A New Route for Synthesis of High-Dimensional Chiral Compounds. Journal of the American Chemical Society, 2007, 129, 10066-10067.	13.7	176
45	Stepwise assembly of metalâ€“organic framework based on a metalâ€“organic polyhedron precursor for drug delivery. Chemical Communications, 2011, 47, 7128.	4.1	170
46	Spontaneous resolution of a 3D chiral polyoxometalate-based polythreaded framework consisting of an achiral ligand. Chemical Communications, 2008, , 58-60.	4.1	169
47	Exceptional Self-Penetrating Networks Containing Unprecedented Quintuple-Stranded Molecular Braid, 9-Fold Meso Helices, and 17-Fold Interwoven Helices. Inorganic Chemistry, 2007, 46, 4158-4166.	4.0	167
48	An Ionothermal Synthetic Approach to Porous Polyoxometalateâ€Based Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 7985-7989.	13.8	165
49	Transesterification of Vegetable Oil to Biodiesel using a Heteropolyacid Solid Catalyst. Advanced Synthesis and Catalysis, 2007, 349, 1057-1065.	4.3	164
50	Carbon nanodots@zeolitic imidazolate framework-8 nanoparticles for simultaneous pH-responsive drug delivery and fluorescence imaging. CrystEngComm, 2014, 16, 3259.	2.6	164
51	Self-Assembly of 2Dâ†'2D Interpenetrating Coordination Polymers Showing Polyrotaxane- and Polycatenane-like Motifs: Influence of Various Ligands on Topological Structural Diversity. Inorganic Chemistry, 2008, 47, 10600-10610.	4.0	162
52	Controllable Fabrication of Carbon Nanotube and Nanobelt with a Polyoxometalate-Assisted Mild Hydrothermal Process. Journal of the American Chemical Society, 2005, 127, 6534-6535.	13.7	160
53	pH-Dependent Assembly of Hybrids Based on Wells-Dawson POM/Ag Chemistry. Inorganic Chemistry, 2008, 47, 5145-5153.	4.0	159
54	Quantum chemical design of nonlinear optical materials by sp2-hybridized carbon nanomaterials: issues and opportunities. Journal of Materials Chemistry C, 2013, 1, 5439.	5.5	155

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55	L-cysteine functionalized gold nanoparticles for the colorimetric detection of Hg²⁺induced by ultraviolet light. Nanotechnology, 2010, 21, 025501.	2.6	154
56	A Microporous Anionic Metalâ€“Organic Framework for Sensing Luminescence of Lanthanide(III) Ions and Selective Absorption of Dyes by Ionic Exchange. Chemistry - A European Journal, 2014, 20, 5625-5630.	3.3	154
57	Utilizing dâ€“pÏ€ Bonds for Ultralong Organic Phosphorescence. Angewandte Chemie - International Edition, 2019, 58, 6645-6649.	13.8	154
58	Two Highly Water-Stable Imidazole-Based Ln-MOFs for Sensing Fe³⁺,Cr₂O₇^{2â€“}/CrO₄^{2â€“} in a Water Environment. Inorganic Chemistry, 2020, 59, 2005-2010.	4.0	154
59	Influence of Neutral Ligands on the Structures of Silver(I) Sulfonates. Inorganic Chemistry, 2005, 44, 9374-9383.	4.0	151
60	An unprecedented fivefold interpenetrated lvt network containing the exceptional racemic motifs originated from nine interwoven helices. Chemical Communications, 2005, , 5450.	4.1	148
61	An unusual polyoxometalate-encapsulating 3D polyrotaxane framework formed by molecular squares threading on a twofold interpenetrated diamondoid skeleton. Chemical Communications, 2007, , 4245.	4.1	148
62	Supramolecular Isomerism with Polythreaded Topology Based on [Mo₈O₂₆]⁴⁻ Isomers. Inorganic Chemistry, 2008, 47, 529-534.	4.0	148
63	Dinuclear metal complexes: multifunctional properties and applications. Chemical Society Reviews, 2020, 49, 765-838.	38.1	148
64	A Practicable Li/Naâ€Ion Hybrid Full Battery Assembled by a Highâ€Voltage Cathode and Commercial Graphite Anode: Superior Energy Storage Performance and Working Mechanism. Advanced Energy Materials, 2018, 8, 1702504.	19.5	142
65	Enhanced proton and electron reservoir abilities of polyoxometalate grafted on graphene for high-performance hydrogen evolution. Energy and Environmental Science, 2016, 9, 1012-1023.	30.8	138
66	Two Dawson-Templated Three-Dimensional Metalâ^'Organic Frameworks Based on Oxalate-Bridged Binuclear Cobalt(II)/Nickel(II) SBUs and Bpy Linkers. Inorganic Chemistry, 2008, 47, 7133-7138.	4.0	132
67	Rationally Designed, Polymeric, Extended Metal-Ciprofloxacin Complexes. Chemistry - A European Journal, 2005, 11, 6673-6686.	3.3	131
68	Theoretical characterization and design of small molecule donor material containing naphthodithiophene central unit for efficient organic solar cells. Journal of Computational Chemistry, 2013, 34, 1611-1619.	3.3	130
69	Protein-Sized Chiral Fe₁₆₈ Cages with NbO-Type Topology. Journal of the American Chemical Society, 2009, 131, 14600-14601.	13.7	128
70	Precise synthesis of unique polydopamine/mesoporous calcium phosphate hollow Janus nanoparticles for imaging-guided chemo-photothermal synergistic therapy. Chemical Science, 2017, 8, 8067-8077.	7.4	125
71	An Interpenetrating Architecture Based on the Wellsâ€“Dawson Polyoxometalate and AgIÂ·Â·Â·AgIInteractions. Crystal Growth and Design, 2011, 11, 2736-2742.	3.0	124
72	Two Multi-Copper-Containing Heteropolyoxotungstates Constructed from the Lacunary Keggin Polyoxoanion and the High-Nuclear Spin Cluster. Inorganic Chemistry, 2007, 46, 8162-8169.	4.0	123

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73	Spontaneous Resolution of Chiral Polyoxometalateâ€Based Compounds Consisting of 3D Chiral Inorganic Skeletons Assembled from Different Helical Units. Chemistry - A European Journal, 2008, 14, 9999-10006.	3.3	123
74	Highly sensitive oxygen sensors based on Cu(i) complexâ€“polystyrene composite nanofibrous membranes prepared by electrospinning. Chemical Communications, 2009, , 5868.	4.1	123
75	Oxidative Polyoxometalates Modified Graphitic Carbon Nitride for Visible-Light CO₂ Reduction. ACS Applied Materials & Interfaces, 2017, 9, 11689-11695.	8.0	122
76	A three-dimensional porous metalâ€“organic framework with the rutile topology constructed from triangular and distorted octahedral building blocks. Chemical Communications, 2005, , 2402.	4.1	121
77	A Series of Lead(II)-Organic Frameworks Based on Pyridyl Carboxylate Acid N-Oxide Derivatives: Syntheses, Structures, and Luminescent Properties. Crystal Growth and Design, 2008, 8, 3566-3576.	3.0	120
78	A Mixed-Valence Tinâ€“Oxygen Cluster Containing Six Peripheral Ferrocene Units. Angewandte Chemie - International Edition, 2004, 43, 2409-2411.	13.8	119
79	A multifunctional microporous anionic metalâ€“organic framework for column-chromatographic dye separation and selective detection and adsorption of Cr³⁺. Journal of Materials Chemistry A, 2015, 3, 23426-23434.	10.3	117
80	Enhanced CO2 photoreduction via tuning halides in perovskites. Journal of Catalysis, 2019, 369, 201-208.	6.2	117
81	Using Flexible and Rigid Organic Ligands to Tune Topology Structures Based on Keggin Polyoxometalates. Crystal Growth and Design, 2010, 10, 1104-1110.	3.0	116
82	Multifunctional Hollow Mesoporous Silica Nanocages for Cancer Cell Detection and the Combined Chemotherapy and Photodynamic Therapy. ACS Applied Materials & Interfaces, 2011, 3, 2479-2486.	8.0	116
83	A cationic iridium(<scp>iii</scp>) complex with aggregation-induced emission (AIE) properties for highly selective detection of explosives. Chemical Communications, 2014, 50, 6031-6034.	4.1	115
84	Biorecognition-Driven Self-Assembly of Gold Nanorods: A Rapid and Sensitive Approach toward Antibody Sensing. Chemistry of Materials, 2007, 19, 5809-5811.	6.7	114
85	Mixed-Valence Iron(II, III) Trimesates with Open Frameworks Modulated by Solvents. Inorganic Chemistry, 2007, 46, 7782-7788.	4.0	113
86	Silver/Polyaniline Composite Nanotubes: One-Step Synthesis and Electrocatalytic Activity for Neurotransmitter Dopamine. Journal of Physical Chemistry C, 2009, 113, 15175-15181.	3.1	112
87	Assembly of Multitrack Cuâ^'N Coordination Polymeric Chain-Modified Polyoxometalates Influenced by Polyoxoanion Cluster and Ligand. Crystal Growth and Design, 2007, 7, 2535-2541.	3.0	111
88	The stability and nonlinear optical properties: Encapsulation of an excess electron compound LiCNâ‹¯Li within boron nitride nanotubes. Journal of Materials Chemistry, 2012, 22, 2196-2202.	6.7	111
89	A new type of organicâ€“inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. Dalton Transactions, 2013, 42, 15053.	3.3	111
90	Syntheses, Characterization, and Luminescent Properties of Three 3D Leadâ^'Organic Frameworks with 1D Channels. Crystal Growth and Design, 2007, 7, 513-520.	3.0	110

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91	A DFT Study on The Twoâ€Dimensional Secondâ€Order Nonlinear Optical (NLO) Response of Terpyridineâ€Substituted Hexamolybdates: Physical Insight on 2D Inorganicâ€“Organic Hybrid Functional Materials. European Journal of Inorganic Chemistry, 2012, 2012, 705-711.	2.0	109
92	Structures and Luminescent Properties of a Series of Zinc(II) and Cadmium(II) 4,4â€²-Oxydiphthalate Coordination Polymers with Various Ligands Based on Bis(pyridyl imidazole) under Hydrothermal Conditions. Crystal Growth and Design, 2008, 8, 1610-1616.	3.0	108
93	Controllable synthesis of iridium(iii)-based aggregation-induced emission and/or piezochromic luminescence phosphors by simply adjusting the substitution on ancillary ligands. Journal of Materials Chemistry C, 2013, 1, 1440.	5.5	107
94	Utilizing dâ€“pÏ€ Bonds for Ultralong Organic Phosphorescence. Angewandte Chemie, 2019, 131, 6717-6721.	2.0	107
95	A polyoxometalate-encapsulated 3D porous metalâ€“organic pseudo-rotaxane framework. Chemical Communications, 2010, 46, 5097.	4.1	106
96	Quantum chemical study of benzimidazole derivatives to tune the second-order nonlinear optical molecular switching by proton abstraction. Physical Chemistry Chemical Physics, 2010, 12, 4791.	2.8	106
97	A hexanuclear cobalt metalâ€“organic framework for efficient CO₂ reduction under visible light. Journal of Materials Chemistry A, 2017, 5, 12498-12505.	10.3	106
98	2D Cd(II)â€“Lanthanide(III) Heterometallicâ€“Organic Frameworks Based on Metalloligands for Tunable Luminescence and Highly Selective, Sensitive, and Recyclable Detection of Nitrobenzene. Inorganic Chemistry, 2014, 53, 8105-8113.	4.0	105
99	High-Performance Metalâ€“Organic Framework-Based Single Ion Conducting Solid-State Electrolytes for Low-Temperature Lithium Metal Batteries. ACS Applied Materials & Interfaces, 2019, 11, 43206-43213.	8.0	104
100	Redox-Switchable Second-Order Nonlinear Optical Responses of Pushâ^'Pull Monotetrathiafulvalene-Metalloporphyrins. Inorganic Chemistry, 2009, 48, 6548-6554.	4.0	103
101	Prediction of Remarkably Large Second-Order Nonlinear Optical Properties of Organoimido-Substituted Hexamolybdates. Journal of Physical Chemistry A, 2009, 113, 3576-3587.	2.5	102
102	Electrical conductivity and electroluminescence of a new anthracene-based metalâ€“organic framework with Ï€-conjugated zigzag chains. Chemical Communications, 2016, 52, 2019-2022.	4.1	102
103	Ternary hybrids as efficient bifunctional electrocatalysts derived from bimetallic metalâ€“organic-frameworks for overall water splitting. Journal of Materials Chemistry A, 2018, 6, 5789-5796.	10.3	102
104	Hetero-metallic active sites coupled with strongly reductive polyoxometalate for selective photocatalytic CO₂-to-CH₄ conversion in water. Chemical Science, 2019, 10, 185-190.	7.4	102
105	Building block approach to nanostructures: step-by-step assembly of large lanthanide-containing polytungstoarsenate aggregates. Dalton Transactions, 2007, , 4293.	3.3	101
106	Uniform hollow mesoporous silica nanocages for drug delivery in vitro and in vivo for liver cancer therapy. Journal of Materials Chemistry, 2011, 21, 5299.	6.7	101
107	Expediting the Conversion of Li₂S₂ to Li₂S Enables High-Performance Liâ€“S Batteries. ACS Nano, 2021, 15, 7318-7327.	14.6	101
108	Syntheses and Structures of Organicâ^'Inorganic Hybrid Compounds Based on Metalâ^'Fluconazole Coordination Polymers and the Î²-Mo₈O₂₆ Anion. Inorganic Chemistry, 2007, 46, 8283-8290.	4.0	99

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109	Catenation of Loop-Containing 2D Layers with a 3D pcu Skeleton into a New Type of Entangled Framework Having Polyrotaxane and Polycatenane Character. Inorganic Chemistry, 2008, 47, 5555-5557.	4.0	99
110	Iodine-templated assembly of unprecedented 3dâ€“4f metalâ€“organic frameworks as photocatalysts for hydrogen generation. Chemical Communications, 2013, 49, 3564.	4.1	99
111	An organicâ€“inorganic hybrid material constructed from a three-dimensional coordination complex cationic framework and entrapped hexadecavanadate clusters. Chemical Communications, 2005, , 5023.	4.1	98
112	An unprecedented (6,8)-connected self-penetrating network based on two distinct zinc clusters. Chemical Communications, 2007, , 4863.	4.1	98
113	Unusual microporous polycatenane-like metalâ€“organic frameworks for the luminescent sensing of Ln3+ cations and rapid adsorption of iodine. Chemical Communications, 2012, 48, 5919.	4.1	96
114	Entangled structures in polyoxometalate-based coordination polymers. Coordination Chemistry Reviews, 2014, 279, 141-160.	18.8	96
115	Metalâ€“organic replica of Î³-Pu: the first uninodal 10-connected coordination network based on pentanuclear cadmium clusters. Chemical Communications, 2009, , 410-412.	4.1	95
116	Uniform Pomegranateâ€Like Nanoclusters Organized by Ultrafine Transition Metal Oxide@Nitrogenâ€Doped Carbon Subunits with Enhanced Lithium Storage Properties. Advanced Energy Materials, 2018, 8, 1702347.	19.5	95
117	Design and syntheses of blue luminescent zinc(II) and cadmium(II) complexes with bidentate or tridentate pyridyl-imidazole ligands. Polyhedron, 2006, 25, 635-644.	2.2	94
118	Realization of High-Energy Emission from [Cu(Nâˆ’N)(Pâˆ’P)]⁺ Complexes for Organic Light-Emitting Diode Applications. Journal of Physical Chemistry C, 2009, 113, 13968-13973.	3.1	94
119	Investigation of Dibenzoboroles Having Ï€-Electrons: Toward a New Type of Two-Dimensional NLO Molecular Switch?. Journal of Physical Chemistry C, 2009, 113, 12551-12557.	3.1	94
120	A 2D bilayered metalâ€“organic framework as a fluorescent sensor for highly selective sensing of nitro explosives. Dalton Transactions, 2015, 44, 7822-7827.	3.3	94
121	First principles study for the key electronic, optical and nonlinear optical properties of novel donor-acceptor chalcones. Journal of Molecular Graphics and Modelling, 2017, 72, 58-69.	2.4	94
122	Spectroscopic and Excited-State Properties of Luminescent Rhenium(I) N-Heterocyclic Carbene Complexes Containing Aromatic Diimine Ligands. Organometallics, 1998, 17, 1622-1630.	2.3	93
123	Reversible piezochromic behavior of two new cationic iridium(iii) complexes. Chemical Communications, 2012, 48, 2000.	4.1	93
124	Polyoxometalate-based crystalline tubular microreactor: redox-active inorganicâ€“organic hybrid materials producing gold nanoparticles and catalytic properties. Chemical Science, 2012, 3, 705-710.	7.4	93
125	A stable luminescent anionic porous metalâ€“organic framework for moderate adsorption of CO₂ and selective detection of nitro explosives. Journal of Materials Chemistry A, 2015, 3, 7224-7228.	10.3	93
126	A luminescent dye@MOF as a dual-emitting platform for sensing explosives. Chemical Communications, 2015, 51, 17521-17524.	4.1	93

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127	Graphene-coated hybrid electrocatalysts derived from bimetallic metalâ€“organic frameworks for efficient hydrogen generation. Journal of Materials Chemistry A, 2017, 5, 5000-5006.	10.3	92
128	Diamondoid-structured polymolybdate-based metalâ€“organic frameworks as high-capacity anodes for lithium-ion batteries. Chemical Communications, 2017, 53, 5204-5207.	4.1	92
129	Luminescent Metalâ€“Organic Frameworks with Anthracene Chromophores: Small-Molecule Sensing and Highly Selective Sensing for Nitro Explosives. Crystal Growth and Design, 2016, 16, 4374-4382.	3.0	91
130	Self-Assembly of Goldberg Polyhedra from a Concave [WV₅O₁₁(RCO₂)₅(SO₄)]^{3â€“} Building Block with 5-Fold Symmetry. Journal of the American Chemical Society, 2018, 140, 17365-17368.	13.7	91
131	Controllable synthesis of isoreticular pillared-layer MOFs: gas adsorption, iodine sorption and sensing small molecules. Journal of Materials Chemistry A, 2014, 2, 14827-14834.	10.3	89
132	The preparation of new covalent organic framework embedded with silver nanoparticles and its applications in degradation of organic pollutants from waste water. Dalton Transactions, 2019, 48, 1051-1059.	3.3	89
133	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
134	Three neutral metalâ€“organic frameworks with micro- and meso-pores for adsorption and separation of dyes. Journal of Materials Chemistry A, 2013, 1, 13060.	10.3	88
135	The Excess Electron in a Boron Nitride Nanotube: Pyramidal NBO Charge Distribution and Remarkable First Hyperpolarizability. Chemistry - A European Journal, 2012, 18, 11350-11355.	3.3	87
136	AIE Multinuclear Ir(III) Complexes for Biocompatible Organic Nanoparticles with Highly Enhanced Photodynamic Performance. Advanced Science, 2019, 6, 1802050.	11.2	87
137	HKUST-1 modified ultrastability cellulose/chitosan composite aerogel for highly efficient removal of methylene blue. Carbohydrate Polymers, 2021, 255, 117402.	10.2	87
138	Novel butterfly pyrene-based organic semiconductors for field effect transistors. Chemical Communications, 2006, , 755.	4.1	86
139	A stable metalâ€“organic framework with suitable pore sizes and rich uncoordinated nitrogen atoms on the internal surface of micropores for highly efficient CO₂ capture. Journal of Materials Chemistry A, 2015, 3, 7361-7367.	10.3	86
140	Improved Photoreduction of CO₂ with Water by Tuning the Valence Band of Covalent Organic Frameworks. ChemSusChem, 2020, 13, 2973-2980.	6.8	86
141	Precise Molecularâ€Level Modification of Nafion with Bismuth Oxide Clusters for Highâ€performance Protonâ€Exchange Membranes. Angewandte Chemie - International Edition, 2021, 60, 6076-6085.	13.8	86
142	A new molybdenum-oxide-based organicâ€“inorganic hybrid framework templated by double-Keggin anions. Chemical Communications, 2007, , 2593-2595.	4.1	85
143	Selective sensing of 2,4,6-trinitrophenol (TNP) in aqueous media with â€œaggregation-induced emission enhancementâ€•(AIEE)-active iridium(<scp>iii</scp>) complexes. Chemical Communications, 2018, 54, 1730-1733.	4.1	85
144	Obtaining carbon nanotubes from grass. Nanotechnology, 2005, 16, 1192-1195.	2.6	84

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145	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.	2.6	84
146	Assembly of a luminescent coreâ€“shell nanocluster featuring a Ag34S26 shell and a W6O216â¸ polyoxoanion core. Chemical Communications, 2012, 48, 5844.	4.1	84
147	Derivation and Decoration of Nets with Trigonal-Prismatic Nodes: A Unique Route to Reticular Synthesis of Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 5299-5307.	13.7	84
148	Redox and Photoisomerization Switching the Second-Order Nonlinear Optical Properties of a Tetrathiafulvalene Derivative Across Six States: A DFT Study. Journal of Physical Chemistry C, 2011, 115, 23946-23954.	3.1	83
149	Assembly of Cerium(III)â€Stabilized Polyoxotungstate Nanoclusters with SeO₃^{2â¸}/TeO₃^{2â¸} Templates: From Single Polyoxoanions to Inorganic Hollow Spheres in Dilute Solution. Chemistry - A European Journal, 2013, 19, 11007-11015.	3.3	83
150	Keggin POMs Modified by Bonding to Multitrack Cu(bipy) Chains through Linearly Arrayed Terminal and Bridging Oxygen Atoms of the M3O13 Triad. European Journal of Inorganic Chemistry, 2007, 2007, 1268-1274.	2.0	82
151	Tailored Surfaces on 2D Material: UFOâ€Like Cyclodextrinâ€Pd Nanosheet/Metal Organic Framework Janus Nanoparticles for Synergistic Cancer Therapy. Advanced Functional Materials, 2018, 28, 1803815.	14.9	82
152	Novel rare-earth(III)-based water soluble emitters for Fe(III) detection. Sensors and Actuators B: Chemical, 2010, 143, 595-599.	7.8	81
153	A stable Alq3@MOF composite for white-light emission. Chemical Communications, 2016, 52, 3288-3291.	4.1	81
154	Directed Copper-Catalyzed Intermolecular Aminative Difunctionalization of Unactivated Alkenes. Journal of the American Chemical Society, 2019, 141, 18475-18485.	13.7	81
155	Capturing a Synergistic Effect of a Conical Push and an Inward Pull in Fluoro Derivatives of Li@B₁₀H₁₄ Basket: Toward a Higher Vertical Ionization Potential and Nonlinear Optical Response. Journal of Physical Chemistry A, 2011, 115, 923-931.	2.5	80
156	A polyoxometalate-based single-molecule magnet with a mixed-valent {MnIV2MnIII6MnII4} core. Chemical Communications, 2013, 49, 2515.	4.1	80
157	A dual-emitting mixed-lanthanide MOF with high water-stability for ratiometric fluorescence sensing of Fe³⁺ and ascorbic acid. Journal of Materials Chemistry C, 2021, 9, 562-568.	5.5	80
158	A Stable Polyoxometalateâ€Pillared Metalâ€“Organic Framework for Protonâ€Conducting and Colorimetric Biosensing. Chemistry - A European Journal, 2015, 21, 11894-11898.	3.3	79
159	Versatile frameworks constructed from divalent metals and 1,2,3,4-butanetetracarboxylate anion: syntheses, crystal structures, luminescence and magnetic properties. CrystEngComm, 2008, 10, 894.	2.6	78
160	Iridium(iii) complexes adopting 1,2-diphenyl-1H-benzoimidazole ligands for highly efficient organic light-emitting diodes with low efficiency roll-off and non-doped feature. Journal of Materials Chemistry C, 2014, 2, 2150.	5.5	78
161	Enhanced Visible Photovoltaic Response of TiO₂ Thin Film with an All-Inorganic Donorâ€“Acceptor Type Polyoxometalate. ACS Applied Materials & Interfaces, 2015, 7, 13714-13721.	8.0	78
162	A (3,12)-Connected 3D Metal-Organic Framework Based on Nanosized Octanuclear Zinc Clusters. Crystal Growth and Design, 2008, 8, 3490-3492.	3.0	77

#	Article	IF	Citations
163	A Stable Porous Anionic Metalâ€“Organic Framework for Luminescence Sensing of Ln³⁺ Ions and Detection of Nitrobenzene. Chemistry - an Asian Journal, 2014, 9, 749-753.	3.3	77
164	Assembly of organicâ€“inorganic hybrid materials constructed from polyoxometalate and metalâ€“1,2,4-triazole units: synthesis, structures, magnetic, electrochemical and photocatalytic properties. CrystEngComm, 2015, 17, 2176-2189.	2.6	77
165	Encapsulating Red Phosphorus in Ultralarge Pore Volume Hierarchical Porous Carbon Nanospheres for Lithium/Sodium-Ion Half/Full Batteries. ACS Nano, 2019, 13, 13513-13523.	14.6	77
166	Bottomâ€Up Construction and Reversible Structural Transformation of Supramolecular Isomers based on Large Truncated Tetrahedra. Angewandte Chemie - International Edition, 2019, 58, 780-784.	13.8	77
167	pH-dependent self-assembly of divalent metals with a new ligand containing polycarboxylate: syntheses, crystal structures, luminescent and magnetic properties. CrystEngComm, 2010, 12, 2157.	2.6	76
168	The interplay of intermolecular interactions, packing motifs and electron transport properties in perylene diimide related materials: a theoretical perspective. Journal of Materials Chemistry, 2012, 22, 20840.	6.7	76
169	Theoretical studies on organoimido-substituted hexamolybdates dyes for dye-sensitized solar cells (DSSC). Dyes and Pigments, 2013, 99, 440-446.	3.7	74
170	Quasi-Solid-State Sodium-Ion Full Battery with High-Power/Energy Densities. ACS Applied Materials & Interfaces, 2018, 10, 17903-17910.	8.0	74
171	Promoted Photocharge Separation in 2D Lateral Epitaxial Heterostructure for Visibleâ€Lightâ€Driven CO₂ Photoreduction. Advanced Materials, 2020, 32, e2004311.	21.0	74
172	Construction and property investigation of transition-metal complexes modified octamolybdate hybrid materials based on V-shaped organic ligands. CrystEngComm, 2010, 12, 434-445.	2.6	73
173	Creation of cationic iridium(iii) complexes with aggregation-induced phosphorescent emission (AIPE) properties by increasing rotation groups on carbazole peripheries. Dalton Transactions, 2011, 40, 2947.	3.3	73
174	Selectedâ€Control Synthesis of Monodisperse Fe₃O₄@C Coreâ€“Shell Spheres, Chains, and Rings as Highâ€Performance Anode Materials for Lithiumâ€Ion Batteries. Chemistry - A European Journal, 2012, 18, 11417-11422.	3.3	73
175	Fluorescent hollow/rattle-type mesoporous Au@SiO2 nanocapsules for drug delivery and fluorescence imaging of cancer cells. Journal of Colloid and Interface Science, 2011, 358, 109-115.	9.4	72
176	Designed Fabrication of Unique Eccentric Mesoporous Silica Nanocluster-Based Coreâ€“Shell Nanostructures for pH-Responsive Drug Delivery. ACS Applied Materials & Interfaces, 2013, 5, 7282-7290.	8.0	72
177	A luminescent metal organic framework with high sensitivity for detecting and removing copper ions from simulated biological fluids. Dalton Transactions, 2017, 46, 2456-2461.	3.3	72
178	Electronic structures and chemical bonding in transition metal monosilicides MSi (M=3d, 4d, 5d) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 1	3.0	71
179	Controllable colours and shapes of silver nanostructures based on pH: application to surface-enhanced Raman scattering. Nanotechnology, 2007, 18, 325602.	2.6	71
180	Boron/Nitrogen Substitution of the Central Carbon Atoms of the Biphenalenyl Diradical Ï€ Dimer: A Novel 2eâ€“12c Bond and Large NLO Responses. Chemistry - A European Journal, 2011, 17, 11773-11779.	3.3	71

#	Article	IF	Citations
181	An unprecedented organicâ€“inorganic hybrid based on the first {Nb₁₀V₄O₄₀(OH)₂}¹²^{â^'}clusters and copper cations. Chemical Communications, 2012, 48, 103-105.	4.1	71
182	A Novel Carboxyethyltin Functionalized Sandwich-type Germanotungstate: Synthesis, Crystal Structure, Photosensitivity, and Application in Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2014, 6, 7876-7884.	8.0	71
183	An Anionic Interpenetrated Zeoliteâ€Like Metalâ€“Organic Framework Composite As a Tunable Dualâ€Emission Luminescent Switch for Detecting Volatile Organic Molecules. Chemistry - A European Journal, 2016, 22, 17298-17304.	3.3	71
184	Recent progress in phosphorescent Ir(III) complexes for nondoped organic light-emitting diodes. Coordination Chemistry Reviews, 2020, 413, 213283.	18.8	71
185	Preparation and Formation Mechanism of Different Î±-Fe2O3Morphologies from Snowflake to Paired Microplates, Dumbbell, and Spindle Microstructures. Journal of Physical Chemistry C, 2007, 111, 9049-9054.	3.1	70
186	Quantum Chemical Research on Structures, Linear and Nonlinear Optical Properties of the Li@n-Acenes Salt (n = 1, 2, 3, and 4). Journal of Physical Chemistry A, 2011, 115, 2035-2040.	2.5	70
187	Controllable synthesis of a non-interpenetrating microporous metalâ€“organic framework based on octahedral cage-like building units for highly efficient reversible adsorption of iodine. Chemical Communications, 2012, 48, 10001.	4.1	70
188	Self-assembled arrays of polyoxometalate-based metalâ€“organic nanotubes for proton conduction and magnetism. Chemical Communications, 2015, 51, 11313-11316.	4.1	70
189	Anderson-like alkoxo-polyoxovanadate clusters serving as unprecedented second building units to construct metalâ€“organic polyhedra. Chemical Communications, 2016, 52, 9632-9635.	4.1	70
190	Self-organization towards complex multi-fold meso-helices in the structures of Wellsâ€“Dawson polyoxometalate-based hybrid materials for lithium-ion batteries. Journal of Materials Chemistry A, 2017, 5, 3371-3376.	10.3	70
191	Construction of different dimensional inorganicâ€“organic hybrid materials based on polyoxometalates and metalâ€“organic units via changing metal ions: from non-covalent interactions to covalent connections. Dalton Transactions, 2008, , 3824.	3.3	69
192	Two eight-connected self-penetrating porous metalâ€“organic frameworks: configurational isomers caused by different linking modes between terephthalate and binuclear nickel building units. CrystEngComm, 2009, 11, 274-277.	2.6	68
193	Remarkable solvent-size effects in constructing novel porous 1,3,5-benzenetricarboxylate metalâ€“organic frameworks. CrystEngComm, 2012, 14, 5596.	2.6	68
194	A neutral dinuclear Ir(iii) complex for anti-counterfeiting and data encryption. Chemical Communications, 2017, 53, 3022-3025.	4.1	68
195	Facile preparation of fluorescent Au nanoclusters-based test papers for recyclable detection of Hg2+ and Pb2+. Sensors and Actuators B: Chemical, 2017, 241, 592-600.	7.8	68
196	Polyaniline as interface layers promoting the in-situ growth of zeolite imidazole skeleton on regenerated cellulose aerogel for efficient removal of tetracycline. Journal of Colloid and Interface Science, 2020, 579, 119-127.	9.4	68
197	Charge Carrier Transporting, Photoluminescent, and Electroluminescent Properties of Zinc(II)-2-(2-hydroxyphenyl)benzothiazolate Complex. Chemistry of Materials, 2007, 19, 1740-1748.	6.7	67
198	Two Heterometallic Aggregates Constructed from the {P₂W₁₂}-Based Trimeric Polyoxotungstates and 3d-4f Heterometals. Crystal Growth and Design, 2010, 10, 135-139.	3.0	67

#	Article	IF	Citations
199	How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene. Journal of Physical Chemistry C, 2010, 114, 19792-19798.	3.1	67
200	Adsorption of volatile organic compounds in porous metalâ€“organic frameworks functionalized by polyoxometalates. Journal of Solid State Chemistry, 2011, 184, 3034-3039.	2.9	67
201	Influence of anionic sulfonate-containing co-ligands on the solid structures of silver complexes supported by 4,4â€²-bipyridine bridges. Dalton Transactions, 2008, , 5331.	3.3	66
202	Facâ€Alq₃ and Merâ€Alq₃ Nano/Microcrystals with Different Emission and Chargeâ€Transporting Properties. Advanced Materials, 2010, 22, 1631-1634.	21.0	66
203	Theoretical Insight into the Origin of Large Stokes Shift and Photophysical Properties of Anilidoâ€Pyridine Boron Difluoride Dyes. ChemPhysChem, 2012, 13, 3714-3722.	2.1	66
204	Control of interpenetration in S-containing metalâ€“organic frameworks for selective separation of transition metal ions. Chemical Communications, 2013, 49, 1088.	4.1	66
205	A highly stable polyoxometalate-based metalâ€“organic framework with an ABW zeolite-like structure. Chemical Communications, 2017, 53, 10054-10057.	4.1	66
206	Structural Study of Silver(I) Sulfonate Complexes with Pyrazine Derivatives. Inorganic Chemistry, 2007, 46, 7299-7311.	4.0	65
207	A Ligand Exchange Route to Highly Luminescent Surfaceâ€Functionalized ZnS Nanoparticles and Their Transparent Polymer Nanocomposites. Advanced Functional Materials, 2008, 18, 3070-3079.	14.9	65
208	Modulation on charge recombination and light harvesting towardÂhigh-performance benzothiadiazole-based sensitizers in dye-sensitized solar cells: A theoretical investigation. Journal of Power Sources, 2014, 267, 300-308.	7.8	65
209	Facile and Scalable Synthesis of Novel Spherical Au Nanocluster Assemblies@Polyacrylic Acid/Calcium Phosphate Nanoparticles for Dualâ€Modal Imagingâ€Guided Cancer Chemotherapy. Small, 2015, 11, 3162-3173.	10.0	65
210	d10-Metal coordination polymers based on analogue di(pyridyl)imidazole derivatives and 4,4â€²-oxydibenzoic acid: influence of flexible and angular characters of neutral ligands on structural diversity. Dalton Transactions, 2008, , 6796.	3.3	64
211	A theoretical discussion on the relationships among molecular packings, intermolecular interactions, and electron transport properties for naphthalene tetracarboxylic diimide derivatives. Journal of Materials Chemistry, 2011, 21, 15558.	6.7	64
212	Intramolecular Ï€-stacking in cationic iridium(iii) complexes with a triazoleâ€“pyridine type ancillary ligand: synthesis, photophysics, electrochemistry properties and piezochromic behavior. Journal of Materials Chemistry, 2012, 22, 12736.	6.7	64
213	A series of pillar-layer metalâ€“organic frameworks based on 5-aminoisophthalic acid and 4,4â€²-bipyridine. Dalton Transactions, 2012, 41, 1047-1053.	3.3	64
214	Pillared metal organic frameworks for the luminescence sensing of small molecules and metal ions in aqueous solutions. Dalton Transactions, 2015, 44, 1754-1760.	3.3	64
215	Supercapacitor with high cycling stability through electrochemical deposition of metalâ€“organic frameworks/polypyrrole positive electrode. Dalton Transactions, 2018, 47, 13472-13478.	3.3	64
216	Polyaniline Nanotubes Prepared Using Fiber Mats Membrane as the Template and their Gas-response Behavior. Journal of Physical Chemistry C, 2008, 112, 8215-8222.	3.1	63

#	Article	IF	Citations
217	pH-Dependent Binary Metalâ"Organic Compounds Assembled from Different Helical Units: Structural Variation and Supramolecular Isomers. Crystal Growth and Design, 2010, 10, 1699-1705.	3.0	63
218	New AIE-active dinuclear Ir(<scp>iii</scp>) complexes with reversible piezochromic phosphorescence behaviour. Chemical Communications, 2015, 51, 13036-13039.	4.1	63
219	Covalently crosslinked zirconium-based metal-organic framework aerogel monolith with ultralow-density and highly efficient Pb(II) removal. Journal of Colloid and Interface Science, 2020, 561, 211-219.	9.4	63
220	pH-tuned synthesis of gold nanostructures from gold nanorods with different aspect ratios. Nanotechnology, 2005, 16, 2555-2560.	2.6	62
221	Effects of starch nanocrystals on structure and properties of waterborne polyurethane-based composites. Carbohydrate Polymers, 2011, 85, 824-831.	10.2	62
222	Piezochromic luminescent (PCL) behavior and aggregation-induced emission (AIE) property of a new cationic iridium(iii) complex. Dalton Transactions, 2012, 41, 9590.	3.3	62
223	A promising anchor group for efficient organic dye sensitized solar cells with iodine-free redox shuttles: a theoretical evaluation. Journal of Materials Chemistry A, 2013, 1, 14000.	10.3	62
224	Solid-state structural transformation doubly triggered by reaction temperature and time in 3D metal-organic frameworks: great enhancement of stability and gas adsorption. Chemical Science, 2014, 5, 1368.	7.4	62
225	Ultrafast and Noninvasive Long-Term Bioimaging with Highly Stable Red Aggregation-Induced Emission Nanoparticles. Analytical Chemistry, 2019, 91, 3467-3474.	6.5	62
226	Heterogeneous hydroxylation catalyzed by multi-walled carbon nanotubes at low temperature. Applied Catalysis A: General, 2006, 299, 212-217.	4.3	61
227	Second-Order Nonlinear Optical Properties of Transition-Metal-Trisubstituted Polyoxometalateâ"Diphosphate Complexes: A Donorâ"Conjugated Bridgeâ"Acceptor Paradigm for Totally Inorganic Nonlinear Optical Materials. Journal of Physical Chemistry C, 2009, 113, 19672-19676.	3.1	61
228	Metalâ"Organic Frameworks Based on Different Benzimidazole Derivatives: Effect of Length and Substituent Groups of the Ligands on the Structures. Crystal Growth and Design, 2010, 10, 1161-1170.	3.0	61
229	New ionic dinuclear Ir(iii) Schiff base complexes with aggregation-induced phosphorescent emission (AIPE). Chemical Communications, 2014, 50, 6977-6980.	4.1	61
230	A bimetallic-MOF catalyst for efficient CO₂ photoreduction from simulated flue gas to value-added formate. Journal of Materials Chemistry A, 2020, 8, 11712-11718.	10.3	61
231	Theoretical interpretation of different nanotube morphologies among Group III (B, Al, Ga) nitrides. Chemical Physics Letters, 2005, 408, 145-149.	2.6	60
232	Density Functional Theory Study on the First Hyperpolarizabilities of Organoimido Derivatives of Hexamolybdates. Journal of Physical Chemistry B, 2005, 109, 22332-22336.	2.6	59
233	Three-dimensional mesomeric networks assembled from helix-linked sheets: syntheses, structures, and magnetisms. Dalton Transactions, 2005, , 2609.	3.3	59
234	A 3D chiral nanoporous coordination framework consisting of homochiral nanotubes assembled from octuple helices. Chemical Communications, 2007, , 4620.	4.1	59

#	Article	IF	Citations
235	A new electrodeposition approach for preparing polyoxometalates-based electrochromic smart windows. Journal of Materials Chemistry A, 2013, 1, 216-220.	10.3	59
236	A stable mixed lanthanide metalâ€“organic framework for highly sensitive thermometry. Dalton Transactions, 2019, 48, 3723-3729.	3.3	59
237	Theoretical Study on the Second-Order Nonlinear Optical Properties of Asymmetric Spirosilabifluorene Derivatives. Journal of Physical Chemistry A, 2006, 110, 4817-4821.	2.5	58
238	Facile and fast synthesis of urchin-shaped Fe3O4@Bi2S3 core-shell hierarchical structures and their magnetically recyclable photocatalytic activity. Journal of Materials Chemistry, 2012, 22, 4832.	6.7	58
239	Polyoxometalateâ€“anatase TiO2 composites are introduced into the photoanode of dye-sensitized solar cells to retard the recombination and increase the electron lifetime. Dalton Transactions, 2013, 42, 2691.	3.3	58
240	The facile synthesis of hollow Au nanoflowers for synergistic chemo-photothermal cancer therapy. Chemical Communications, 2015, 51, 14338-14341.	4.1	58
241	Highly Fluorescent Cadmium Based Metalâ€“Organic Frameworks for Rapid Detection of Antibiotic Residues, Fe³⁺ and Cr₂O₇^{2â€“} Ions. Inorganic Chemistry, 2021, 60, 9148-9156.	4.0	58
242	Two Novel One-Dimensional Î±-Keggin-Based Coordination Polymers with Argentophilic {Ag3}3+/{Ag4}4+ Clusters. Crystal Growth and Design, 2009, 9, 2110-2116.	3.0	57
243	A new triazine-based covalent organic polymer for efficient photodegradation of both acidic and basic dyes under visible light. Dalton Transactions, 2018, 47, 4191-4197.	3.3	57
244	HKUSTâ€1 Derived Hollow Câ€Cu_{2â^'x}S Nanotube/gâ€C₃N₄ Composites for Visibleâ€Light CO₂ Photoreduction with H₂O Vapor. Chemistry - A European Journal, 2019, 25, 379-385.	3.3	57
245	Two carboxyethyltin functionalized polyoxometalates for assembly on carbon nanotubes as efficient counter electrode materials in dye-sensitized solar cells. Chemical Communications, 2014, 50, 14678-14681.	4.1	56
246	Assembly of Organicâ^'Inorganic Hybrid Materials Based on Dawson-Type Polyoxometalate and Multinuclear Copperâ^'Phen Complexes with Unique Magnetic Properties. Crystal Growth and Design, 2009, 9, 3655-3660.	3.0	55
247	Fluorescent Gold Nanoprobes for the Sensitive and Selective Detection for Hg2+. Nanoscale Research Letters, 2010, 5, 1856-1860.	5.7	55
248	Chirality and magnetism of an open-framework cobalt phosphite containing helical channels from achiral materials. Chemical Communications, 2010, 46, 2614.	4.1	55
249	Selfâ€Assembly versus Stepwise Synthesis: Heterometalâ€“Organic Frameworks Based on Metalloligands with Tunable Luminescence Properties. Chemistry - A European Journal, 2013, 19, 11279-11286.	3.3	55
250	Assembly of Fe-substituted Dawson-type nanoscale selenotungstate clusters with photocatalytic H₂evolution activity. Chemical Communications, 2014, 50, 13265-13267.	4.1	55
251	Ligand-Directed Assembly of Polyoxovanadate-Based Metalâ€“Organic Polyhedra. Inorganic Chemistry, 2016, 55, 8770-8775.	4.0	55
252	From Octahedral to Icosahedral Metalâ€“Organic Polyhedra Assembled from Two Types of Polyoxovanadate Clusters. Angewandte Chemie - International Edition, 2019, 58, 4649-4653.	13.8	55

#	Article	IF	Citations
253	Effect of Ï€-Conjugated Length of Bridging Ligand on the Optoelectronic Properties of Platinum(II) Dimers. Inorganic Chemistry, 2008, 47, 2347-2355.	4.0	54
254	Three novel 3D (3,8)-connected metalâ€“organic frameworks constructed from flexible-rigid mixed ligands. CrystEngComm, 2009, 11, 1842.	2.6	54
255	Study of a hydrothermal reaction system of copper, imidazole and polyoxometalates: selective assembly of a 3D porous metalâ€“organic pseudo-rotaxane framework and encapsulation of polyoxometalate clusters. CrystEngComm, 2011, 13, 7079.	2.6	54
256	Nitrogen-doped carbon dots for the detection of mercury ions in living cells and visualization of latent fingerprints. New Journal of Chemistry, 2018, 42, 6824-6830.	2.8	54
257	A two-dimensional conductive Mo-based covalent organic framework as an efficient electrocatalyst for nitrogen fixation. Journal of Materials Chemistry A, 2020, 8, 23599-23606.	10.3	54
258	Electronic Properties and Stability of DititaniumIV Substituted Î±-Keggin Polyoxotungstate with Heteroatom Phosphorus by DFT. Inorganic Chemistry, 2005, 44, 100-107.	4.0	53
259	Theoretical Characterization of a Typical Hole/Exciton-Blocking Material Bathocuproine and Its Analogues. Journal of Physical Chemistry A, 2008, 112, 9097-9103.	2.5	53
260	Efficient Lightâ€Emitting Electrochemical Cells (LECs) Based on Ionic Iridium(III) Complexes with 1,3,4â€Oxadiazole Ligands. Advanced Functional Materials, 2013, 23, 4667-4677.	14.9	53
261	A Highly Energetic Nâ€Rich Zeoliteâ€Like Metalâ€Organic Framework with Excellent Air Stability and Insensitivity. Advanced Science, 2015, 2, 1500150.	11.2	53
262	An Amineâ€Functionalized Zirconium Metalâ€“Organic Polyhedron Photocatalyst with High Visibleâ€Light Activity for Hydrogen Production. Chemistry - A European Journal, 2019, 25, 2824-2830.	3.3	53
263	Rational design of iridiumâ€“porphyrin conjugates for novel synergistic photodynamic and photothermal therapy anticancer agents. Chemical Science, 2021, 12, 5918-5925.	7.4	53
264	Inorganicâ€“organic hybrid materials with different dimensions constructed from copperâ€“fluconazole metalâ€“organic units and Keggin polyanion clusters. Dalton Transactions, 2008, , 2015.	3.3	52
265	Complexâ€“Surfactantâ€Assisted Hydrothermal Synthesis and Properties of Hierarchical Wormâ€Like Cobalt Sulfide Microtubes Assembled by Hexagonal Nanoplates. Chemistry - A European Journal, 2010, 16, 6625-6631.	3.3	52
266	An orange iridium(iii) complex with wide-bandwidth in electroluminescence for fabrication of high-quality white organic light-emitting diodes. Journal of Materials Chemistry C, 2013, 1, 7371.	5.5	52
267	Spontaneous chiral resolution of a rare 3D self-penetration coordination polymer for sensitive aqueous-phase detection of picric acid. Dalton Transactions, 2015, 44, 18386-18394.	3.3	52
268	How does hybrid bridging core modification enhance the nonlinear optical properties in donorâ€Ïâ€acceptor configuration? A case study of dinitrophenol derivatives. Journal of Computational Chemistry, 2015, 36, 118-128.	3.3	52
269	Syntheses, Structures, and Luminescent Properties of Zinc(II) and Cadmium(II) Coordination Complexes Based on Different (Pyridyl)imidazole Derivatives and 1,4-Benzenedicarboxylate. Crystal Growth and Design, 2009, 9, 1353-1360.	3.0	51
270	White light emission from Mn2 +doped ZnS nanocrystals through the surface chelating of 8-hydroxyquinoline-5-sulfonic acid. Nanotechnology, 2010, 21, 115702.	2.6	51

#	Article	IF	Citations
271	Widening or Lengthening? Enhancing the First Hyperpolarizability of Tubiform Multilithium Salts. Journal of Physical Chemistry C, 2011, 115, 16340-16346.	3.1	51
272	A novel class of Zn(II) Schiff base complexes with aggregation-induced emission enhancement (AIEE) properties: Synthesis, characterization and photophysical/electrochemical properties. Dyes and Pigments, 2013, 96, 467-474.	3.7	51
273	A designed bithiopheneimide-based conjugated polymer for organic photovoltaic with ultrafast charge transfer at donor/PC71BM interface: theoretical study and characterization. Physical Chemistry Chemical Physics, 2014, 16, 25799-25808.	2.8	51
274	An ultrastable {Ag₅₅Mo₆} nanocluster with a Ag-centered multishell structure. Chemical Communications, 2014, 50, 11934-11937.	4.1	51
275	Metalâ€“organic framework composites with luminescent gold(<scp>iii</scp>) complexes. Strongly emissive and long-lived excited states in open air and photo-catalysis. Chemical Science, 2015, 6, 7105-7111.	7.4	51
276	Recent advances in oligomers/polymers with unconventional chromophores. Materials Chemistry Frontiers, 2021, 5, 60-75.	5.9	51
277	Theoretical study of the bridging effect on the charge carrier transport properties of cyclooctatetrathiophene and its derivatives. Journal of Materials Chemistry, 2012, 22, 6907.	6.7	50
278	Theoretical study and design of triphenylamine-malononitrile-based p-type organic dyes with different Ï€-linkers for dyes-sensitized solar cells. Dyes and Pigments, 2014, 108, 106-114.	3.7	50
279	ZIF-8 templated fabrication of rhombic dodecahedron-shaped ZnO@SiO2, ZIF-8@SiO2 yolkâ€“shell and SiO2 hollow nanoparticles. CrystEngComm, 2014, 16, 6534.	2.6	50
280	Two-State Reactivity Mechanism of Benzene Câ€“C Activation by Trinuclear Titanium Hydride. Journal of the American Chemical Society, 2016, 138, 11069-11072.	13.7	50
281	Theoretical Design of Perylene Diimide Dimers with Different Linkers and Bridged Positions as Promising Non-Fullerene Acceptors for Organic Photovoltaic Cells. Journal of Physical Chemistry C, 2017, 121, 2125-2134.	3.1	50
282	Electronic Structures of 5d Transition Metal Monoxides by Density Functional Theory. Theoretical Chemistry Accounts, 2006, 117, 115-122.	1.4	49
283	Keplerate-type polyoxometalate/semiconductor composite electrodes with light-enhanced conductivity towards highly efficient photoelectronic devices. Journal of Materials Chemistry A, 2016, 4, 14025-14032.	10.3	49
284	Photoreduction of carbon dioxide under visible light by ultra-small Ag nanoparticles doped into Co-ZIF-9. Nanotechnology, 2018, 29, 284003.	2.6	49
285	Nitrogen- and sulfur-doped carbon dots as peroxidase mimetics: colorimetric determination of hydrogen peroxide and glutathione, and fluorimetric determination of lead(II). Mikrochimica Acta, 2019, 186, 604.	5.0	49
286	Improving the Accuracy of Density-Functional Theory Calculation:Â The Statistical Correction Approach. Journal of Physical Chemistry A, 2004, 108, 8514-8525.	2.5	48
287	Knot-Isomers of MÃ¶bius Cyclacene: How Does the Number of Knots Influence the Structure and First Hyperpolarizability?. Journal of Physical Chemistry C, 2009, 113, 15380-15383.	3.1	48
288	A cationic iridium(<scp>iii</scp>) complex showing aggregation-induced phosphorescent emission (AIPE) in the solid state: synthesis, characterization and properties. Dalton Transactions, 2012, 41, 523-530.	3.3	48

#	Article	IF	Citations
289	Theoretical investigation of structural and electronic propertyies of [PW12O40]3â^' on graphene layer. Dalton Transactions, 2012, 41, 4602.	3.3	48
290	Theoretical study on charge transport properties of cyanovinyl-substituted oligothiophenes. Organic Electronics, 2012, 13, 1213-1222.	2.6	48
291	Modification on C219 by coumarin donor toward efficient sensitizer for dye sensitized solar cells: A theoretical study. Dyes and Pigments, 2013, 99, 127-135.	3.7	48
292	Ultrasmall C-TiO_{2â^'x} nanoparticle/g-C₃N₄ composite for CO₂ photoreduction with high efficiency and selectivity. Journal of Materials Chemistry A, 2018, 6, 21596-21604.	10.3	48
293	Two-Dimensional Cobaltporphyrin-based Cobaltâ€“Organic Framework as an Efficient Photocatalyst for CO₂ Reduction Reaction: A Computational Study. ACS Sustainable Chemistry and Engineering, 2019, 7, 14102-14110.	6.7	48
294	Water-stable lanthanide-based metalâ€“organic gel for the detection of organic amines and white-light emission. Journal of Materials Chemistry C, 2020, 8, 13648-13654.	5.5	48
295	A (4,8)-Connected Fluorite Topology Framework Based on Mononuclear and Dinuclear Metal Centers. Crystal Growth and Design, 2008, 8, 2055-2057.	3.0	47
296	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.	4.0	47
297	Computational Study on Redox-Switchable 2D Second-Order Nonlinear Optical Properties of Pushâ^'Pull Mono-tetrathiafulvalene-Bis(Salicylaldiminato) Zn(II) Schiff Base Complexes. Journal of Physical Chemistry C, 2011, 115, 6024-6032.	3.1	47
298	Secondary ligand-directed assembly of metalâ€“organic coordination polymers based on a 2-(pyridin-4-yl)-1H-imidazole-4,5-dicarboxylic acid ligand: Syntheses, structures and photoluminescent properties. CrystEngComm, 2012, 14, 1865.	2.6	47
299	Effect of alkyl chain length on piezochromic luminescence of iridium(<scp>iii</scp>)-based phosphors adopting 2-phenyl-1H-benzoimidazole type ligands. Journal of Materials Chemistry C, 2014, 2, 7648-7655.	5.5	47
300	Polyoxovanadate-based organicâ€“inorganic hybrids: from {V₅O₉Cl} clusters to nanosized octahedral cages. Dalton Transactions, 2016, 45, 3698-3701.	3.3	47
301	Control of bulk homochirality and proton conductivity in isostructural chiral metalâ€“organic frameworks. Chemical Communications, 2017, 53, 1892-1895.	4.1	47
302	Planar NiC₃ as a reversible anode material with high storage capacity for lithium-ion and sodium-ion batteries. Journal of Materials Chemistry A, 2019, 7, 13356-13363.	10.3	47
303	Synthesis of an Organotin Oligomer Containing a Heptanuclear Tin Phosphonate Cluster by Debenzylation Reactions:Â X-ray Crystal Structure of {Na6(CH3OH)2(H2O)}-{[(BzSn)3(PhPO3)5(Î¼3-O)(CH3O)]2Bz2Sn}Â·CH3OH. Organometallics, 2007, 26, 2125-2128.	2.3	46
304	Second-Order Nonlinear Optical Properties of Trisubstituted Keggin and Wellsâ^'Dawson Polyoxometalates: Density Functional Theory Investigation of the Inorganic Donor-Conjugated Bridgeâ^'Acceptor Structure. Inorganic Chemistry, 2009, 48, 8115-8119.	4.0	46
305	Prediction of second-order optical nonlinearity of porphyrinâ€“metalâ€“polyoxometalate sandwich compounds. Dalton Transactions, 2010, 39, 7645.	3.3	46
306	Chiral salen-metal derivatives of polyoxometalates with asymmetric catalytic and photocatalytic activities. Dalton Transactions, 2011, 40, 9964.	3.3	46

#	Article	IF	Citations
307	Conformational Supramolecular Isomerism in Two-Dimensional Fluorescent Coordination Polymers Based on Flexible Tetracarboxylate Ligand. Crystal Growth and Design, 2013, 13, 4092-4099.	3.0	46
308	Schiff-base as highly sensitive and reversible chemosensors for HCl gas. Sensors and Actuators B: Chemical, 2013, 177, 41-49.	7.8	46
309	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
310	Alkali Metals-Substituted Adamantanes Lead to Visible Light Absorption: Large First Hyperpolarizability. Journal of Physical Chemistry C, 2014, 118, 6952-6958.	3.1	46
311	In situ assembly of monodispersed Ag nanoparticles in the channels of ordered mesopolymers as a highly active and reusable hydrogenation catalyst. Journal of Materials Chemistry A, 2015, 3, 4307-4313.	10.3	46
312	Theoretical design and characterization of pyridalthiadiazole-based chromophores with fast charge transfer at donor/acceptor interface toward small molecule organic photovoltaics. RSC Advances, 2015, 5, 29401-29411.	3.6	46
313	A cascaded QSAR model for efficient prediction of overall power conversion efficiency of all-organic dye-sensitized solar cells. Journal of Computational Chemistry, 2015, 36, 1036-1046.	3.3	46
314	Tuning Emission of AIE-Active Organometallic Ir(III) Complexes by Simple Modulation of Strength of Donor/Acceptor on Ancillary Ligands. Organometallics, 2016, 35, 3996-4001.	2.3	46
315	Theoretical Study on the Considerable Second-Order Nonlinear Optical Properties of Naphthylimido-Substituted Hexamolybdates. Journal of Physical Chemistry A, 2008, 112, 9919-9923.	2.5	45
316	Construction of a Three-Dimensional Polynuclear Zinc Compound Based on Unique Metallophthalocyanine-like Subunits. Inorganic Chemistry, 2009, 48, 10-12.	4.0	45
317	Three-propeller-blade-shaped electride: remarkable alkali-metal-doped effect on the first hyperpolarizability. Theoretical Chemistry Accounts, 2011, 128, 241-248.	1.4	45
318	Alkylene-Chain Effect on Microwire Growth and Crystal Packing of Ï€-Moieties. Chemistry of Materials, 2012, 24, 1944-1949.	6.7	45
319	A comparative study of a fluorene-based non-fullerene electron acceptor and PC61BM in an organic solar cell at a quantum chemical level. RSC Advances, 2016, 6, 81164-81173.	3.6	45
320	NIR-responsive NaYF 4 :Yb,Er,Gd fluorescent upconversion nanorods for the highly sensitive detection of blood fingerprints. Dyes and Pigments, 2016, 134, 178-185.	3.7	45
321	Thermally Activated Delayed Fluorescence in Cu^I Complexes Originating from Restricted Molecular Vibrations. Chemistry - A European Journal, 2017, 23, 11761-11766.	3.3	45
322	How Does Iridium(III) Photocatalyst Regulate Nickel(II) Catalyst in Metallaphotoredox-Catalyzed Câ€“S Cross-Coupling? Theoretical and Experimental Insights. ACS Catalysis, 2019, 9, 3858-3865.	11.2	45
323	Electrochemical reduction of carbon dioxide on the twoâ€“dimensional M3(Hexaiminotriphenylene)2 sheet: A computational study. Applied Surface Science, 2019, 467-468, 98-103.	6.1	45
324	Prediction of Second-Order Optical Nonlinearity of Trisorganotin-Substituted Î²-Keggin Polyoxotungstate. Inorganic Chemistry, 2006, 45, 7864-7868.	4.0	44

#	Article	IF	Citations
325	Hydrogen Adsorption in Polyoxometalate Hybrid Compounds Based on Porous Metalâ€Organic Frameworks. European Journal of Inorganic Chemistry, 2010, 2010, 3756-3761.	2.0	44
326	DFT/TD-DFT Study on the Electronic Structures and Optoelectronic Properties of Several Blue-Emitting Iridium(III) Complexes. Journal of Physical Chemistry A, 2010, 114, 6559-6564.	2.5	44
327	Forward molecular design for highly efficient OLED emitters: A theoretical analysis of photophysical properties of platinum(ii) complexes with N-heterocyclic carbene ligands. Dalton Transactions, 2011, 40, 4480.	3.3	44
328	An AIE-active phosphorescent Ir(<scp>iii</scp>) complex with piezochromic luminescence (PCL) and its application for monitoring volatile organic compounds (VOCs). Journal of Materials Chemistry C, 2017, 5, 12189-12193.	5.5	44
329	Introduction of Molecular Building Blocks to Improve the Stability of Metalâ€“Organic Frameworks for Efficient Mercury Removal. Inorganic Chemistry, 2018, 57, 6118-6123.	4.0	44
330	All-inorganic perovskite/graphitic carbon nitride composites for CO₂ photoreduction into C1 compounds under low concentrations of CO₂. Dalton Transactions, 2019, 48, 14115-14121.	3.3	44
331	Carbon/Binderâ€Free NiO@NiO/NF with In Situ Formed Interlayer for Highâ€Arealâ€Capacity Lithium Storage. Advanced Energy Materials, 2019, 9, 1803690.	19.5	44
332	Ultrahigh capacity 2D anode materials for lithium/sodium-ion batteries: an entirely planar B₇P₂ monolayer with suitable pore size and distribution. Journal of Materials Chemistry A, 2020, 8, 10301-10309.	10.3	44
333	A novel (4,8)-connected 3D polyoxometalate-based metalâ€“organic framework containing an in situ ligand. CrystEngComm, 2008, 10, 1129.	2.6	43
334	Molecular tectonics of metalâ€“organic frameworks based on ligand-modulated polynuclear zinc SBUs and aromatic multicarboxylic acids. CrystEngComm, 2011, 13, 889-896.	2.6	43
335	A Rational Design for Dye Sensitizer: Density Functional Theory Study on the Electronic Absorption Spectra of Organoimido-Substituted Hexamolybdates. Journal of Physical Chemistry C, 2013, 117, 2245-2251.	3.1	43
336	Generalized Approach to the Synthesis of Reversible Concentric and Eccentric Polymerâ€Coated Nanostructures. Small, 2013, 9, 825-830.	10.0	43
337	Anion-specific aggregation induced phosphorescence emission (AIPE) in an ionic iridium complex in aqueous media. Chemical Communications, 2015, 51, 16924-16927.	4.1	43
338	Facile one-pot synthesis of carbon/calcium phosphate/Fe₃O₄ composite nanoparticles for simultaneous imaging and pH/NIR-responsive drug delivery. Chemical Communications, 2016, 52, 11068-11071.	4.1	43
339	Lanthanide-MOFs as multifunctional luminescent sensors. Inorganic Chemistry Frontiers, 2022, 9, 3259-3266.	6.0	43
340	Density Functional Studies of Diatomic LaO to LuO. Journal of Cluster Science, 2007, 18, 444-458.	3.3	42
341	Theoretical studies on the hole transport property of tetrathienoarene derivatives: The influence of the position of sulfur atom, substituent and Ï€-conjugated core. Organic Electronics, 2014, 15, 602-613.	2.6	42
342	pH-Controlled and Sulfite Anion-Directed Assembly of a Family of Cerium(III)-Containing Polyoxotungstates Clusters. Inorganic Chemistry, 2014, 53, 9486-9497.	4.0	42

#	Article	IF	Citations
343	The Enhancement on Proton Conductivity of Stable Polyoxometalateâ€Based Coordination Polymers by the Synergistic Effect of MultiProton Units. Chemistry - A European Journal, 2016, 22, 9299-9304.	3.3	42
344	Encapsulation of an iridium complex in a metalâ€“organic framework to give a composite with efficient white light emission. Inorganic Chemistry Frontiers, 2017, 4, 547-552.	6.0	42
345	One-pot controllable synthesis of CoFe₂O₄solid, hollow and multi-shell hollow nanospheres as superior anode materials for lithium ion batteries. Journal of Materials Chemistry A, 2017, 5, 21994-22003.	10.3	42
346	The substitution effect of heterocyclic rings to tune the optical and nonlinear optical properties of hybrid chalcones: A comparative study. Journal of Molecular Graphics and Modelling, 2018, 81, 25-31.	2.4	42
347	Orange emissive carbon dots for colorimetric and fluorescent sensing of 2,4,6-trinitrophenol by fluorescence conversion. RSC Advances, 2018, 8, 16095-16102.	3.6	42
348	Recent advances in luminescent dinuclear iridium(III) complexes and their application in organic electroluminescent devices. Polyhedron, 2018, 140, 146-157.	2.2	42
349	A water-stable terbium metalâ€“organic framework with functionalized ligands for the detection of Fe³⁺ and Cr₂O₇^{2â^’} ions in water and picric acid in seawater. CrystEngComm, 2020, 22, 3638-3643.	2.6	42
350	Maximized Schottky Effect: The Ultrafine V₂O₃/Ni Heterojunctions Repeatedly Arranging on Monolayer Nanosheets for Efficient and Stable Waterâ€toâ€Hydrogen Conversion. Small, 2021, 17, e2005769.	10.0	42
351	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.	2.5	41
352	DFT study on second-order nonlinear optical properties of a series of mono Schiff-base M(II) (M=Ni,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.6	41
353	Unexpected 1D self-assembly of carbonate-templated sandwich-like macrocycle-based Ag₂₀S₁₀luminescent nanoclusters. CrystEngComm, 2014, 16, 7860.	2.6	41
354	Polyurethane derivatives for highly sensitive and selective fluorescence detection of 2,4,6-trinitrophenol (TNP). Journal of Materials Chemistry C, 2018, 6, 11287-11291.	5.5	41
355	Spadix-Bract Structured Nanobowls for Bimodal Imaging-Guided Multidrug Chemo-Photothermal Synergistic Therapy. Chemistry of Materials, 2018, 30, 3722-3733.	6.7	41
356	Electronic structures of 4d transition metal monoxides by density functional theory. Theoretical Chemistry Accounts, 2007, 117, 407-415.	1.4	40
357	Syntheses and characterizations of four metal coordination polymers constructed by the pyridine-3,5-dicarboxylate ligand. Polyhedron, 2008, 27, 583-592.	2.2	40
358	Quantum Chemical Studies on High-Valent Metal Nitrido Derivatives of Keggin-Type Polyoxometalates ([PW11O39{MVIN}]4â^’ (M = Ru, Os, Re)): MVIâ^’N Bonding and Electronic Structures. Inorganic Chemistry, 2009, 48, 541-548.	4.0	40
359	Controllable synthesis of microporous, nanotubular and mesocage-like metalâ€“organic frameworks by adjusting the reactant ratio and modulated luminescence properties of Alq3@MOF composites. Journal of Materials Chemistry, 2012, 22, 17947.	6.7	40
360	Rational molecular design of aggregation-induced emission cationic Ir(<scp>iii</scp>) phosphors achieving supersensitive and selective detection of nitroaromatic explosives. Journal of Materials Chemistry C, 2017, 5, 10847-10854.	5.5	40

#	Article	IF	Citations
361	Two-dimensional Ï€-conjugated metal bis(dithiolene) nanosheets as promising electrocatalysts for carbon dioxide reduction: a computational study. Journal of Materials Chemistry A, 2019, 7, 15341-15346.	10.3	40
362	Bright red aggregation-induced emission nanoparticles for multifunctional applications in cancer therapy. Chemical Science, 2020, 11, 2369-2374.	7.4	40
363	Improving the accuracy of density-functional theory calculation: The genetic algorithm and neural network approach. Journal of Chemical Physics, 2007, 126, 144101.	3.0	39
364	Synthesis, Characterization, and Crystal Structures of Double-Cubane-Substituted and Asymmetric Penta-Ni-Substituted Dimeric Polyoxometalates. Crystal Growth and Design, 2007, 7, 1305-1311.	3.0	39
365	Electronic structures and chemical bonding in diatomic ScX to ZnX (X = S, Se, Te). Journal of Computational Chemistry, 2007, 28, 703-714.	3.3	39
366	Metalâ€“Organic Frameworks Containing Flexible Bis(benzimidazole) Ligands. European Journal of Inorganic Chemistry, 2008, 2008, 745-755.	2.0	39
367	Assembly of a Chiral Bikitaite Zeolite Metalâ€'Organic Framework Based on the Asymmetrical Tetrahedral Building Blocks. Crystal Growth and Design, 2008, 8, 2986-2989.	3.0	39
368	Two unprecedented porous anionic frameworks: organoammonium templating effects and structural diversification. Dalton Transactions, 2009, , 8562.	3.3	39
369	Polyoxometalate-Based Porous Framework with Perovskite Topology. Crystal Growth and Design, 2010, 10, 4227-4230.	3.0	39
370	A series of novel chiral lanthanide coordination polymers with channels constructed from 16Ln-based cage-like building units. CrystEngComm, 2010, 12, 1147-1152.	2.6	39
371	An unprecedented (3,4,24)-connected heteropolyoxozincate organic framework as heterogeneous crystalline Lewis acid catalyst for biodiesel production. Scientific Reports, 2013, 3, 2616.	3.3	39
372	Assembly of Keggin-/Dawson-type Polyoxotungstate Clusters with Different Metal Units and SeO₃^{2â€“} Heteroanion Templates. Crystal Growth and Design, 2014, 14, 5099-5110.	3.0	39
373	Exploring what prompts ITIC to become a superior acceptor in organic solar cell by combining molecular dynamics simulation with quantum chemistry calculation. Physical Chemistry Chemical Physics, 2017, 19, 31227-31235.	2.8	39
374	Polyoxometalates/Active Carbon Thin Separator for Improving Cycle Performance of Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2018, 10, 35911-35918.	8.0	39
375	Continuous detection of HCl and NH₃ gases with a high-performance fluorescent polymer sensor. New Journal of Chemistry, 2018, 42, 13367-13374.	2.8	39
376	Nitrogen and Sulfur-Codoped Porous Carbon Nanospheres with Hierarchical Micromesoporous Structures and an Ultralarge Pore Volume for High-Performance Supercapacitors. ACS Applied Materials & Interfaces, 2020, 12, 8225-8232.	8.0	39
377	Luminescent Cd(â…¡) metal-organic frameworks with anthracene nitrogen-containing organic ligands as novel multifunctional chemosensors for the detection of picric acid, pesticides, and ferric ions. Dyes and Pigments, 2021, 185, 108834.	3.7	39
378	Establishing the Principal Descriptor for Electrochemical Urea Production via the Dispersed Dualâ€Metals Anchored on the Nâ€Ðecorated Graphene. Advanced Science, 2022, 9, e2105697.	11.2	39

#	Article	IF	Citations
379	Why Does Disubstituted Hexamolybdate with Arylimido Prefer to Form an Orthogonal Derivative? Analysis of Stability, Bonding Character, and Electronic Properties on Molybdate Derivatives by Density Functional Theory (DFT) Study. Journal of Physical Chemistry B, 2004, 108, 17337-17343.	2.6	38
380	Two-Dimensional Lanthanide Heteropolyvanadates of Manganese(IV) and Nickel(IV) Containing Two Types of Heteropoly Anions with 1:13 and 1:12 Stoichiometry. Inorganic Chemistry, 2006, 45, 8036-8040.	4.0	38
381	Intercalation and Photophysical Properties of the Tetra-(8-hydroxyquinolinato) Boron Complex and 3,3â€˜,4,4â€˜-Benzophenone Tetracarboxylic Anion into Mgâˆ’Al Layered Double Hydroxides. Inorganic Chemistry, 2006, 45, 4364-4371.	4.0	38
382	Quantum Chemical Study of Structures, Electronic Spectrum, and Nonlinear Optical Properties of Goldâˆ’Pentacene Complexes. Organometallics, 2007, 26, 2082-2087.	2.3	38
383	Theoretical Study on Photophysical Properties of Phenolpyridyl Boron Complexes. Journal of Physical Chemistry A, 2007, 111, 2739-2744.	2.5	38
384	Inorganicâ€“organic hybrid compounds based on the co-existence of different isomers or forms of polymolybdate. CrystEngComm, 2010, 12, 3684.	2.6	38
385	Synthesis and characterization of two {Mo₆}-based/templated metalâ€“organic frameworks. CrystEngComm, 2011, 13, 1461-1466.	2.6	38
386	3D Racemic Microporous Frameworks and 3D Chiral Supramolecular Architectures Based on Evansâ€“Showell-Type Polyoxometalates Controlled by the Temperature. Crystal Growth and Design, 2015, 15, 164-175.	3.0	38
387	Berylliumâ€“beryllium double-Ï€ bonds in the octahedral cluster of Be₂(Î¼₂-X)₄ (X = Li, Cu, BeF). Physical Chemistry Chemical Physics, 2018, 20, 23898-23902.	2.8	38
388	Atomic Nb Anchoring on Graphdiyne as a New Potential Electrocatalyst for Nitrogen Fixation: A Computational View. Advanced Theory and Simulations, 2019, 2, 1900132.	2.8	38
389	From Octahedral to Icosahedral Metalâ€“Organic Polyhedra Assembled from Two Types of Polyoxovanadate Clusters. Angewandte Chemie, 2019, 131, 4697-4701.	2.0	38
390	Highly Efficient Photoreduction of Lowâ€Concentration CO₂to Syngas by Using a Polyoxometalates/Ru^{II}Composite. Chemistry - A European Journal, 2020, 26, 2735-2740.	3.3	38
391	An intriguing window opened by a metallic two-dimensional Lindqvist-cobaltporphyrin organic framework as an electrochemical catalyst for the CO₂reduction reaction. Journal of Materials Chemistry A, 2020, 8, 14807-14814.	10.3	38
392	From Racemic Compound to Spontaneous Resolution: A Linkerâ€Imposed Evolution of Chiral [MnMo₉O₃₂]^{6âˆ’}â€Based Polyoxometalate Compounds. Chemistry - A European Journal, 2009, 15, 10940-10947.	3.3	37
393	Rational design and characterization of high-efficiency planar Aâ€“Ï€â€“Dâ€“Ï€â€“A type electron donors in small molecule organic solar cells: A quantum chemical approach. Materials Chemistry and Physics, 2014, 145, 387-396.	4.0	37
394	Simultaneous modification of N-alkyl chains on cyclometalated and ancillary ligands of cationic iridium(iii) complexes towards efficient piezochromic luminescence properties. Journal of Materials Chemistry C, 2015, 3, 2341-2349.	5.5	37
395	A carbon-free polyoxometalate molecular catalyst with a cobaltâ€“arsenic core for visible light-driven water oxidation. Chemical Communications, 2016, 52, 9514-9517.	4.1	37
396	Pure inorganic Dâ€“A type polyoxometalate/reduced graphene oxide nanocomposite for the photoanode of dye-sensitized solar cells. Journal of Materials Chemistry A, 2016, 4, 3297-3303.	10.3	37

#	Article	IF	Citations
397	Self-Assembly of Nanoscale Lanthanoid-Containing Selenotungstates: Synthesis, Structures, and Magnetic Studies. Inorganic Chemistry, 2019, 58, 12895-12904.	4.0	37
398	A tetraphenylethylene-based covalent organic polymer for highly selective and sensitive detection of Fe³⁺ and as a white light emitting diode. Chemical Communications, 2019, 55, 12328-12331.	4.1	37
399	Green synthesis of carbon dots by celery leaves for use as fluorescent paper sensors for the detection of nitrophenols. New Journal of Chemistry, 2020, 44, 1500-1507.	2.8	37
400	Synthesis of a Magnetic 2D Co@NC-600 Material by Designing a MOF Precursor for Efficient Catalytic Reduction of Water Pollutants. Inorganic Chemistry, 2020, 59, 12672-12680.	4.0	37
401	Rational design of well-dispersed ultrafine CoS₂ nanocrystals in microâ€“mesoporous carbon spheres with a synergistic effect for high-performance lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2020, 8, 10885-10890.	10.3	37
402	ZIF-8/covalent organic framework for enhanced CO2 photocatalytic reduction in gas-solid system. Chemical Engineering Journal, 2022, 450, 138040.	12.7	37
403	Synthesis and characterization of one- to three-dimensional compounds composed of paradodecatungstate-B cluster and transition metals as linkers. Journal of Solid State Chemistry, 2006, 179, 2093-2100.	2.9	36
404	An unprecedented 3D 8-connected pure inorganic framework based on nanosized {[Na12PO16H24]âŠ‚[P4Mo6O31H6]4}15âˆ’ clusters and zinc cations. Chemical Communications, 2011, 47, 2832.	4.1	36
405	New heteropolyniobates based on a bicapped Keggin-type {VNb₁₄} cluster with selective adsorption and photocatalytic properties. CrystEngComm, 2014, 16, 9582-9585.	2.6	36
406	A novel 3D inorganic heteropoly blue as visible light responsive photocatalyst. Dalton Transactions, 2014, 43, 10005.	3.3	36
407	Stepwise modulation of the electron-donating strength of ancillary ligands: understanding the AIE mechanism of cationic iridium(<scp>iii</scp>) complexes. Chemical Communications, 2014, 50, 10986-10989.	4.1	36
408	Evidence of Amineâ€“CO₂ Interactions in Two Pillaredâ€Layer MOFs Probed by Xâ€ray Crystallography. Chemistry - A European Journal, 2015, 21, 7238-7244.	3.3	36
409	Metalâ€“Organic Framework with Aromatic Rings Tentacles: High Sulfur Storage in Liâ€“S Batteries and Efficient Benzene Homologues Distinction. ACS Applied Materials & Interfaces, 2016, 8, 33183-33188.	8.0	36
410	Flexible blue-green and white light-emitting electrochemical cells based on cationic iridium complex. Organic Electronics, 2016, 28, 314-318.	2.6	36
411	Metalâ€“organic framework composites with luminescent pincer platinum(<scp>ii</scp>) complexes:³MMLCT emission and photoinduced dehydrogenation catalysis. Chemical Science, 2018, 9, 2357-2364.	7.4	36
412	Ir^{III}/Ni^{II}-Metallaphotoredox catalysis: the oxidation state modulation mechanism versus the radical mechanism. Chemical Communications, 2018, 54, 5968-5971.	4.1	36
413	Facile synthesis of conjugated microporous polymer-based porphyrin units for adsorption of CO₂ and organic vapors. Polymer Chemistry, 2019, 10, 819-822.	3.9	36
414	Tuning Second-Order Non-linear (NLO) Optical Response of Organoimido-Substituted Hexamolybdates through Halogens: Quantum Design of Novel Organic-Inorganic Hybrid NLO Materials. Australian Journal of Chemistry, 2010, 63, 836.	0.9	35

#	Article	IF	Citations
415	Highâ€Performance Oxygen Sensors Based on Eu^{III} Complex/Polystyrene Composite Nanofibrous Membranes Prepared by Electrospinning. ChemPhysChem, 2011, 12, 349-355.	2.1	35
416	Polyoxometalate/TiO₂ Interfacial Layer with the Function of Accelerating Electron Transfer and Retarding Recombination for Dye-Sensitized Solar Cells. Industrial & Engineering Chemistry Research, 2014, 53, 150-156.	3.7	35
417	Rational design of a highly sensitive and selective â€œturn-onâ€•fluorescent sensor for PO₄^{3â^'} detection. Dalton Transactions, 2015, 44, 20830-20833.	3.3	35
418	Assembly of two novel 3D organicâ€“inorganic hybrids based on Keggin-type polyoxometalates: syntheses, crystal structures and properties. CrystEngComm, 2016, 18, 6370-6377.	2.6	35
419	Single Metalâ€“Organic Cage Decorated with an Ir(III) Complex for CO₂ Photoreduction. ACS Catalysis, 2021, 11, 7241-7248.	11.2	35
420	On the Origin of the Relative Stability of Wellsâ€“Dawson Isomers: A DFT Study of Î±-, Î²-, Î³-, Î±*-, Î²*-, and Î³*-[(PO₄)₂W₁₈O₅₄]^{6â€“}Anions. Inorganic Chemistry, 2011, 50, 4967-4977.	4.0	34
421	Designed preparation of polyacrylic acid/calcium carbonate nanoparticles with high doxorubicin payload for liver cancer chemotherapy. CrystEngComm, 2015, 17, 4768-4773.	2.6	34
422	Cluster-based metalâ€“organic frameworks as sensitive and selective luminescent probes for sensing nitro explosives. New Journal of Chemistry, 2015, 39, 7858-7862.	2.8	34
423	Synthesis, structures, and magnetic properties of metalâ€“organic polyhedra based on unprecedented {V₇} isopolyoxometalate clusters. Dalton Transactions, 2016, 45, 14898-14901.	3.3	34
424	Functionalized polyoxometalate-based metalâ€“organic cuboctahedra for selective adsorption toward cationic dyes in aqueous solution. Dalton Transactions, 2018, 47, 12979-12983.	3.3	34
425	Non-metal boron atoms on a CuB₁₂ monolayer as efficient catalytic sites for urea production. Chemical Science, 2022, 13, 1342-1354.	7.4	34
426	A novel strong fluorescent three-dimensional supramolecular coordination polymer based on bridging terephthalate. Inorganic Chemistry Communication, 2004, 7, 260-263.	3.9	33
427	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.	2.0	33
428	Electronic structures and chemical bonding in 4d transition metal monohalides. Journal of Computational Chemistry, 2007, 28, 2190-2202.	3.3	33
429	Two novel lead-carboxylate complexes based on nicotinic acid N-oxide: Synthesis, crystal structures and luminescent properties. Inorganic Chemistry Communication, 2007, 10, 410-414.	3.9	33
430	A theoretical investigation of intermolecular interaction of a phthalimide based â€œonâ€“offâ€•sensor with different halide ions: tuning its efficiency and electro-optical properties. Theoretical Chemistry Accounts, 2009, 122, 77-86.	1.4	33
431	3d - 4f Heterometallic Complexes for the Construction of POM-based Inorganic - Organic Hybrid Compounds: from Nanoclusters to One-Dimensional Ladder-Like Chains. Australian Journal of Chemistry, 2010, 63, 1389.	0.9	33
432	Three Cobalt(II)â€Linked {P₈W₄₈} Network Assemblies: Syntheses, Structures, and Magnetic and Photocatalysis Properties. Chemistry - an Asian Journal, 2014, 9, 470-478.	3.3	33

#	Article	IF	Citations
433	Switchable NLO response induced by rotation of metallacarboranes [NiIII/IV(C2B9H11)2]â^'/0 and C-,B-functionalized derivatives. Dalton Transactions, 2014, 43, 5069.	3.3	33
434	A novel strategy to fabricate multifunctional Fe3O4@C@TiO2 yolkâ€“shell structures as magnetically recyclable photocatalysts. Nanoscale, 2014, 6, 6603.	5.6	33
435	Multilithiation Effect on the First Hyperpolarizability of Carbonâ€“Boronâ€“Nitride Heteronanotubes: Activating Segment versus Connecting Pattern. Journal of Physical Chemistry C, 2014, 118, 14185-14191.	3.1	33
436	Steamâ€Assisted Synthesis of an Extraâ€Stable Polyoxometalateâ€Encapsulating Metal Azolate Framework: Applications in Reagent Purification and Proton Conduction. Chemistry - A European Journal, 2015, 21, 13058-13064.	3.3	33
437	Metalâ€“Organic Rotaxane Frameworks Assembly by Cucurbit[6]uril-Based Pseudorotaxanes and Mixed Ligands. Crystal Growth and Design, 2015, 15, 4311-4317.	3.0	33
438	Metalâ€“organic frameworks constructed from tib and carboxylate acid ligands: selective sensing of nitro explosives and magnetic properties. Dalton Transactions, 2017, 46, 7567-7576.	3.3	33
439	A stable pillared-layer Cu(<scp>ii</scp>) metalâ€“organic framework with magnetic properties for dye adsorption and separation. New Journal of Chemistry, 2017, 41, 3661-3666.	2.8	33
440	Computational Study on M₁/POM Single-Atom Catalysts (M = Cu, Zn, Ag, and Au; POM =) Tj ETQq0 0 0 rgBT /Overlock 10 for Alkene Epoxidation. Inorganic Chemistry, 2017, 56, 10496-10504.	4.0	33
441	Aggregation-Induced Long-Lived Phosphorescence in Nonconjugated Polyurethane Derivatives at 77 K. Macromolecules, 2018, 51, 4178-4184.	4.8	33
442	A metal-free covalent organic framework as a photocatalyst for CO₂ reduction at low CO₂ concentration in a gasâ€“solid system. Journal of Materials Chemistry A, 2021, 9, 24895-24902.	10.3	33
443	Theoretical Study on the Relationship between Spin Multiplicity Effects and Nonlinear Optical Properties of the Pyrrole Radical (C4H4NÂ·). Journal of Physical Chemistry A, 2008, 112, 83-88.	2.5	32
444	Theoretical Investigation of the Reactions of CF₃CHFOCF₃ with the OH Radical and Cl Atom. Journal of Physical Chemistry A, 2010, 114, 417-424.	2.5	32
445	A long-term stable Pt counter electrode modified by POM-based multilayer film for high conversion efficiency dye-sensitized solar cells. Dalton Transactions, 2012, 41, 2227.	3.3	32
446	Metal ion directed metalâ€“organic rotaxane frameworks with intrinsic features of self-penetration and interpenetration. Chemical Communications, 2013, 49, 8555.	4.1	32
447	Modification of iridium(III) complexes for fabrication of high-performance non-doped organic light-emitting diode. Dyes and Pigments, 2015, 112, 8-16.	3.7	32
448	A machine learning correction for DFT non-covalent interactions based on the S22, S66 and X40 benchmark databases. Journal of Cheminformatics, 2016, 8, 24.	6.1	32
449	A Wellâ€Established POMâ€based Singleâ€Crystal Protonâ€Conducting Model Incorporating Multiple Weak Interactions. Chemistry - A European Journal, 2018, 24, 2365-2369.	3.3	32
450	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.	2.6	31

#	Article	IF	Citations
451	Syntheses and characterizations of three coordination polymers based on dipyridylbenzoates and 1,4-bezenedicarboxylate. Polyhedron, 2009, 28, 975-979.	2.2	31
452	The influence of thienyl-S,S-dioxidation on the photoluminescence and charge transport properties of dithienothiophenes: a theoretical study. Theoretical Chemistry Accounts, 2011, 129, 247-255.	1.4	31
453	Li doped effect of through novel noncovalent charge transfer on nonlinear optical properties. Dyes and Pigments, 2014, 106, 7-13.	3.7	31
454	A pillar-layer MOF for detection of small molecule acetone and metal ions in dilute solution. RSC Advances, 2015, 5, 48881-48884.	3.6	31
455	The composite material based on Dawson-type polyoxometalate and activated carbon as the supercapacitor electrode. Inorganic Chemistry Communication, 2015, 55, 149-152.	3.9	31
456	Theoretical studies on POM-based organicâ€“inorganic hybrids containing double Dâ€“A1â€“Ï€â€“A2 chains for high-performance p-type, dye-sensitized solar cells (DSSCs). Physical Chemistry Chemical Physics, 2015, 17, 5459-5465.	2.8	31
457	A fluorescent sensor for highly selective sensing of nitro explosives and Hg(<scp>ii</scp>) ions based on a 3D porous layer metalâ€“organic framework. CrystEngComm, 2016, 18, 4765-4771.	2.6	31
458	Changes of coordination modes of Cu-based coordination complexes as tuneable proton-conducting solid electrolytes. Journal of Materials Chemistry A, 2017, 5, 1085-1093.	10.3	31
459	Bimetallic Phosphides as High-Efficient Electrocatalysts for Hydrogen Generation. Inorganic Chemistry, 2021, 60, 1624-1630.	4.0	31
460	Facile method to detect oligonucleotides with functionalized polydiacetylene vesicles. Sensors and Actuators B: Chemical, 2006, 113, 510-515.	7.8	30
461	A chiral 3D polymer with right- and left-helices based on 2,2â€²-biimidazole: Synthesis, crystal structure and fluorescent property. Inorganic Chemistry Communication, 2007, 10, 720-723.	3.9	30
462	Studies on the interactions of Ti-containing polyoxometalates (POMs) with SARS-CoV 3CLpro by molecular modeling. Journal of Inorganic Biochemistry, 2007, 101, 89-94.	3.5	30
463	Prediction of robustly large molecular second-order nonlinear optical properties of terpyridine-substituted hexamolybdates: Structural modelling towards a rational entry to NLO materials. Journal of Molecular Graphics and Modelling, 2010, 28, 735-745.	2.4	30
464	Theoretical study on the electron transfer and phosphorescent properties of iridium(iii) complexes with 2-phenylpyridyl and 8-hydroxyquinolate ligands. Dalton Transactions, 2010, 39, 7733.	3.3	30
465	Step-wise synthesis of inorganicâ€“organic hybrid based on Î³-octamolybdate-based tectons. Dalton Transactions, 2011, 40, 3176.	3.3	30
466	Functional heterometallic coordination polymers with metalloligands as tunable luminescent crystalline materials. Journal of Materials Chemistry, 2012, 22, 19673.	6.7	30
467	Chiroptical, linear, and second-order nonlinear optical properties of binaphthol derivatives. Organic and Biomolecular Chemistry, 2012, 10, 8418.	2.8	30
468	Inorganic Crown Ethers: Sulfateâ€Based Preyssler Polyoxometalates. Chemistry - A European Journal, 2012, 18, 9184-9188.	3.3	30

#	Article	IF	Citations
469	DFT characterization on the mechanism of water splitting catalyzed by single-Ru-substituted polyoxometalates. Dalton Transactions, 2013, 42, 10617.	3.3	30
470	Exploring the influence of electron donating/withdrawing groups on hexamolybdate-based derivatives for efficient p-type dye-sensitized solar cells (DSSCs). RSC Advances, 2015, 5, 39821-39827.	3.6	30
471	The assembly of vanadium(<scp>iv</scp>)-substituted Keggin-type polyoxometalate/graphene nanocomposite and its application in photovoltaic system. Journal of Materials Chemistry A, 2015, 3, 10174-10178.	10.3	30
472	Theoretical study and design of multifunctional phosphorescent platinum(<scp>ii</scp>) complexes containing triarylboron moieties for efficient OLED emitters. Physical Chemistry Chemical Physics, 2015, 17, 2438-2446.	2.8	30
473	Achieving High Performances of Nondoped OLEDs Using Carbazole and Diphenylphosphoryl-Functionalized Ir(III) Complexes as Active Components. Inorganic Chemistry, 2017, 56, 9979-9987.	4.0	30
474	Sulfur-containing bimetallic metal organic frameworks with multi-fold helix as anode of lithium ion batteries. Dalton Transactions, 2018, 47, 4827-4832.	3.3	30
475	Tuning the Excited-State Properties of Luminescent Rhenium(V) Benzylidyne Complexes Containing Phosphorus and Nitrogen Donor Ligands. Organometallics, 1998, 17, 1946-1955.	2.3	29
476	Synthesis, Structure, Electronic State, and Luminescent Properties of Novel Blueâ€Lightâ€Emitting Arylâ€Substituted 9,9â€Di(4â€(diâ€pâ€tolyl)aminophenyl)fluorenes. Advanced Functional Materials, 2008, 18, 2335-2347.	14.9	29
477	Computational Study on Second-Order Nonlinear Response of a Series of Two-Dimensional Carbazole-Cored Chromophores. Journal of Physical Chemistry C, 2008, 112, 7021-7028.	3.1	29
478	Synthesis and characterization of new bifunctional nanocomposites possessing upconversion and oxygen-sensing properties. Nanotechnology, 2010, 21, 285701.	2.6	29
479	Anion-directed genuine meso-helical supramolecular isomers of two 1D Ag(i) complexes based on arene-linked bis(pyrazolyl)methane ligands. CrystEngComm, 2010, 12, 3458.	2.6	29
480	A new organicâ€“inorganic hybrid based on the crescent-shaped polyoxoanion [H6SiNb18O54]8â^' and copperâ€“organic cations. Dalton Transactions, 2012, 41, 6075.	3.3	29
481	Cyano or o-nitrophenyl? Which is the optimal electron-withdrawing group for the acrylic acid acceptor of D-Ï€-A sensitizers in DSSCs? A density functional evaluation. Journal of Molecular Modeling, 2013, 19, 1597-1604.	1.8	29
482	New cationic Ir(<scp>iii</scp>) complexes without â€œany soft substituentsâ€• aggregation-induced emission and piezochromic luminescence. Journal of Materials Chemistry C, 2018, 6, 12217-12223.	5.5	29
483	TMC (TM = Co, Ni, and Cu) monolayers with planar pentacoordinate carbon and their potential applications. Journal of Materials Chemistry C, 2019, 7, 6406-6413.	5.5	29
484	Tinâ€“Oxo Clusters Based on Aryl Arsonate Anions. Chemistry - A European Journal, 2008, 14, 4093-4103.	3.3	28
485	Unprecedented interweaving of single-helical chains into a chiral metalâ€“organic framework based on a flexible ligand. CrystEngComm, 2009, 11, 1711.	2.6	28
486	Mechanistic and Kinetic Study of CH₂O+O₃ Reaction. Journal of Physical Chemistry A, 2010, 114, 3516-3522.	2.5	28

#	Article	IF	Citations
487	Novel Trumpet-Shaped Conjugation Bridge (Carbon Nanocone) for Nonlinear Optical Materials. Journal of Physical Chemistry C, 2011, 115, 18545-18551.	3.1	28
488	Auxiliary ligand induced structural allomorphism in nanotubular microporous metalâ€“organic frameworks based on discrete magnesium clusters. Dalton Transactions, 2012, 41, 2231-2233.	3.3	28
489	Theoretical investigation on redoxâ€switchable secondâ€order nonlinear optical responses of pushâ€“pull Cp*CoEt₂C₂B₄H₃â€expanded (metallo)porphyrins. Journal of Computational Chemistry, 2012, 33, 211-219.	3.3	28
490	Enhancing the luminescence properties and stability of cationic iridium(iii) complexes based on phenylbenzoimidazole ligand: a combined experimental and theoretical study. Dalton Transactions, 2013, 42, 11056.	3.3	28
491	Assembly of Zn-metal organic frameworks based on a N-rich ligand: selective sorption for CO₂ and luminescence sensing of nitro explosives. RSC Advances, 2015, 5, 49606-49613.	3.6	28
492	Highly tuneable proton-conducting coordination polymers derived from a sulfonate-based ligand. CrystEngComm, 2017, 19, 7050-7056.	2.6	28
493	A simple strategy to achieve remarkable mechanochromism of cationic Ir(<scp>iii</scp>) phosphors through subtle ligand modification. Journal of Materials Chemistry C, 2018, 6, 11686-11693.	5.5	28
494	The electronic and optical properties of carbon nitride derivatives: A first principles study. Applied Surface Science, 2018, 453, 442-448.	6.1	28
495	in situ engineered ultrafine NiS₂-ZnS heterostructures in microâ€“mesoporous carbon spheres accelerating polysulfide redox kinetics for high-performance lithiumâ€“sulfur batteries. Nanoscale, 2020, 12, 16201-16207.	5.6	28
496	The roles of polyoxometalates in photocatalytic reduction of carbon dioxide. Materials Today Energy, 2021, 21, 100760.	4.7	28
497	Ferromagnetically Coupled Dimer of CuII-Substituted Î³-Decatungstosilicate. Inorganic Chemistry, 2007, 46, 10041-10043.	4.0	27
498	Combination of POMs and deliberately designed macrocations: a rational approach for synthesis of POM-pillared metalâ€“organic framework. Dalton Transactions, 2009, , 940-947.	3.3	27
499	Theoretical investigation on electronic structure and second-order nonlinear optical properties of novel hexamolybdate-organoimido-(car)borane hybrid. Physical Chemistry Chemical Physics, 2012, 14, 5605.	2.8	27
500	Selectedâ€Control Fabrication of Multifunctional Fluorescentâ€“Magnetic Coreâ€“Shell and Yolkâ€“Shell Hybrid Nanostructures. Chemistry - A European Journal, 2012, 18, 3745-3752.	3.3	27
501	New oxazoline- and thiazoline-containing heteroleptic iridium(iii) complexes for highly-efficient phosphorescent organic light-emitting devices (PhOLEDs): colour tuning by varying the electroluminescence bandwidth. Journal of Materials Chemistry C, 2013, 1, 6800.	5.5	27
502	Theoretical insights into [PMo12O40]3â^' grafted on single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 9177.	2.8	27
503	Theoretical exploration to second-order nonlinear optical properties of new hybrid complexes via coordination interaction between (metallo)porphyrin and [MSiW11O39]3â^' (M=NbV or VV) polyoxometalates. Journal of Molecular Graphics and Modelling, 2013, 46, 59-64.	2.4	27
504	High-Nuclear Vanadoniobate {Nb₄₈V₈} Multiple-Strand Wheel. Inorganic Chemistry, 2015, 54, 11083-11087.	4.0	27

#	Article	IF	Citations
505	A theoretical design and investigation on Zn-porphyrin-polyoxometalate hybrids with different Ï€-linkers for searching high performance sensitizers of p-type dye-sensitized solar cells. Dyes and Pigments, 2016, 130, 168-175.	3.7	27
506	Aggregation-induced emission (AIE) active iridium complexes toward highly efficient single-layer non-doped electroluminescent devices. Journal of Materials Chemistry C, 2016, 4, 10464-10470.	5.5	27
507	Exploring more effective polymer donors for the famous non-fullerene acceptor ITIC in organic solar cells by increasing electron-withdrawing ability. Organic Electronics, 2018, 53, 308-314.	2.6	27
508	Fluorescence, Phosphorescence, or Delayed Fluorescence?â€”A Theoretical Exploration on the Reason Why a Series of Similar Organic Molecules Exhibit Different Luminescence Types. Journal of Physical Chemistry C, 2018, 122, 23091-23101.	3.1	27
509	Theoretical Insight into Multiple Charge-Transfer Mechanisms at the P3HT/Nonfullerenes Interface in Organic Solar Cells. ACS Sustainable Chemistry and Engineering, 2019, 7, 19699-19707.	6.7	27
510	Rational Design of Efficient Organometallic Ir(III) Complexes for High-Performance, Flexible, Monochromatic, and White Light-Emitting Electrochemical Cells. ACS Applied Materials & Interfaces, 2020, 12, 4649-4658.	8.0	27
511	Mn-doped CsPb(Br/Cl)₃ mixed-halide perovskites for CO₂ photoreduction. Nanotechnology, 2020, 31, 215605.	2.6	27
512	Preparation and electrochemical hydrogen storage properties of Ti49Zr26Ni25 alloy covered with porous polyaniline. International Journal of Hydrogen Energy, 2020, 45, 11675-11685.	7.1	27
513	Bimetallic Metalâ€“Organic Framework-Derived Graphitic Carbon-Coated Small Co/VN Nanoparticles as Advanced Trifunctional Electrocatalysts. ACS Applied Materials & Interfaces, 2021, 13, 2462-2471.	8.0	27
514	Anion-directed assembly of two novel cadmium(II) complexes constructed by 2,2â€²-(1,4-butanediyl)bis(1H-benzimidazole) ligand. Inorganic Chemistry Communication, 2006, 9, 1207-1211.	3.9	26
515	Quantum Chemical Design for Enhanced Secondâ€Order NLO Response of Terpyridineâ€Substituted Hexamolybdates. European Journal of Inorganic Chemistry, 2010, 2010, 3466-3472.	2.0	26
516	Theoretical Study on the Chiroptical Optical Properties of Chiral Fullerene C₆₀Derivative. Journal of Physical Chemistry A, 2011, 115, 13356-13363.	2.5	26
517	Assembly of Sandwich-Like Supermolecules Li Salts CpLi-C₆₀: Structures, Stabilities, and Nonlinear Optical Properties. Organometallics, 2012, 31, 4409-4414.	2.3	26
518	Hydrothermal synthesis and structural characterization of a new inorganicâ€“organic hybrid compound with photocatalytic activity based on Keggin-type polyanion and cadmium-1, 2, 4-triazolate units. Inorganic Chemistry Communication, 2012, 20, 273-276.	3.9	26
519	An efficient strategy for improving carrier transport performance â€“ Introducing fluorine into aryl substituted tetracene. Organic Electronics, 2013, 14, 1359-1369.	2.6	26
520	Self-assembly of metalâ€“organic frameworks based on N-donor ligand and flexible tricarboxylic acids with different angular characters. CrystEngComm, 2013, 15, 8214.	2.6	26
521	A photovoltaic system composed of a keplerate-type polyoxometalate and a water-soluble poly(p-phenylenevinylene) derivative. Journal of Materials Chemistry A, 2013, 1, 6727.	10.3	26
522	BN Segment Doped Effect on the First Hyperpolarizibility of Heteronanotubes: Focused on an Effective Connecting Pattern. Journal of Physical Chemistry C, 2013, 117, 10039-10044.	3.1	26

#	Article	IF	Citations
523	Prediction of second-order nonlinear optical properties of Wellsâ€“Dawson polyoxometalate derivatives [Xâ€“C(CH₂O)₃P₂Mâ€²₃M₁₅O₅₉]^{6â^'}(X = Chemistry Frontiers, 2014, 1, 65-70.	6.0	26
524	Designed Synthesis of Lipidâ€Coated Polyacrylic Acid/Calcium Phosphate Nanoparticles as Dual pHâ€Responsive Drugâ€Delivery Vehicles for Cancer Chemotherapy. Chemistry - A European Journal, 2017, 23, 6586-6595.	3.3	26
525	Polyoxometalatesâ€Based Metalâ€“Organic Frameworks Made by Electrodeposition and Carbonization Methods as Cathodes and Anodes for Asymmetric Supercapacitors. Chemistry - A European Journal, 2019, 25, 16617-16624.	3.3	26
526	Visible-light CO₂ photoreduction of polyoxometalate-based hybrids with different cobalt clusters. CrystEngComm, 2019, 21, 6423-6431.	2.6	26
527	Achieving highly electrochemically active maricite NaFePO4 with ultrafine NaFePO4@C subunits for high rate and low temperature sodium-ion batteries. Chemical Engineering Journal, 2021, 405, 126689.	12.7	26
528	Metalâ€“organic framework (MOF) composite materials for photocatalytic CO₂ reduction under visible light. Dalton Transactions, 2021, 50, 3186-3192.	3.3	26
529	Polyoxotungstates containing uranyl group: Germanotungstates with Keggin sandwich structure. Inorganic Chemistry Communication, 2006, 9, 1331-1334.	3.9	25
530	Theoretical studies on the electronic structure and spectral properties of versatile diarylethene-containing 1,10-phenanthroline ligands and their rhenium(I) complexes. Journal of Organometallic Chemistry, 2007, 692, 5368-5374.	1.8	25
531	Coordination between [H2P2W12O48]12â^' and antimony(iii): synthesis and characterization of sandwich complex derived from the new {P2W13O51} fragment. Dalton Transactions, 2010, 39, 8033.	3.3	25
532	pH-Tuned self-assembly of organicâ€“inorganic hybrids based on different vanadate chains, Zn(<scp>ii</scp>) ions and flexible ligands: crystallizing in polar and centrosymmetric space group. CrystEngComm, 2011, 13, 779-786.	2.6	25
533	Preparation and Application of Multipleâ€Componentâ€Doped Keggin Polyoxometalate Microtubesâ€”Towards a Componentâ€Tunable Hollow Structure. Chemistry - A European Journal, 2011, 17, 3657-3662.	3.3	25
534	The research of a new polyoxometalates based photosensitizer on dye sensitized solar cell. Inorganic Chemistry Communication, 2013, 38, 78-82.	3.9	25
535	A strategy for breaking the MOF template to obtain small-sized and highly dispersive polyoxometalate clusters loaded on solid films. Journal of Materials Chemistry A, 2015, 3, 14573-14577.	10.3	25
536	Controlled synthesis of mesoporous hollow SnO₂ nanococoons with enhanced lithium storage capability. Journal of Materials Chemistry A, 2015, 3, 22021-22025.	10.3	25
537	Self-assembly and photocatalytic H₂ evolution activity of two unprecedented polytantalotungstates based on the largest {Ta₁₈} and {Ta₁₈Yb₂} clusters. Chemical Communications, 2016, 52, 13787-13790.	4.1	25
538	Construction of porous covalent organic polymer as photocatalysts for RhB degradation under visible light. Science Bulletin, 2017, 62, 931-937.	9.0	25
539	Exploiting aggregation induced emission and twisted intramolecular charge transfer in a BODIPY dye for selective sensing of fluoride in aqueous medium and living cells. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 358, 274-283.	3.9	25
540	Uniform NiCo2O4/NiFe2O4 hollow nanospheres with excellent properties for Li-ion batteries and supercapacitors. Journal of Alloys and Compounds, 2018, 767, 223-231.	5.5	25

#	Article	IF	Citations
541	Supramolecular oligourethane gel as a highly selective fluorescent â€œonâ€“offâ€“onâ€•sensor for ions. Journal of Materials Chemistry C, 2020, 8, 11540-11545.	5.5	25
542	Faceâ€Directed Assembly of Molecular Cubes: In Situ Substitution of a Predetermined Concave Cluster. Angewandte Chemie - International Edition, 2020, 59, 22034-22038.	13.8	25
543	Single-atom catalysts on supported silicomolybdic acid for CO₂ electroreduction: a DFT prediction. Journal of Materials Chemistry A, 2022, 10, 6178-6186.	10.3	25
544	Luminescent compounds diphenylboron analogs of Alq3 and its methyl substituents: A theoretical investigation of their electronic and spectroscopic properties. International Journal of Quantum Chemistry, 2005, 103, 775-780.	2.0	24
545	Density functional study of protonation sites of Î±-Keggin isopolyanions. International Journal of Quantum Chemistry, 2006, 106, 1860-1864.	2.0	24
546	Improved performance of electrophosphorescent devices based on Re(CO)3Clâ€dipyrido[3,2â€:2â€²,3â€²â€]phenazine. Applied Physics Letters, 2006, 88, 093507.	3.3	24
547	ITO electrode modified with chitosan nanofibers loading polyoxometalate by one step self-assembly method and its electrocatalysis. Electrochemistry Communications, 2007, 9, 2224-2228.	4.7	24
548	Photoluminescent metal-organic framework with hex topology constructed from infinite rod-shaped secondary building units and single e,e-trans-1,4-cyclohexanedicarboxylic dianion. Inorganica Chimica Acta, 2007, 360, 3108-3112.	2.4	24
549	A Quantum Chemical Study of the Structure, Bonding Characteristics and Nonlinear Optical Properties of Aryloxido and Salicylaldehydo Derivatives of [XW₅O₁₈]^{3â€“} (X = Zr or Ti). European Journal of Inorganic Chemistry, 2009, 2009, 2529-2535.	2.0	24
550	Carbazolyl-contained phenol-pyridyl boron complexes: syntheses, structures, photoluminescent and electroluminescent properties. Dalton Transactions, 2010, 39, 5123.	3.3	24
551	Ionothermal synthesis of a new open-framework zinc phosphite NIS-3 with low framework density. CrystEngComm, 2010, 12, 1401.	2.6	24
552	Syntheses, structures and luminescent properties of a series of 3D lanthanide coordination polymers with tripodal semirigid ligand. Journal of Solid State Chemistry, 2011, 184, 373-378.	2.9	24
553	Computational Design of Host Materials Suitable for Green-(Deep) Blue Phosphors through Effectively Tuning the Triplet Energy While Maintaining the Ambipolar Property. Journal of Physical Chemistry C, 2013, 117, 8420-8428.	3.1	24
554	A polyrotaxane-like metalâ€“organic framework exhibiting luminescent sensing of Eu3+cations and proton conductivity. CrystEngComm, 2014, 16, 6882-6888.	2.6	24
555	The relationship between intermolecular interactions and charge transport properties of trifluoromethylated polycyclic aromatic hydrocarbons. Organic Electronics, 2014, 15, 1896-1905.	2.6	24
556	TiO2 film decorated with highly dispersed polyoxometalate nanoparticles synthesized by micelle directed method for the efficiency enhancement of dye-sensitized solar cells. Journal of Power Sources, 2016, 328, 1-7.	7.8	24
557	Latent harmony in dicarbon between VB and MO theories through orthogonal hybridization of 3Ï*f*_g and 2Ï*f*_u. Chemical Science, 2016, 7, 1028-1032.	7.4	24
558	A difunctional metalâ€“organic framework with Lewis basic sites demonstrating turn-off sensing of Cu²⁺ and sensitization of Ln³⁺. Journal of Materials Chemistry C, 2018, 6, 7874-7879.	5.5	24

#	Article	IF	Citations
559	Degradation of azo dyes under visible light with stable MOF based on tetrastyrene imidazole ligand. Dalton Transactions, 2020, 49, 4352-4357.	3.3	24
560	Photocatalytic C(sp³)â€“O/N Cross-Couplings by Nalâ€“PPh₃/CuBr Cooperative Catalysis: Computational Design and Experimental Verification. ACS Catalysis, 2021, 11, 6633-6642.	11.2	24
561	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.	3.0	23
562	A novel pentanuclear Zn(II) coordination polymer with double helices: Synthesis, structure and luminescent property. Inorganic Chemistry Communication, 2008, 11, 1246-1249.	3.9	23
563	The effect of phenyl group on the electronic and phosphorescent properties of cyclometalated analogues of platinum(II) terpyridine complexes: a theoretical study. Theoretical Chemistry Accounts, 2009, 124, 29-36.	1.4	23
564	Synthesis and photovoltaic properties of low-bandgap polymers based on N-arylcarbazole. Polymer, 2011, 52, 1748-1754.	3.8	23
565	Phenylcarbazole and phosphine oxide/sulfide hybrids as host materials for blue phosphors: effectively tuning the charge injection property without influencing the triplet energy. Physical Chemistry Chemical Physics, 2012, 14, 1685-1693.	2.8	23
566	pH variation induced construction of a series of entangled frameworks based on bi- and tri-metallic cores as nodes. CrystEngComm, 2012, 14, 124-130.	2.6	23
567	Spiral Intramolecular Charge Transfer and Large First Hyperpolarizability in MÃ¶bius Cyclacenes: New Insight into the Localized Ï€ Electrons. ChemPhysChem, 2012, 13, 2349-2353.	2.1	23
568	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
569	Theoretical Studies on Metalloporphyrinâ€“Polyoxometalates Hybrid Complexes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2014, 118, 29623-29628.	3.1	23
570	Ir(III) Phosphors Modified with Fluorine Atoms in Pyridine-1,2,4-triazolyl Ligands for Efficient OLEDs Possessing Low-Efficiency Roll-off. Organometallics, 2016, 35, 3870-3877.	2.3	23
571	Influence of Aggregation on the Structure and Fluorescent Properties of a Tetraphenylethylene Derivative: a Theoretical Study. ChemPhysChem, 2017, 18, 755-762.	2.1	23
572	Monodisperse and Tiny Co₂N_{0.67} Nanocrystals Uniformly Embedded over Two Curving Surfaces of Hollow Carbon Microfibers as Efficient Electrocatalyst for Oxygen Evolution Reaction. ACS Applied Nano Materials, 2018, 1, 4461-4473.	5.0	23
573	Towards red-light o-carborane derivatives with both aggregation induced emission and thermally activated delayed fluorescence combining quantum chemistry calculation with molecular dynamics simulation. Journal of Materials Chemistry C, 2019, 7, 2699-2709.	5.5	23
574	Controllable Synthesis of Metalâ€“Organic Frameworks Based on Anthracene Ligands for High-Sensitivity Fluorescence Sensing of Fe³⁺, Cr₂O₇^{2â€“}, and TNP. Crystal Growth and Design, 2022, 22, 2954-2963.	3.0	23
575	A DFT Study on the Electronic and Redox Properties of [PW11O39(ReN)]nâ€“(n = 3, 4, 5) and [PW11O39(OsN)]2â€“. European Journal of Inorganic Chemistry, 2006, 2006, 5126-5129.	2.0	22
576	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.	2.5	22

#	Article	IF	Citations
577	A series of inorganicâ€“organic hybrid compounds constructed from bis(undecatungstophosphate) lanthanates and copper-organic units. Inorganica Chimica Acta, 2010, 363, 3823-3831.	2.4	22
578	Synthesis and characterization of two self-catenated networks and one case of pcu topology based on the mixed ligands. CrystEngComm, 2012, 14, 4205.	2.6	22
579	Redox-active polyoxometalate-based crystalline material-immobilized noble metal nanoparticles: spontaneous reduction and synergistic catalytic activity. Journal of Materials Chemistry, 2012, 22, 21040.	6.7	22
580	Multipoint interactions enhanced H2 storage and organosulfur removal in a microporous metalâ€“organic framework. Journal of Materials Chemistry A, 2013, 1, 11111.	10.3	22
581	Influence of alkyl chain lengths on the properties of iridium(III)-based piezochromic luminescent dyes with triazole-pyridine type ancillary ligands. Dyes and Pigments, 2013, 99, 1082-1090.	3.7	22
582	The Application of ZnO Nanoparticles Containing Polyoxometalates in Dye-Sensitized Solar Cells. European Journal of Inorganic Chemistry, 2013, 2013, 1951-1959.	2.0	22
583	An accurate and efficient method to predict the electronic excitation energies of BODIPY fluorescent dyes. Journal of Computational Chemistry, 2013, 34, 566-575.	3.3	22
584	Intramolecular Ï€ Stacking in Cationic Iridium(III) Complexes with Phenylâ€Functionalized Cyclometalated Ligands: Synthesis, Structure, Photophysical Properties, and Theoretical Studies. European Journal of Inorganic Chemistry, 2014, 2014, 2376-2382.	2.0	22
585	Two hybrid materials assembled from transition metal mono-substituted Keggin polyoxoanions as photocatalysts under visible light. CrystEngComm, 2014, 16, 9163-9167.	2.6	22
586	Syntheses, crystal structures and properties of inorganicâ€“organic hybrids constructed from Keggin-type polyoxometalates and silver coordination compounds. CrystEngComm, 2014, 16, 7410-7418.	2.6	22
587	Assembly of tetrameric dimethyltin-functionalized selenotungstates: from nanoclusters to one-dimensional chains. Chemical Communications, 2015, 51, 2433-2436.	4.1	22
588	Three Kegginâ€Type Transition Metalâ€Substituted Polyoxometalates as Pure Inorganic Photosensitizers for pâ€Type Dyeâ€Sensitized Solar Cells. Chemistry - A European Journal, 2016, 22, 3234-3238.	3.3	22
589	Self-assembly and photocatalytic properties of Ta/W mixed-addendum polyoxometalate and transition-metal cations. CrystEngComm, 2016, 18, 8722-8725.	2.6	22
590	Self-assembly and photocatalytic H₂ evolution activity of two nanoscale polytantalotungstates based on unprecedented {Cr₃Ta₆} and {Cr₄Ta₁₂} clusters. Journal of Materials Chemistry A, 2017, 5, 22970-22974.	10.3	22
591	Design of Hexabenzocoronene Derivatives as Non-Fullerene Acceptors in Organic Photovoltaics by Bridging Dimers and Modulating Structural Twists. Solar Rrl, 2017, 1, 1700060.	5.8	22
592	Nonfullerene Acceptors for Organic Photovoltaics: From Conformation Effect to Power Conversion Efficiencies Prediction. Solar Rrl, 2019, 3, 1900258.	5.8	22
593	A triazine-based metal-organic framework with solvatochromic behaviour and selectively sensitive photoluminescent detection of nitrobenzene and Cu2+ ions. Dyes and Pigments, 2019, 163, 159-167.	3.7	22
594	Copper Dimer Anchored in gâ€CN Monolayer as an Efficient Electrocatalyst for CO₂ Reduction Reaction: A Computational Study. Advanced Theory and Simulations, 2020, 3, 2000218.	2.8	22

#	Article	IF	Citations
595	Preparation and electrochemical hydrogen storage properties of <scp> Co ₉ S ₈ </scp> alloy coated with cobalt/graphene composite. International Journal of Energy Research, 2020, 44, 11742-11755.	4.5	22
596	A novel 3D cobalt(II) metalâ€“organic framework to activate peroxymonosulfate for degradation of organic dyes in water. Journal of Solid State Chemistry, 2020, 289, 121443.	2.9	22
597	Rh@C8N8 monolayer as a promising single-atom-catalyst for overall water splitting. Applied Surface Science, 2021, 549, 149320.	6.1	22
598	An unprecedented fully reduced {Mo^V₆₀} polyoxometalate: from an all-inorganic molecular light-absorber model to improved photoelectronic performance. Chemical Science, 2022, 13, 4573-4580.	7.4	22
599	Two unprecedented 1D coordination polymer chains based on tetranuclear copper(II) building blocks. Journal of Solid State Chemistry, 2008, 181, 2406-2411.	2.9	21
600	Two unusual self-threading frameworks self-assembled from mixed ligands and cobalt/zinc ions. CrystEngComm, 2011, 13, 325-329.	2.6	21
601	3D Chiral Microporous (10,3)-a Topology Metalâ€“Organic Framework Containing Large Helical Channels. Crystal Growth and Design, 2011, 11, 2510-2514.	3.0	21
602	Hydrothermal synthesis and luminescence properties of hierarchical SrF2 and SrF2:Ln3+ (Ln=Er, Nd,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	5.2	21
603	Polyoxometalate supported complexes as effective electron-transfer mediators in dye-sensitized solar cells. Dalton Transactions, 2014, 43, 1493-1497.	3.3	21
604	Coordination assemblies of seven metal-organic frameworks based on a bent connector: structural diversity and properties. CrystEngComm, 2015, 17, 3129-3138.	2.6	21
605	Assembly of Mn-Containing Unprecedented Selenotungstate Clusters with Photocatalytic H₂ Evolution Activity. Crystal Growth and Design, 2016, 16, 2481-2486.	3.0	21
606	Tailored Synthesis of Octopusâ€type Janus Nanoparticles for Synergistic Activelyâ€Targeted and Chemoâ€Photothermal Therapy. Angewandte Chemie, 2016, 128, 2158-2161.	2.0	21
607	Rational design and synthesis of cationic Ir(III) complexes with triazolate cyclometalated and ancillary ligands for multi-color tuning. Dyes and Pigments, 2017, 139, 524-532.	3.7	21
608	Near-infrared light and pH-responsive Au@carbon/calcium phosphate nanoparticles for imaging and chemo-photothermal cancer therapy of cancer cells. Dalton Transactions, 2017, 46, 14746-14751.	3.3	21
609	A mechanochromic cyclemetalated cationic Ir(<scp>iii</scp>) complex with AIE activity by strategic modification of ligands. Dalton Transactions, 2020, 49, 13066-13071.	3.3	21
610	Integration of zirconium-based metalâ€“organic framework with CdS for enhanced photocatalytic conversion of CO₂ to CO. Nanoscale, 2021, 13, 16977-16985.	5.6	21
611	Structure, stability, and aromaticity of M?SubPc (M?B, Al, and Ga): Computational study. International Journal of Quantum Chemistry, 2005, 103, 54-59.	2.0	20
612	An accurate density functional theory calculation for electronic excitation energies: The least-squares support vector machine. Journal of Chemical Physics, 2009, 130, 184104.	3.0	20

#	Article	IF	Citations
613	Metalâ€“organic replica of chiral natural material Î²-SnF₂: an enantiopure binodal (3,5)-connected net based on triangular and trigonal bipyramidal coordination. Chemical Communications, 2010, 46, 604-606.	4.1	20
614	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.	1.4	20
615	Synthesis of cationic iridium(III) complexes with high quantum yield via enhancing the steric hindrance of ligands. Journal of Organometallic Chemistry, 2012, 702, 27-35.	1.8	20
616	Controlled synthesis and magnetically separable photocatalytic properties of magnetic iron oxides@SnO2 yolkâ€“shell nanocapsules. Journal of Materials Chemistry, 2012, 22, 13380.	6.7	20
617	Selfâ€Assembly and Visibleâ€Light Photocatalytic Properties of W/Nb Mixedâ€Addendum Polyoxometalate and Transitionâ€Metal Cations. ChemPlusChem, 2013, 78, 775-779.	2.8	20
618	After the electronic field: Structure, bonding, and the first hyperpolarizability of HArF. Journal of Computational Chemistry, 2013, 34, 952-957.	3.3	20
619	Theoretical Exploration of Photoisomerization-Switchable Second-Order Nonlinear Optical Responses of Two-Dimendional Î›- and W-Shaped Polyoxometalate Derivatives of Dithienylperfluorocyclopentene. Journal of Physical Chemistry A, 2013, 117, 10783-10789.	2.5	20
620	Redox-controlled Î´-Dawson {Mn2IIIW17} polyoxometalate with photocatalytic H2 evolution activity. Chemical Communications, 2014, 50, 5961.	4.1	20
621	Synthesis, crystal structure, and application of an acenaphtho[1,2-k] fluoranthene diimide derivative. Science China Chemistry, 2015, 58, 364-369.	8.2	20
622	Simple molecular structure design of iridium(III) complexes: Achieving highly efficient non-doped devices with low efficiency roll-off. Organic Electronics, 2016, 35, 142-150.	2.6	20
623	Syntheses, crystal structures and properties of metalâ€“organic rotaxane frameworks with cucurbit[6]uril. CrystEngComm, 2016, 18, 2327-2336.	2.6	20
624	Effect of polyoxometalate in organic-inorganic hybrids on charge transfer and absorption spectra towards sensitizers. Dyes and Pigments, 2017, 142, 379-386.	3.7	20
625	Reversible tricolour luminescence switching based on a piezochromic iridium(<scp>iii</scp>) complex. Chemical Communications, 2019, 55, 14582-14585.	4.1	20
626	A hydrazone-based covalent organic framework/iridium (III) complex for photochemical CO2 reduction with enhanced efficiency and durability. Journal of Catalysis, 2020, 392, 49-55.	6.2	20
627	Organic Supramolecular Zippers with Ultralong Organic Phosphorescence by a Dexter Energy Transfer Mechanism. Angewandte Chemie - International Edition, 2022, 61, .	13.8	20
628	Chiral self-sorting and guest recognition of porous aromatic cages. Nature Communications, 2022, 13, .	12.8	20
629	Synthesis, structure and characterization of a new cobalt-containing germanotungstate with open Wells-Dawson structure: K13[{Co(H2O)}(Î¼-H2O)2K(Ge2W18O66)]. Journal of Molecular Structure, 2006, 785, 170-175.	3.6	19
630	A Quantum Mechanical Study of the Second-Order Nonlinear Optical Properties of Aryldiazenido-Substituted Hexamolybdates: A Surprising Charge Transfer. European Journal of Inorganic Chemistry, 2009, 2009, 5181-5188.	2.0	19

#	Article	IF	Citations
631	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.	1.4	19
632	Macroscopic single-crystal tubes assembled with porous supramolecular architecture of water-soluble calixarene and phenanthroline. Chemical Communications, 2009, , 1861.	4.1	19
633	Theoretical studies on nitrido ruthenium (VI) porphyrin and high valent ruthenium nitrido derivatives of Keggin typical polyoxometalate ([PW11O39{RuVIN}]4â^'): electronic structures and bonding features. Dalton Transactions, 2009, , 6208.	3.3	19
634	Identification of nonplanar small molecule for G-quadruplex grooves: Molecular docking and molecular dynamic study. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 6969-6972.	2.2	19
635	Quantum chemical study of structures, electronic spectrum, and nonlinear optical properties of polynuclear lithium compounds. Computational and Theoretical Chemistry, 2011, 966, 14-19.	2.5	19
636	TDDFT Studies on the Electronic Structures and Chiroptical Properties of Mono-Tin-Substituted Wellsâ€“Dawson Polyoxotungstates. Journal of Physical Chemistry A, 2012, 116, 4152-4158.	2.5	19
637	The encapsulated lithium effect of Li@C60Cl8 remarkably enhances the static first hyperpolarizability. RSC Advances, 2013, 3, 13348.	3.6	19
638	Green Oxidative Degradation of Methyl Orange with Copper(II) Schiff Base Complexes as Photoâ€Fentonâ€Like Catalysts. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2014, 640, 2035-2040.	1.2	19
639	Synthesis of red-emitting cationic Ir (III) complex and its application in white light-emitting electrochemical cells. Organic Electronics, 2017, 42, 303-308.	2.6	19
640	Di-/trinuclear cationic Ir(III) complexes: Design, synthesis and application for highly sensitive and selective detection of TNP in aqueous solution. Sensors and Actuators B: Chemical, 2017, 244, 314-322.	7.8	19
641	Intra- and Intermolecular Charge Transfer in a Novel Dimer: Cooperatively Enhancing Second-Order Optical Nonlinearity. Journal of Physical Chemistry C, 2017, 121, 25472-25478.	3.1	19
642	A metal-organic framework based on nanosized hexagonal channels as fluorescent indicator for detection of nitroaromatic explosives. Journal of Solid State Chemistry, 2018, 258, 781-785.	2.9	19
643	Honeycomb-patterned hybrid films of surfactant-encapsulated polyoxometalates by a breath figure method and its electrocatalysis for BrO₃^{â^'}. Dalton Transactions, 2018, 47, 105-111.	3.3	19
644	A 3D pillared-layer metalâ€“organic framework with fluorescence property for detection of nitroaromatic explosives. New Journal of Chemistry, 2019, 43, 963-969.	2.8	19
645	Ligand-Induced Tunable Dual-Color Emission Based on Lead Halide Perovskites for White Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2019, 11, 15898-15904.	8.0	19
646	Bottomâ€Up Construction and Reversible Structural Transformation of Supramolecular Isomers based on Large Truncated Tetrahedra. Angewandte Chemie, 2019, 131, 790-794.	2.0	19
647	Element table of TM-substituted polyoxotungstates for direct electrocatalytic reduction of nitric oxide to ammonia: a DFT guideline for experiments. Inorganic Chemistry Frontiers, 2020, 7, 4507-4516.	6.0	19
648	A tetraphenylethylene-based covalent organic framework for waste gas adsorption and highly selective detection of Fe³⁺. CrystEngComm, 2021, 23, 5569-5574.	2.6	19

#	Article	IF	Citations
649	Stepwise Construction of Multivariate Metalâ€“Organic Frameworks from a Predesigned Zr ₁₆ Cluster. CCS Chemistry, 2021, 3, 287-293.	7.8	19
650	Synergetic effect of H⁺ adsorption and ethylene functional groups of covalent organic frameworks on the CO₂ photoreduction in aqueous solution. Chemical Communications, 2020, 56, 7261-7264.	4.1	19
651	Activating room-temperature phosphorescence of 1,8-naphthalimide by doping into aromatic dicarboxylic acids. Chemical Communications, 2022, 58, 3641-3644.	4.1	19
652	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
653	Colorimetric detection of immunoglobulin G by use of functionalized gold nanoparticles on polyethylenimine film. Analytical and Bioanalytical Chemistry, 2006, 384, 1518-1524.	3.7	18
654	Two New Helical Compounds Based on Pitchâ€Tunable Keggin Clusters. European Journal of Inorganic Chemistry, 2009, 2009, 5175-5180.	2.0	18
655	Synthesis, characterization and crystal structure of a novel Os(II)-supported tungstoarsenate [HAsW7O28Os(dmso)3]6â^'. Journal of Solid State Chemistry, 2009, 182, 83-88.	2.9	18
656	1,2,3,4-Alternate double cone conformational extreme in the supramolecular assemblies of p-sulfonatocalix[8]arene. CrystEngComm, 2009, 11, 1803.	2.6	18
657	Construction of a series of 0D, 2D and 3D inorganicâ€“organic hybrid coordination polymers based on octamolybdate and 2-(2-pyridyl)imidazole and its derivative. Inorganica Chimica Acta, 2010, 363, 118-126.	2.4	18
658	A DFT study on the electronic and redox properties of [X₈V₁₄O₅₀]^{nâ€“} (X = Si^{IV},) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 434-442.	1.1	18
659	Syntheses, structures, and photoluminescence of d10 coordination architectures: From 1D to 3D complexes based on mixed ligands. Solid State Sciences, 2011, 13, 1083-1091.	3.2	18
660	Thermochemical stabilities, electronic structures, and optical properties of C₅₆X₁₀ (X = H, F, and Cl) fullerene compounds. Journal of Computational Chemistry, 2011, 32, 658-667.	3.3	18
661	Theoretical studies on the structure and properties of BN clusters (BN)n and endohedral metallo-BN clusters M@(BN)n. Computational and Theoretical Chemistry, 2011, 964, 56-64.	2.5	18
662	Flowerlike Î³-Fe2O3@NiO hierarchical core-shell nanostructures as superb capability and magnetically separable adsorbents for water treatment. RSC Advances, 2013, 3, 12671.	3.6	18
663	Self-assembly and photocatalytic hydrogen evolution of a niobium-containing polyoxometalate. Inorganic Chemistry Communication, 2014, 44, 195-197.	3.9	18
664	The photovoltaic performance of dye-sensitized solar cells enhanced by using Dawson-type heteropolyacid and heteropoly blue-TiO2 composite films as photoanode. Inorganic Chemistry Communication, 2014, 47, 138-143.	3.9	18
665	Co-sensitization promoted light harvesting with a new mixed-addenda polyoxometalate [Cu(C₁₂H₈N₂)₂]₂[V₂W₄O₁₉ in dye-sensitized solar cells. Dalton Transactions, 2015, 44, 18553-18562.	3.8	18
666	A visible-light responsive zirconium metalâ€“organic framework for living photopolymerization of methacrylates. RSC Advances, 2016, 6, 66444-66450.	3.6	18

#	Article	IF	Citations
667	Theoretical design and characterization of high-efficiency organic dyes with different electron-withdrawing groups based on C275 toward dye-sensitized solar cells. New Journal of Chemistry, 2016, 40, 9320-9328.	2.8	18
668	How does a little difference in structure determine whether molecules have thermally activated delayed fluorescence characteristic or not?. Organic Electronics, 2017, 50, 70-76.	2.6	18
669	Guest exchange in a porous cucurbit[6]uril-based metalâ€“organic rotaxane framework probed by NMR and X-ray crystallography. Chemical Communications, 2018, 54, 5474-5477.	4.1	18
670	A multifunctional microporous metalâ€“organic framework: efficient adsorption of iodine and column-chromatographic dye separation. RSC Advances, 2018, 8, 36400-36406.	3.6	18
671	Metalâ€“Organic Frameworks with Organogold(III) Complexes for Photocatalytic Amine Oxidation with Enhanced Efficiency and Selectivity. Chemistry - A European Journal, 2018, 24, 15089-15095.	3.3	18
672	Beî€,Be triple bond in Be₂X₄Y₂ clusters (X = Li, Na and Y = Li, Na, K) and a perfect classical Beî€,Be triple bond presented in Be₂Na₄K₂. Dalton Transactions, 2019, 48, 14590-14594.	3.3	18
673	Transition metals doped fullerenes: structures â€“ NLO property relationships. Molecular Physics, 2019, 117, 705-711.	1.7	18
674	Equiâ€“size nesting of Platonic and Archimedean metalâ€“organic polyhedra into a twin capsid. Nature Communications, 2020, 11, 4103.	12.8	18
675	Multiâ€functional TiO ₂ nanosheets/carbon nanotubes modified separator enhanced cycling performance for lithiumâ€sulfur batteries. International Journal of Energy Research, 2020, 44, 3231-3240.	4.5	18
676	PL sensor for sensitive and selective detection of 2,4,6-trinitrophenol based on carbazole and tetraphenylsilane polymer. Dyes and Pigments, 2021, 191, 109379.	3.7	18
677	Organicâ€“inorganic hybrids constructed by Anderson-type polyoxoanions and copper coordination complexes. Journal of Solid State Chemistry, 2009, 182, 49-54.	2.9	17
678	Synthesis, crystal structures and nonlinear optical properties of three TCF-based chromophores. CrystEngComm, 2009, 11, 589-596.	2.6	17
679	An equatorial tri-iron substituted Wellsâ€“Dawson type tungstophosphate with magnetic and bifunctional electrocatalytic properties. Inorganica Chimica Acta, 2010, 363, 718-722.	2.4	17
680	Electronic Properties of Unprecedented Bridging Organoimido-Substituted Hexamolybdate: New Insights from Density Functional Theory Study. Journal of Physical Chemistry B, 2010, 114, 3754-3758.	2.6	17
681	Quantum chemical characterization of the generation of high-valent oxoruthenium species of Keggin type polyoxometalates: electronic structure and bonding features. Dalton Transactions, 2011, 40, 2967.	3.3	17
682	A series of POM-based entangled frameworks with the rigid ligand 1,4-bis(1-imidazolyl)benzene and different isomers of octamolybdate. Journal of Solid State Chemistry, 2011, 184, 1141-1147.	2.9	17
683	Bonding Interactions between Nitrous Oxide (N₂O) and Monoâ€Ruthenium Substituted Kegginâ€Type Polyoxometalates: Electronic Structures of Ruthenium/N₂O Adducts. European Journal of Inorganic Chemistry, 2011, 2011, 489-494.	2.0	17
684	Synthesis and characterizations of novel spindle-like terphenyl-type chromophores for non-linear optical materials. Tetrahedron, 2011, 67, 4110-4117.	1.9	17

#	Article	IF	Citations
685	Nonaqueous synthesis of uniform polyaniline nanospheres Via cellulose acetate template. Journal of Polymer Science Part A, 2012, 50, 912-917.	2.3	17
686	An effective method for accurate prediction of the first hyperpolarizability of alkalides. Journal of Computational Chemistry, 2012, 33, 231-236.	3.3	17
687	Superatoms (Li₃O and BeF₃) induce phenalenyl radical Ï€-dimer: fascinating interlayer charge-transfer and large NLO responses. Dalton Transactions, 2014, 43, 12657-12662.	3.3	17
688	Theoretical studies on organic D-Ï€-A sensitizers with planar triphenylamine donor and different Ï€-linkers for dyes-sensitized solar cells. Journal of Molecular Modeling, 2014, 20, 2309.	1.8	17
689	POM-based inorganicâ€“organic hybrid compounds: synthesis, structures, highly-connected topologies and photodegradation of organic dyes. RSC Advances, 2015, 5, 59093-59098.	3.6	17
690	A sulfur-free iridium(<scp>iii</scp>) complex for highly selective and multi-signaling mercury(<scp>ii</scp>)-chemosensors. Dalton Transactions, 2015, 44, 19997-20003.	3.3	17
691	Connecting effect on the first hyperpolarizability of armchair carbonâ€“boronâ€“nitride heteronanotubes: pattern versus proportion. Physical Chemistry Chemical Physics, 2016, 18, 13954-13959.	2.8	17
692	The conversion of donor to acceptor and rational design for diketopyrrolopyrrole-containing small molecule acceptors by introducing nitrogen-atoms for organic solar cells. RSC Advances, 2017, 7, 31800-31806.	3.6	17
693	Supramolecular hydrogen-bonded organic networks through acidâ€“base pairs as efficient proton-conducting electrolytes. CrystEngComm, 2019, 21, 4996-5001.	2.6	17
694	Copper cyanide polymers with controllable dimensions modulated by rigid and flexible bis-(imidazole) ligands: synthesis, crystal structure and fluorescence properties. CrystEngComm, 2019, 21, 1242-1249.	2.6	17
695	Photosensitizers based on Ir(III) complexes for highly efficient photocatalytic hydrogen generation. Dyes and Pigments, 2019, 170, 107547.	3.7	17
696	Theoretical mechanistic study of metallaphotoredox catalysis: Câ€“N cross-coupling via Ni(<scp>ii</scp>)-mediated Ï*f*-bond metathesis. Organic Chemistry Frontiers, 2020, 7, 2168-2178.	4.5	17
697	Theoretical study on C32 fullerenes and derivatives. Chemical Physics Letters, 2006, 428, 148-151.	2.6	16
698	Hydrothermal syntheses, crystal structures and properties of three coordination frameworks based on a new semirigid ligand and benzenedicarboxylate. Journal of Solid State Chemistry, 2008, 181, 2378-2385.	2.9	16
699	Self-assembly of zinc polymers based on a flexible linear ligand at different pH values: Syntheses, structures and fluorescent properties. Solid State Sciences, 2009, 11, 635-642.	3.2	16
700	Theoretical investigation of structures, electronic spectra and nonlinear optical properties of gold-pentacene (Au2C22H14) complexes. Journal of Organometallic Chemistry, 2009, 694, 1266-1272.	1.8	16
701	Improving the accuracy of low level quantum chemical calculation for absorption energies: the genetic algorithm and neural network approach. Physical Chemistry Chemical Physics, 2009, 11, 5124.	2.8	16
702	Building block approach to a series of substituted Keggin-type inorganicâ€“organic hybrids. Solid State Sciences, 2011, 13, 1115-1121.	3.2	16

#	Article	IF	Citations
703	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
704	Theoretical Study on the Rectifying Performance of Organoimido Derivatives of Hexamolybdates. ChemPhysChem, 2013, 14, 610-617.	2.1	16
705	Helical Carbon Segment in Carbonâ€“Boronâ€“Nitride Heteronanotubes: Structure and Nonlinear Optical Properties. ChemPlusChem, 2014, 79, 732-736.	2.8	16
706	Theoretical exploration on switchable NLO response induced by photochromic properties of covalently connected unsymmetrical spiropyranâ€“polyoxometalate complex. Dyes and Pigments, 2014, 106, 105-110.	3.7	16
707	A series of coordination compounds containing rigid multi-pyridine based ligands: syntheses, structures and properties. CrystEngComm, 2014, 16, 2754.	2.6	16
708	Large Size Color-tunable Electroluminescence from Cationic Iridium Complexes-based Light-emitting Electrochemical Cells. Scientific Reports, 2016, 6, 27613.	3.3	16
709	A novel Ta/W mixed-addendum polyoxometalate with photocatalytic properties. Dalton Transactions, 2017, 46, 10177-10180.	3.3	16
710	Tuning the inter-molecular charge transfer, second-order nonlinear optical and absorption spectra properties of a Ï€-dimer under an external electric field. Physical Chemistry Chemical Physics, 2017, 19, 31958-31964.	2.8	16
711	Strategic modification of ligands for remarkable piezochromic luminescence (PCL) based on a neutral Ir(<scp>iii</scp>) phosphor. Journal of Materials Chemistry C, 2019, 7, 10876-10880.	5.5	16
712	Mechanistic insight into electroreduction of carbon dioxide on FeN_x (x = 0â€“4) embedded graphene. Physical Chemistry Chemical Physics, 2019, 21, 23638-23644.	2.8	16
713	Precise Molecularâ€Level Modification of Nafion with Bismuth Oxide Clusters for Highâ€performance Protonâ€Exchange Membranes. Angewandte Chemie, 2021, 133, 6141-6150.	2.0	16
714	Elongated heterometal double-sites promote nitrogen reduction on two-dimensional MMâ€²B₇ monolayers. Journal of Materials Chemistry A, 2021, 9, 10855-10868.	10.3	16
715	Mechanistic insight into photocatalytic CO₂ reduction by a Z-scheme g-C₃N₄/TiO₂ heterostructure. New Journal of Chemistry, 2021, 45, 11474-11480.	2.8	16
716	Study on the electronic structure of phenylene vinylene dimers with different substituents. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2001, 85, 165-168.	3.5	15
717	Hierarchical self-assembling of dendriticâ€“linear diblock complex based on hydrogen bonding. Polymer, 2007, 48, 3759-3770.	3.8	15
718	Theoretical predication of third-order optical nonlinearities of [Al4MAl4] nâ¯ (nÂ= 0â€“2, M = Ti, V and) Tj ETQq0 0 0 rgBT /Overlock 10	1.4	15
719	A metalâ€“organic framework containing meso-helical chains: Synthesis, characterization and luminescent property. Inorganic Chemistry Communication, 2008, 11, 1181-1183.	3.9	15
720	The self-assembly mechanism of the Lindqvist anion [W6O19]2â¯ in aqueous solution: a density functional theory study. Dalton Transactions, 2012, 41, 11361.	3.3	15

#	Article	IF	Citations
721	Synthesis, structure and photophysical properties of cationic Ir(III) complexes with functionalized 1,10-phenanthroline ancillary ligands. Journal of Organometallic Chemistry, 2012, 713, 20-26.	1.8	15
722	Probing the linear and nonlinear optical properties of nitrogen-substituted carbon nanotube. Journal of Molecular Modeling, 2012, 18, 3219-3225.	1.8	15
723	Theoretical studies on the photoisomerization-switchable second-order nonlinear optical responses of DTE-linked polyoxometalate derivatives. Journal of Molecular Graphics and Modelling, 2013, 40, 110-115.	2.4	15
724	Bonding interactions between sulfur dioxide (SO₂) and mono-ruthenium(<scp>ii</scp>)-substituted Keggin-type polyoxometalates: electronic structures of rutheniumâ€“SO₂adducts. Physical Chemistry Chemical Physics, 2014, 16, 18017.	2.8	15
725	Facile Fabrication of Wellâ€Dispersed Pt Nanoparticles in Mesoporous Silica with Large Open Spaces and Their Catalytic Applications. Chemistry - A European Journal, 2016, 22, 9293-9298.	3.3	15
726	Orthogonal reactivity of Ni(<scp>i</scp>)/Pd(0) dual catalysts for Ullmann Câ€“C cross-coupling: theoretical insight. Chemical Communications, 2018, 54, 7959-7962.	4.1	15
727	Phosphorescent iridium(III) complex based photoluminescence sensor for sensitive and selective detection of picric acid. Dyes and Pigments, 2020, 172, 107799.	3.7	15
728	Assembly of tetra-nuclear YbIII-containing selenotungstate clusters: synthesis, structures, and magnetic properties. Dalton Transactions, 2021, 50, 11535-11541.	3.3	15
729	Computational evaluation of FeMo heteroatom coeffect induced high electroreduction activity of N2-to-NH3. Applied Surface Science, 2022, 579, 152214.	6.1	15
730	Electronic structure and molecular orbital study of the first excited state of the high-efficiency blue OLED material bis(2-methyl-8-quinolinolato)aluminum(III) hydroxide complex from ab initio and TD-B3LYP. International Journal of Quantum Chemistry, 2004, 97, 992-1001.	2.0	14
731	Self-assembling structures and thin-film microscopic morphologies of amphiphilic rodâ€“coil block oligomers. Journal of Colloid and Interface Science, 2005, 289, 488-497.	9.4	14
732	â€˜One-stepâ€™ controllable synthesis of Ag and Ag2S nanocrystals on a large scale. Nanotechnology, 2006, 17, 5681-5685.	2.6	14
733	Synthesis and self-assembly of silica-coated anisotropic gold nanoparticle films. Nanotechnology, 2006, 17, 1819-1824.	2.6	14
734	A novel chiral 3D supramolecular framework based on organooxotin cluster. Inorganic Chemistry Communication, 2008, 11, 220-224.	3.9	14
735	DFT study on second-order nonlinear optical properties of the derivatives of 7-vertex cobaltâ€“carborane metallocenyl. Computational and Theoretical Chemistry, 2008, 863, 66-72.	1.5	14
736	Unprecedented Dinuclear Tin Derivative of Deprotonated Î²-Cyclodextrins. Inorganic Chemistry, 2008, 47, 2931-2933.	4.0	14
737	Theoretical study on the secondâ€order nonlinear optical properties of nonconjugated Dâ€Ï€â€A chromophores. International Journal of Quantum Chemistry, 2009, 109, 1553-1559.	2.0	14
738	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.	1.4	14

#	Article	IF	Citations
739	Broad absorbing low-bandgap polythiophene derivatives incorporating separate and content-tunable benzothiadiazole and carbazole moieties for polymer solar cells. European Polymer Journal, 2010, 46, 1770-1777.	5.4	14
740	A en-templated 3D coordination polymer based on H2pzdc with macrometallocycles. Inorganic Chemistry Communication, 2010, 13, 1227-1230.	3.9	14
741	On the Origin of the Inverted Stability Order of the Reverse-Keggin [(MnO₄)(CH₃)₁₂Sb₁₂O₂₄]^{6â^'}: A DFT Study of Î±, Î², Î³, Î´, and Îµ Isomers. Inorganic Chemistry, 2010, 49, 5472-5481.	4.0	14
742	Theoretical study on the tetranuclear endohedral vanadyl carboxylates with guest-switchable redox properties and large polarizability. Dalton Transactions, 2010, 39, 3706.	3.3	14
743	Time-Dependent Current Distributions of a Two-Terminal Carbon Nanotube-Based Electronic Device. Journal of Physical Chemistry B, 2011, 115, 5519-5525.	2.6	14
744	Ab initio and density functional study on fullerene C44 and its derivatives. Computational and Theoretical Chemistry, 2011, 978, 166-171.	2.5	14
745	N-Methylbenzoaza-18-crown-6-ether derivatives as efficient alkali metal cations sensors: the dipole moment and first hyperpolarizability. RSC Advances, 2014, 4, 24433-24438.	3.6	14
746	Syntheses, structures, magnetic and luminescence properties of a series of coordination polymers constructed from 1,4-naphthalenedicarboxylate and N-donor ligands. CrystEngComm, 2015, 17, 4517-4524.	2.6	14
747	Modulating the Charge Transfer of Dâ€“Sâ€“A Molecules: Structures and NLO Properties. Journal of Physical Chemistry A, 2015, 119, 767-773.	2.5	14
748	Theoretical design of three-dimensional non-fullerene acceptor materials based on an arylenediimide unit towards high efficiency organic solar cells. New Journal of Chemistry, 2017, 41, 3857-3864.	2.8	14
749	Simple and efficient polyoxomolybdate-mediated synthesis of novel graphene and metal nanohybrids for versatile applications. Journal of Colloid and Interface Science, 2018, 514, 507-516.	9.4	14
750	Fabrication of a Flowerlike Ag Microsphere Film with Applications in Catalysis and as a SERS Substrate. European Journal of Inorganic Chemistry, 2018, 2018, 2835-2840.	2.0	14
751	An unprecedented {CuII14TeIV10} core incorporated in a 36-tungsto-4-silicate polyoxometalate with visible light-driven catalytic hydrogen evolution activity. Dalton Transactions, 2018, 47, 16403-16407.	3.3	14
752	Stimulating intra- and intermolecular charge transfer and nonlinear optical response for biphenalenyl biradicaloid dimer under an external electric field. Physical Chemistry Chemical Physics, 2018, 20, 18699-18706.	2.8	14
753	An Updated Strategy for Designing Non-Fullerene Acceptors by the Lowest Singlet and Triplet States Excitation: Influence of Periodical Substitution from O, S, and Se to Te for BAE Derivatives. Journal of Physical Chemistry C, 2019, 123, 11397-11405.	3.1	14
754	All Boron Atoms in a ScB₁₂ Monolayer Contribute to the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 23221-23229.	3.1	14
755	A luminescent metalâ€“organic framework with tetragonal nanochannels as an efficient chemosensor for nitroaromatic explosives detection. CrystEngComm, 2021, 23, 3901-3906.	2.6	14
756	2D luminescent metalâ€“organic framework: efficient and highly selective detection of 2,4,6-trinitrophenol at the ppb level. CrystEngComm, 2021, 23, 929-934.	2.6	14

#	Article	IF	Citations
757	Self-assembly of bimetallic polyoxometalates and dicyandiamide to form Co/WC@NC for efficient electrochemical hydrogen generation. New Journal of Chemistry, 2021, 46, 178-184.	2.8	14
758	Synthesis, structure and luminescent properties of two three-dimensional d10 metal complexes constructed from pyridine-3,4-dicarboxylic acid with new network topologies. Journal of Molecular Structure, 2006, 796, 172-178.	3.6	13
759	MP2 theory investigation on the halides of D6hC36:C36Xn (X=F,Cl,Br; n=2,4,6,12). Journal of Chemical Physics, 2006, 124, 144108.	3.0	13
760	Synthesis and characterization of a new trifunctional magneticâ€“photoluminescentâ€“oxygen-sensing nanomaterial. Nanotechnology, 2008, 19, 495709.	2.6	13
761	Theoretical study on the two-dimensional second-order nonlinear optical properties: a series of charge-transfer covalently bonded organoimido derived hexamolybdate complexes. Theoretical Chemistry Accounts, 2009, 122, 217-226.	1.4	13
762	A novel luminescent 3D metalâ€“organic framework possessing 4-fold interpenetrating (3,4)-connected net. Inorganic Chemistry Communication, 2009, 12, 969-971.	3.9	13
763	Tin Alkylarsonate Clusters: Câˆ'HÂ·Â·Â·X (X = Cl, O, and Ï€) Interaction-Mediated Supramolecular Formation. Crystal Growth and Design, 2009, 9, 3881-3888.	3.0	13
764	Triphenylamine-based pH chemosensor: Synthesis, crystal structure, photophysical properties and computational studies. Synthetic Metals, 2009, 159, 2497-2501.	3.9	13
765	DFT study on the secondâ€order nonlinear optical property of 12â€vertex closoâ€carborane derivatives. International Journal of Quantum Chemistry, 2011, 111, 1039-1047.	2.0	13
766	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
767	Theoretical investigation on the 2e/12c bond and second hyperpolarizability of azaphenalenyl radical dimers: Strength and effect of dimerization. Journal of Chemical Physics, 2013, 139, 124314.	3.0	13
768	Ag(<scp>i</scp>)-mediated formation of a 2D cyano-bridged multinuclear silver(<scp>i</scp>) alkynyl network coupled with the Câ€“C bond cleavage of acetonitrile. CrystEngComm, 2014, 16, 10376-10379.	2.6	13
769	Assembly of Large Purely Inorganic Ceâ€Stabilized/Bridged Selenotungstates: From Nanoclusters to Layers. Chemistry - an Asian Journal, 2015, 10, 1184-1191.	3.3	13
770	The effect of ring sizes and alkali metal cations on interaction energy, charge transfer and nonlinear optical properties of crown ether derivatives. RSC Advances, 2015, 5, 30107-30119.	3.6	13
771	Theoretical study on the charge transfer mechanism at donor/acceptor interface: Why TTF/TCNQ is inadaptable to photovoltaics?. Journal of Chemical Physics, 2016, 145, 244705.	3.0	13
772	A noncovalently connected metalâ€“organic framework assembled from a Ni(<scp>iii</scp>)-supported polyoxometalateâ€“imidazolate hybrid. CrystEngComm, 2017, 19, 1721-1724.	2.6	13
773	Low-cost p-type dye-sensitized solar cells based on Dawson-type transition metal-substituted polyoxometalate inorganic co-sensitizers. Inorganic Chemistry Frontiers, 2017, 4, 1187-1191.	6.0	13
774	Boron/nitrogen substituted the staggered hetero-dimers: Fascinating intermolecular charge-transfer and large NLO responses. Dyes and Pigments, 2017, 145, 21-28.	3.7	13

#	Article	IF	Citations
775	Superatoms-Induced Effects of Phenalenyl Ï€-Dimer on NICS and NLO Properties: Not Always Enhancement. Journal of Physical Chemistry C, 2017, 121, 20419-20425.	3.1	13
776	From blue to full color â€“ theoretical design and characterization of a series of Ir(<scp>iii</scp>) complexes containing azoline ligand with potential application in OLEDs. Dalton Transactions, 2017, 46, 11491-11502.	3.3	13
777	Two polyoxovanadate-based metalâ€“organic polyhedra with undiscovered â€œnear-miss Johnson solidâ€• geometry. Chemical Communications, 2019, 55, 10701-10704.	4.1	13
778	Evidence of two-state reactivity in water oxidation catalyzed by polyoxometalate-based complex [Mn3(H2O)3(SbW9O33)2]12â^'. Journal of Catalysis, 2019, 376, 146-149.	6.2	13
779	Theoretical insights on the rigidified dithiophene effects on the performance of near-infrared cis-squaraine-based dye-sensitized solar cells with panchromatic absorption. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 369, 150-158.	3.9	13
780	Near-infrared-emitting AIE multinuclear cationic Ir(<scp>iii</scp>) complex-assembled nanoparticles for photodynamic therapy. Dalton Transactions, 2020, 49, 15332-15338.	3.3	13
781	A photo-activated process cascaded electrocatalysis for the highly efficient CO₂ reduction over a coreâ€“shell ZIF-8@Co/C. Journal of Materials Chemistry A, 2020, 8, 16616-16623.	10.3	13
782	Structural, Optical and Mechanical Properties and Cracking Factors of Large-Sized KBr:Ce3+ Single Crystal. Journal of Electronic Materials, 2020, 49, 4785-4793.	2.2	13
783	Blue-emitting thermoreversible oligourethane gelators with aggregation-induced emission properties. Journal of Materials Chemistry C, 2020, 8, 5137-5142.	5.5	13
784	An EPR-independent therapeutic strategy: Cancer cell-mediated dual-drug delivery depot for diagnostics and prevention of hepatocellular carcinoma metastasis. Biomaterials, 2021, 268, 120541.	11.4	13
785	PMO₁₂@ZIF-8/ZnO-derived hierarchical porous molybdenum carbide as efficient electrocatalysts for hydrogen evolution. New Journal of Chemistry, 2021, 45, 9456-9461.	2.8	13
786	The second-order nonlinear optical property of hydrazones-based photochromic complexes: A DFT study. Journal of Molecular Liquids, 2021, 327, 114882.	4.9	13
787	Metallic subnanometer porous silicon: A theoretical prediction. Physical Review B, 2021, 103, .	3.2	13
788	A novel cobalt-anchored covalent organic framework for photocatalytic conversion of CO₂ into widely adjustable syngas. Journal of Materials Chemistry A, 2022, 10, 13418-13427.	10.3	13
789	Theoretical studies on the one- and two-photon absorption of symmetrical stilbene derivatives. Computational and Theoretical Chemistry, 2000, 531, 169-174.	1.5	12
790	Electronic properties of Strandberg anions: A DFT study of [X2Mo5O23]nâ^', (X = PV, SVI, AsV, SeVI), and [(RP)2Mo5O21]4â^' (R = H, CH3, C2H5). International Journal of Quantum Chemistry, 2005, 105, 37-42.	2.0	12
791	A Series of New Organotinâ^'Cyanometalate Compounds Based on Triorganotin, Diorganotin, and Organooxotin Clusters. Organometallics, 2006, 25, 5996-6006.	2.3	12
792	ITO electrode modified by self-assembling multilayer film of polyoxometallate on poly(vinyl alcohol) nanofibers and its electrocatalytic behavior. Electrochimica Acta, 2007, 53, 569-574.	5.2	12

#	Article	IF	Citations
793	Interpenetrating metal-organic frameworks formed by self-assembly of tetrahedral and octahedral building blocks. Journal of Solid State Chemistry, 2009, 182, 3105-3112.	2.9	12
794	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.	1.4	12
795	A theoretical study on the efficient reversible redox-based switching of the second-order polarizabilities of two-dimensional nonlinear optical-active donorâ€“acceptor phenanthroline-hexamolybdate. Journal of Molecular Graphics and Modelling, 2010, 29, 13-20.	2.4	12
796	Helical channels, low framework density and structure-directing effect: a novel non-centrosymmetric zinc phosphate NIS-4 prepared by ionothermal reaction. CrystEngComm, 2010, 12, 3448.	2.6	12
797	Theoretical Study of Isomerism/Phase Dependent Charge Transport Properties in Tris(8-hydroxyquinolinato)aluminum(III). Journal of Physical Chemistry A, 2011, 115, 9259-9264.	2.5	12
798	Quantum chemical studies of Lindqvist-type polyoxometalates containing late 3d transition metals ([(py)MIIW5O18]4â¯ (MÂ=ÂFe, Co, Ni)): MIIâ€“N bonding and second-order nonlinear optical properties. Theoretical Chemistry Accounts, 2011, 130, 1043-1053.	1.4	12
799	Structures and fluorescence properties of two novel metal-organic frameworks based on the bis(2-benzimidazole) and aromatic carboxylate ligands. Inorganic Chemistry Communication, 2011, 14, 1077-1081.	3.9	12
800	A new luminescent 3-D metal-organic framework of diamond-like network possessing 8-fold interpenetration. Journal of Coordination Chemistry, 2011, 64, 1578-1585.	2.2	12
801	Improving the Accuracy of Density Functional Theory (DFT) Calculation for Homolysis Bond Dissociation Energies of Y-NO Bond: Generalized Regression Neural Network Based on Grey Relational Analysis and Principal Component Analysis. International Journal of Molecular Sciences, 2011, 12, 2242-2261.	4.1	12
802	The structureâ€“property relationship of chiral 1,1â€²-binaphthyl-based polyoxometalates: TDDFT studies on the static first hyperpolarizabilities and the ECD spectra. Journal of Molecular Graphics and Modelling, 2012, 32, 1-8.	2.4	12
803	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
804	TDDFT Studies on the Determination of the Absolute Configurations and Chiroptical Properties of Strandberg-Type Polyoxometalates. Journal of Physical Chemistry A, 2013, 117, 2492-2498.	2.5	12
805	SnO₂@Nâ€Doped Carbon Hollow Nanoclusters for Advanced Lithiumâ€Ion Battery Anodes. European Journal of Inorganic Chemistry, 2016, 2016, 812-817.	2.0	12
806	Trimeric hexa-dimethyltin-functionalized selenotungstate [{Sn(CH₃)₂(CH₃COO)}₃{Sn(CH₃)₂₃<sub>{Se<s CrystEngComm, 2016, 18, 2820-2824.	2.6	12
807	Phenalenyl Ï€-Dimer under the External Electric Field: Two-Electron/12-Center Bonding Breaking and Emergence of Electrostatic Interaction. Journal of Physical Chemistry C, 2017, 121, 3765-3770.	3.1	12
808	Electrochemical and diffuse reflectance study on tetrahedral Îµ-Keggin-based metalâ€“organic frameworks. RSC Advances, 2017, 7, 31544-31548.	3.6	12
809	Conductive metal adatoms adsorbed on graphene nanoribbons: a first-principles study of electronic structures, magnetization and transport properties. Journal of Materials Chemistry C, 2017, 5, 4053-4062.	5.5	12
810	Two nanoscale Nb containing polyoxometalates based on {P₂W₁₅Nb₃O₆₂} clusters and chromium cations. Dalton Transactions, 2017, 46, 13345-13348.	3.3	12

#	Article	IF	Citations
811	A theoretical exploration of the effect of fluorine and cyano substitutions in diketopyrrolopyrrole-based polymer donor for organic solar cells. Journal of Molecular Graphics and Modelling, 2017, 77, 9-16.	2.4	12
812	Redox-switchable structures and NLO property: Li2 doped into the cavity of pyridine helix. Organic Electronics, 2018, 57, 68-73.	2.6	12
813	An ultra-stable porous coordination polymer for water-mediated proton conduction. Inorganic Chemistry Communication, 2018, 96, 153-158.	3.9	12
814	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
815	Molecular Engineering of Phenylbenzimidazole-Based Orange Ir(III) Phosphors toward High-Performance White OLEDs. Inorganic Chemistry, 2018, 57, 6029-6037.	4.0	12
816	Self-assembly and Li-ion storage performance of three new Nb/W mixed-addendum polyoxometalates based on the {SiNb3W9O40} clusters and transition-metal cations. CrystEngComm, 2019, 21, 1862-1866.	2.6	12
817	Tricopper-polyoxometalate catalysts for water oxidation: Redox-inertness of copper center. Journal of Catalysis, 2020, 381, 402-407.	6.2	12
818	Investigation of the Structural and Luminescent Properties and the Chromium Ion Valence of Li2CaGeO4 Crystals Doped with Cr4+ Ions. Crystals, 2020, 10, 1019.	2.2	12
819	Can we utilize the higher Frenkel exciton state in biazulene diimides-based non-fullerene acceptors to promote charge separation at the donor/acceptor interface?. New Journal of Chemistry, 2020, 44, 9767-9774.	2.8	12
820	A ruthenium/polyoxometalate for efficient CO₂ photoreduction under visible light in diluted CO₂. Nanotechnology, 2020, 31, 255402.	2.6	12
821	Reduced graphene oxide/TiO₂(B) nanocomposite-modified separator as an efficient inhibitor of polysulfide shuttling in Liâ€“S batteries. RSC Advances, 2020, 10, 4538-4544.	3.6	12
822	Self-assembly and lithium storage performance of a nanoscale polyoxometalate based on the {MnTa18} cluster. Chemical Communications, 2020, 56, 2403-2406.	4.1	12
823	Synthesis, crystal structure and iodine capture of Zr-based metal-organic polyhedron. Inorganica Chimica Acta, 2021, 516, 120174.	2.4	12
824	Transition-Metal-Modified Vanadoborate Clusters as Stable and Efficient Photocatalysts for CO₂ Reduction. Inorganic Chemistry, 2021, 60, 7364-7371.	4.0	12
825	Two-dimensional graphdiyne analogue containing Mo-coordinated porphyrin covalent organic framework as a high-performance electrocatalyst for nitrogen fixation. Applied Surface Science, 2022, 580, 152359.	6.1	12
826	Copper-Based Metalâ€“Organic Framework with a Tetraphenylethylene-Tetrazole Linker for Visible-Light-Driven CO₂ Photoconversion. Inorganic Chemistry, 2022, 61, 5869-5877.	4.0	12
827	Lanthanide metalâ”organic frameworks based on planar Ï€-conjugated ligands for white light emission, temperature and chemical sensing. Dyes and Pigments, 2022, 202, 110256.	3.7	12
828	Molecular engineering to achieve AIE-active photosensitizers with NIR emission and rapid ROS generation efficiency. Journal of Materials Chemistry B, 2022, 10, 5272-5278.	5.8	12

#	Article	IF	Citations
829	Photoelectric properties of material of N,Nâ€²-bis(4â€²-aminophenyl)-1,4-quinonediimine doped with heteropolyacid. Synthetic Metals, 2002, 129, 15-18.	3.9	11
830	A facile method to produce highly monodispersed nanospheres of cystine aggregates. Nanotechnology, 2006, 17, 5163-5166.	2.6	11
831	Theoretical investigation of electronic structures and excitation energies of doubly N-confused porphyrin and its group 11 transition metal (III) complexes. Journal of Chemical Physics, 2007, 126, 245106.	3.0	11
832	Electronic structures and spectra of porphyrin with fused benzoheterocycles: DFT and TDDFT-PCM investigations. International Journal of Quantum Chemistry, 2007, 107, 1614-1623.	2.0	11
833	Incorporation of Znq2 complexes into mesoporous silica and their transparent polymer luminescent nanocomposites. Journal of Solid State Chemistry, 2009, 182, 1430-1437.	2.9	11
834	Effect of dehydrogenation/hydrogenation on the linear and nonlinear optical properties of Li@porphyrins. Journal of Molecular Modeling, 2012, 18, 4901-4907.	1.8	11
835	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
836	DFT study of ionic peapod structures from single-walled carbon nanotubes and Lindqvist tungstates. Dalton Transactions, 2012, 41, 2798.	3.3	11
837	Density functional studies on photophysical properties and chemical reactivities of the triarylboranes: effect of the constraint of planarity. Journal of Molecular Modeling, 2013, 19, 3437-3446.	1.8	11
838	A novel organicâ€“inorganic hybrid constructed from the Nyman-type dititanoniobate [Ti2Nb8O28]8â^' and copperâ€“organic cations. Dalton Transactions, 2014, 43, 9847.	3.3	11
839	One lithium atom binding with P-nitroaniline: lithium salts or lithium electrides?. Journal of Molecular Modeling, 2015, 21, 23.	1.8	11
840	Ammonia borane in an external electric field: structure, charge transfer, and chemical bonding. RSC Advances, 2015, 5, 65991-65997.	3.6	11
841	Syntheses, structures, luminescent and photocatalytic properties of two Zn(II) coordination polymers assembled with mixed bridging N-donors and 2-(4-carboxyphenyl)-4,5-imidazole dicarboxylic acid ligand. Journal of Molecular Structure, 2017, 1134, 504-510.	3.6	11
842	An unprecedented 3D architecture based on a Nb/W mixed-addendum polyoxometalate and lanthanideâ€“organic complex: synthesis, crystal structure and properties. New Journal of Chemistry, 2017, 41, 10532-10536.	2.8	11
843	Synergistic Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Cyanoesterification: Effect of Lewis Acid. Organometallics, 2017, 36, 4713-4720.	2.3	11
844	Theoretical insights into the catalytic mechanism for the oxygen reduction reaction on M₃(hexaiminotriphenylene)₂ (M = Ni, Cu). Physical Chemistry Chemical Physics, 2018, 20, 1821-1828.	2.8	11
845	The regulation of hydroboration of olefins by oriented external electric field. New Journal of Chemistry, 2018, 42, 18402-18408.	2.8	11
846	Theoretical Insight into the Performance of Mn^{II/III}-Monosubstituted Heteropolytungstates as Water Oxidation Catalysts. Inorganic Chemistry, 2019, 58, 15751-15757.	4.0	11

#	Article	IF	Citations
847	Syntheses and magnetic properties of high-dimensional cucurbit[6]uril-based metalâ€“organic rotaxane frameworks. Dalton Transactions, 2019, 48, 9939-9943.	3.3	11
848	A probe into underlying factors affecting utrafast charge transfer at Donor/IDIC interface of all-small-molecule nonfullerene organic solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 375, 1-8.	3.9	11
849	Allâ€Metallic Zn=Zn Doubleâ€Ï€ Bonded Octahedral Zn 2 M 4 (M=Li, Na) Clusters with Negative Oxidation State of Zinc. ChemPhysChem, 2020, 21, 459-463.	2.1	11
850	A theoretical investigation on promising acceptor groups for POM-based dyes: from electronic structure to photovoltaic conversion efficiency. Journal of Materials Chemistry C, 2020, 8, 219-227.	5.5	11
851	Optical and mechanical properties of NaCl: Ce3+ crystal grown by the Czochralski method. Journal of Materials Science: Materials in Electronics, 2020, 31, 13070-13077.	2.2	11
852	Hydrogen Migration-Triggered Diradicaloid Singlet-Fission Switch. Journal of the American Chemical Society, 2020, 142, 11791-11803.	13.7	11
853	Ferroelectric Metalâ€“Organic Framework as a Host Material for Sulfur to Alleviate the Shuttle Effect of Lithiumâ€“Sulfur Battery. Chemistry - A European Journal, 2020, 26, 13779-13782.	3.3	11
854	Understanding Mechanochromic Luminescence on Account of Molecular Level Based on Phosphorescent Iridium(III) Complex Isomers. Inorganic Chemistry, 2021, 60, 3741-3748.	4.0	11
855	Radical Mechanism of Ir III /Ni II -Metallaphotoredox-Catalyzed C(sp 3)â€“H Functionalization Triggered by Proton-Coupled Electron Transfer: Theoretical Insight. CCS Chemistry, 0, , 1456-1467.	7.8	11
856	Effective CO Migration among Multiabsorbed Sites Achieves the Low-Barrier and High-Selective Conversion to C2 Products on the Ni₂B₅ Monolayer. ACS Applied Materials & Interfaces, 2021, 13, 3845-3855.	8.0	11
857	Ammonium polyphosphate induced bimetallic phosphides nanoparticles coated with porous N-doped carbon for efficiently electrochemical hydrogen evolution. Chemical Engineering Journal, 2022, 431, 133696.	12.7	11
858	Theoretical search of a simple characteristic for long-lived organic room-temperature phosphorescence materials with H aggregation. Journal of Materials Chemistry C, 2022, 10, 5425-5432.	5.5	11
859	Ag Nanoparticle-Modified Polyoxometalate-Based Metalâ€“Organic Framework for Enhanced CO₂ Photoreduction. Inorganic Chemistry, 2022, 61, 11359-11365.	4.0	11
860	Syntheses and Structure of a Novel Layered Lanthanideâ€“Zinc Coordination Polymer: [LaZn(HIDA)(IDA)2Â·0.5H2O]n. Chemistry Letters, 2004, 33, 446-447.	1.3	10
861	Absolute Configuration Determination of a New Chiral Rigid Bisetherketone Macrocycle Containing Binaphthyl and Thioether Moieties by Vibrational Circular Dichroism. Macromolecular Chemistry and Physics, 2005, 206, 1140-1145.	2.2	10
862	A novel cadmium(II) coordination polymer with biphenyl-3,3â€²,4,4â€²-tetracarboxylic acid and 4,4â€²-bipyridine. Acta Crystallographica Section C: Crystal Structure Communications, 2005, 61, m469-m471.	0.4	10
863	Time-dependent density functional theory study on electronic and spectroscopic properties for Ph2Bq and its complexes. Theoretical Chemistry Accounts, 2006, 117, 1-5.	1.4	10
864	Five supramolecular compounds of water-soluble sulfonylcalix[4]arenetetrasulfonate showing two calixarene conformations. CrystEngComm, 2009, 11, 597-604.	2.6	10

#	Article	IF	Citations
865	High luminescence, organicâ€“inorganic nanocomposite films with covalently linked 8-hydroxyquinoline anchored to ZnS nanoparticles. Dyes and Pigments, 2010, 85, 66-72.	3.7	10
866	MnIIIâ€“Salen composite materials based on Keggin heteropolyanions exhibiting photocatalytic and electrocatalytic activities. Inorganic Chemistry Communication, 2011, 14, 1418-1421.	3.9	10
867	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
868	Effects of size and surface modification of multi-walled carbon nanotubes on mechanical properties of polyurethane-based nanocomposites. Journal Wuhan University of Technology, Materials Science Edition, 2012, 27, 608-614.	1.0	10
869	Effect of metal ions on the structures of metalâ€“organic frameworks based on mixed ligands. Inorganic Chemistry Communication, 2012, 15, 288-291.	3.9	10
870	A series of coordination complexes based on unsymmetrical multicarboxylate ligands: syntheses, structures and properties. CrystEngComm, 2013, 15, 6769.	2.6	10
871	Quantum chemical characterization and design of host materials based on phosphine oxide-substituted (triphenylamine) fluorene for (deep) blue phosphors in OLEDs. Physical Chemistry Chemical Physics, 2013, 15, 2351.	2.8	10
872	Influence of Spiral Framework on Nonlinear Optical Materials. ChemPhysChem, 2014, 15, 929-934.	2.1	10
873	Mechanism and kinetic study of 3-fluoropropene with hydroxyl radical reaction. Journal of Molecular Graphics and Modelling, 2014, 48, 18-27.	2.4	10
874	The V-shaped polar molecules encapsulated into C_s (10528)-C₇₂: stability and nonlinear optical response. Dalton Transactions, 2014, 43, 9655-9660.	3.3	10
875	The research of employing polyoxometalates as pure-inorganic electron-transfer mediators on dye-sensitized solar cells. Inorganic Chemistry Communication, 2014, 46, 89-93.	3.9	10
876	Coordination and supramolecular assembly of {Cd₂Ge₈V₁₂O₄₈} building block and cucurbit[6] to form rotaxane-shaped hybrids. Dalton Transactions, 2016, 45, 4989-4992.	3.3	10
877	Controllable synthesis of isoreticular pillared-layer MOFs based on N-rich triangular prism building units: gas adsorption and luminescent properties. New Journal of Chemistry, 2018, 42, 20056-20060.	2.8	10
878	Hierarchical and Highly Stable Conductive Network Cathode for Ultraflexible Liâ€“S Batteries. ACS Applied Energy Materials, 2018, 1, 2689-2697.	5.1	10
879	A remarkable phosphorescent sensor for acidâ€“base vapours based on an AIPE-active Ir(<scp>iii</scp>) complex. Dalton Transactions, 2019, 48, 1955-1959.	3.3	10
880	A triazine-functionalized nanoporous metalâ€“organic framework for the selective adsorption and chromatographic separation of transition metal ions and cationic dyes and white-light emission by Ln³⁺ ion encapsulation. Journal of Materials Chemistry C, 2019, 7, 8861-8867.	5.5	10
881	Terminal Modulation in Search of a Balance between Hole Transport and Electron Transfer at the Interface for BODIPY-Based Organic Solar Cells. Journal of Physical Chemistry C, 2019, 123, 6407-6415.	3.1	10
882	A theoretical mechanistic study of Ir^{III}/Cu^I-metallaphotoredox catalyzed asymmetric radical decarboxylative cyanation. Dalton Transactions, 2020, 49, 15276-15286.	3.3	10

#	Article	IF	Citations
883	Luminescent metalâ€“organic frameworks encapsulating polycyclic aromatic hydrocarbons for energy transfer. Dalton Transactions, 2020, 49, 5087-5091.	3.3	10
884	N-(O-methoxyphenyl)aza-15-crown-5-ether derivatives: Highly efficient and wide range nonlinear optical response based cation recognition. Journal of Molecular Liquids, 2020, 301, 112492.	4.9	10
885	Tuning Second-Order Nonlinear Optical Properties of Cross-Linked Carbon Nanotube via External Electric Field. Journal of Physical Chemistry C, 2020, 124, 3778-3783.	3.1	10
886	Synthesis of novel tetrazol-pyridine based cationic Ir(III) complexes with efficient AIE characteristic and significant mechanochromic luminescence behavior. Dyes and Pigments, 2021, 184, 108817.	3.7	10
887	Self-Assembled Polyoxometalate-Based Metal-Organic Polyhedra as an Effective Heterogeneous Catalyst for Oxidation of Sulfide. Crystal Growth and Design, 2021, 21, 1028-1034.	3.0	10
888	Role of Terminal Positions of Aryl Ring Towards Second-Order Nonlinearity in Arylimido-Substituted Molybdates: An Interesting Quantum Study of Organic-Inorganic Hybrid Composites. Current Physical Chemistry, 2011, 1, 99-105.	0.2	10
889	Origin and Regioselectivity of Direct Hydrogen Atom Transfer Mechanism of C(sp3)â€“H Arylation by [W10O32]4â€“/Ni Metallaphotoredox Catalysis. Inorganic Chemistry, 2021, , .	4.0	10
890	The second-order NLO and TADF properties of a donorâ€“acceptor dihydropyreneâ€“cyclophanediene system: the impact of molecular architecture and polarizable environment. Journal of Materials Chemistry C, 2022, 10, 886-898.	5.5	10
891	Three Cd-MOFs with water stability act as novel fluorescent probes for detecting nitrofuran, nitrofurantoin and Fe3+. Journal of Solid State Chemistry, 2022, 313, 123170.	2.9	10
892	Effective Hamiltonians of polymethineimine, polyazine and polyazoethene: A density matrix variation approach. Journal of Chemical Physics, 1998, 109, 2565-2571.	3.0	9
893	Synthesis, Crystal Structure and Spectroscopic Studies of a Supramolecular Compound [Cu(IDA)(phen)(H2O)]Â·4H2O Built from Ââ€“Â Interactions and Hydrogen Bonds. Transition Metal Chemistry, 2004, 29, 471-476.	1.4	9
894	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.	1.8	9
895	Two novel supramolecular isomers based on 2,2â€²-biimidazole derivative and zinc ions: Syntheses, structures and luminescent properties. Inorganic Chemistry Communication, 2009, 12, 169-172.	3.9	9
896	Synthesis, structure and properties of one 2-D Ag(I) complex based on trinuclear silver(I) cluster and arene-linked bis(pyrazolyl)methane ligand. Inorganic Chemistry Communication, 2011, 14, 347-350.	3.9	9
897	Probing the Chemical Functionalization of Singleâ€Walled Carbon Nanotubes with Multiple Carbon Adâ€Dimer Defects. ChemPhysChem, 2012, 13, 1232-1239.	2.1	9
898	Enhanced quantum efficiency of cationic iridium(III) complexes with carbazole moiety as a steric hindrance unit. Journal of Molecular Structure, 2012, 1026, 59-64.	3.6	9
899	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
900	Carbonyl Amine/Schiff Base Ligands in Manganese Complexes: Theoretical Study on the Mechanism, Capability of NO Release. Inorganic Chemistry, 2012, 51, 3972-3980.	4.0	9

#	Article	IF	Citations
901	Potential of bifluorenylidene derivatives as nonfullerene small-molecule acceptor for heterojunction organic photovoltaics: a density functional theory study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
902	The influence of molecular solid packings on the photoluminescence and carrier transport properties for two bow-shaped thiophene compounds: a theoretical study. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	9
903	Design and construction of porous metalâ€“organic frameworks based on flexible BPH pillars. Journal of Solid State Chemistry, 2013, 198, 143-148.	2.9	9
904	Theoretical exploration to the substituting effect on second-order nonlinear optical properties for lacunary Î³-Keggin polyoxometalates. Chemical Physics Letters, 2013, 557, 123-128.	2.6	9
905	Theoretical study on the transport properties of oligothiopheneâ€“diketopyrrolopyrrole derivatives: quinoidal versus aromatic. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	9
906	Charge transfer and first hyperpolarizability: cage-like radicals C59X and lithium encapsulated Li@C59X (X=B, N). Journal of Molecular Modeling, 2015, 21, 258.	1.8	9
907	The transport properties of silicon and carbon nanotubes at the atomic scale: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 23643-23650.	2.8	9
908	Structure and Frontier Molecular Orbital (FMO) energies of Î±-Keggin-type polyoxometalate [PW12O40]3â^': A systematical study with different functionals of density functional theory. Computational and Theoretical Chemistry, 2016, 1089, 28-34.	2.5	9
909	Theoretical design and study on hexamolybdate-based organic-inorganic hybrids with double D-Ï€-A chains for high performance p-type dye-sensitized solar cells (DSSCs). Dyes and Pigments, 2017, 137, 372-377.	3.7	9
910	Spectroscopic behavior, FMO, NLO and substitution effect of 2-(1H-Benzo[d]imidazole-2-ylthio)-N-o-substituted-acetamides: Experimental and theoretical approach. Dyes and Pigments, 2019, 171, 107742.	3.7	9
911	Cationic dinuclear Ir(III) complexes based on acylhydrazine ligands: Reversible piezochromic luminescence and AIE behaviours. Dyes and Pigments, 2020, 172, 107855.	3.7	9
912	Two Ni/Co-substituted sandwich-type germanomolybdates based on an unprecedented trivacant polyanion [Î±-GeMo₁₀O₃₆]^{8â^'}. Dalton Transactions, 2020, 49, 977-982.	3.3	9
913	Octamolybdate-based hybrid constructed by flexible bis-triazole ligands: synthesis, photocatalytic and electrochemical properties. New Journal of Chemistry, 2020, 44, 13524-13528.	2.8	9
914	Hollow Porous MnFe₂O₄ Sphere Grown on Elmâ€Moneyâ€Derived Biochar towards Energyâ€Saving Full Water Electrolysis. Chemistry - A European Journal, 2020, 26, 14397-14404.	3.3	9
915	Syntheses of cucurbit[6]uril-based metalâ€“organic rotaxane networks by the anion regulation strategy and their proton conduction properties. Dalton Transactions, 2020, 49, 1747-1751.	3.3	9
916	Promoting visible-light-driven hydrogen production of a zirconium-based metal-organic polyhedron decorated by platinum nanoparticles with different spatial locations. Catalysis Communications, 2020, 137, 105930.	3.3	9
917	A luminescent metalâ€“organic framework with mixed-linker strategy for white-light-emitting by iridium-complex encapsulation. Inorganic Chemistry Communication, 2021, 123, 108359.	3.9	9
918	Er, Yb:CeF3 red emission nanoparticles with controllable size and enhanced luminescence properties. Journal of Materials Science: Materials in Electronics, 2021, 32, 8213-8225.	2.2	9

#	Article	IF	Citations
919	Hourglass-Type Polyoxometalate-Based Crystalline Material as an Efficient Proton-Conducting Solid Electrolyte. Inorganic Chemistry, 2021, 60, 18912-18917.	4.0	9
920	Dynamic Interface with Enhanced Visible-Light Absorption and Electron Transfer for Direct Photoreduction of Flue Gas to Syngas. ACS Applied Materials & Interfaces, 2022, 14, 6476-6483.	8.0	9
921	Efficient cobalt-based metal-organic framework derived magnetic Co@C-600 Nanoreactor for peroxymonosulfate activation and oxytetracycline degradation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 648, 129234.	4.7	9
922	Encapsulation of AIEgens within Metalâ€“Organic Framework toward Highâ€Performance White Lightâ€Emitting Diodes. Advanced Optical Materials, 2022, 10, .	7.3	9
923	Electronic property and molecule design for luminescent metal complexes of tris(8-hydroxyquinoline) gallium. Science in China Series B: Chemistry, 2000, 43, 657-669.	0.8	8
924	Controlled cutting carbon nanotube with polyoxometalates assisted renewable method. Materials Letters, 2006, 60, 2266-2269.	2.6	8
925	Theoretical Studies on Electronic Spectra and Second-order Nonlinear Optical Properties of Glucosyl Substituted Barbituric Acid Derivatives. Chinese Journal of Chemistry, 2006, 24, 119-123.	4.9	8
926	THEORETICAL STUDY ON ENDOHEDRAL COMPLEXES C₂H₂â€“C₆₀, C₂H₄â€“C₆₀, AND C₂H₆â€“C₆₀. Journal of Theoretical and Computational Chemistry, 2008, 07, 1-11.	1.8	8
927	The comparative investigation on redox property and second-order nonlinear response of Keggin-type Î±-[PM12O39NPh]3â¯ (M = W and Mo) and Mo6NPh. Science Bulletin, 2009, 54, 203-211.	9.0	8
928	Length-Dependent Direction-Tunable Charge-Transfer Behavior of Second-Order Optical Nonlinearity in Keggin-Type Organosilicone Derivative [PW11O39(RSi)2O]3â¯: A TDDFT Study. Journal of Cluster Science, 2010, 21, 69-80.	3.3	8
929	A novel 3-connected [3 + 3] topological net showing both rotaxane- and catenane-like motifs. CrystEngComm, 2011, 13, 4945.	2.6	8
930	Three-dimensional porous metalâ€“organic replica of natural mineral Î±-Al2O3 based on hexadentate triazine derivative. Inorganic Chemistry Communication, 2011, 14, 893-896.	3.9	8
931	Comparative study of the electrostatic potential of perfect and defective single-walled carbon nanotubes. Computational and Theoretical Chemistry, 2011, 966, 1-8.	2.5	8
932	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
933	Influence of the central atom on the electronic properties of Lindqvist polyoxometalates. Computational and Theoretical Chemistry, 2012, 988, 1-5.	2.5	8
934	First principle investigation of transport properties of Lindqvist derivatives based molecular junction. Journal of Molecular Graphics and Modelling, 2012, 38, 220-225.	2.4	8
935	Theoretical studies on phosphoraniminato derivatives of Keggin-type polyoxometalates [PW11O39{MVNPPh3}]3â¯ (M = Fe, Ru): Electronic structures and bonding features. Science China Chemistry, 2012, 55, 1910-1915.	8.2	8
936	Red- and white-emitting organic light-emitting diodes based on trimetallic dendritic europium (III) complex: Eu3(DBM)9(TMMB). Solid-State Electronics, 2012, 69, 67-71.	1.4	8

#	Article	IF	Citations
937	The symmetric and asymmetric thiophene-fused benzocarborane: structures and first hyperpolarizabilities. Journal of Molecular Modeling, 2013, 19, 3741-3747.	1.8	8
938	Theoretical investigation of second-order nonlinear optical response by linking hexamolybdate with graphene in the donorâ€“acceptor (Dâ€“A) framework. Molecular Simulation, 2013, 39, 214-219.	2.0	8
939	Synthesis, structure, and photoluminescent property of a trinuclear CdII complex based on semi-rigid bis(imidazole-4,5-dicarboxylate) ligand. Inorganic Chemistry Communication, 2014, 42, 15-19.	3.9	8
940	Superalkali atoms bonding to the phenalenyl radical: structures, intermolecular interaction and nonlinear optical properties. Journal of Molecular Modeling, 2015, 21, 209.	1.8	8
941	Rational synthesis, structural characterization and theoretical exploration on third-order nonlinear optical properties of isolated Ag (nÂ=Â5, 8, 12) alkynyl clusters. Dyes and Pigments, 2015, 113, 299-306.	3.7	8
942	1,4-Azaborine as a controller of triplet energy, exciton distribution, and aromaticity in [6]cycloparaphenylenes. Journal of Materials Chemistry C, 2017, 5, 9088-9097.	5.5	8
943	Theoretical study on the optical response behavior to hydrogen chloride gas of a series of Schiff-base-based star-shaped structures. Journal of Molecular Modeling, 2018, 24, 58.	1.8	8
944	Metalâ€“oxygen clusters as peroxidase mimics for their multifarious applications in colorimetric sensors. New Journal of Chemistry, 2019, 43, 13430-13436.	2.8	8
945	Engineering of Yin Yang-like nanocarriers for varisized guest delivery and synergistic eradication of patient-derived hepatocellular carcinoma. Nanoscale Horizons, 2019, 4, 1046-1055.	8.0	8
946	A substrate-free Mo₂C-based electrocatalyst by facile glucose-blowing for efficient hydrogen production. New Journal of Chemistry, 2019, 43, 18970-18974.	2.8	8
947	A BPt4S4 cluster: a planar tetracoordinate boron system with three charges all at their global energy minima. New Journal of Chemistry, 2020, 44, 767-772.	2.8	8
948	High-Performance and Stable Warm White OLEDs Based on Orange Iridium(III) Phosphors Modified with Simple Alkyl Groups. Organometallics, 2020, 39, 3384-3393.	2.3	8
949	Robust Electrodes for Flexible Energy Storage Devices Based on Bimetallic Encapsulated Coreâ€“Multishell Structures. Advanced Science, 2021, 8, e2100911.	11.2	8
950	Co/WC@NC electrocatalysts derived from polyoxometalates (POM) for efficient hydrogen evolution. Nanotechnology, 2021, 32, 375602.	2.6	8
951	Boosting ultralong organic phosphorescence performance by synergistic heavy-atom effect and multiple intermolecular interactions in molecular crystal. Journal of Materials Chemistry C, 2022, 10, 6334-6340.	5.5	8
952	Rational Design of Ir(III) Phosphors to Strategically Manage Charge Recombination for High-Performance White Organic Light-Emitting Diodes. Inorganic Chemistry, 2022, 61, 3736-3745.	4.0	8
953	A Poreâ€Forming Strategy Toward Porous Carbonâ€Based Substrates for High Performance Flexible Lithium Metal Full Batteries. Energy and Environmental Materials, 2023, 6, .	12.8	8
954	Construction of multi-hydroxyl/ketone lanthanide metalâ€“organic frameworks for understanding mechanochromic luminescence and high proton conductivity. Inorganic Chemistry Frontiers, 2022, 9, 4376-4384.	6.0	8

#	Article	IF	Citations
955	Bimetallic polyoxometalate derived Co/WN composite as electrocatalyst for high-efficiency hydrogen evolution. International Journal of Hydrogen Energy, 2022, 47, 27452-27459.	7.1	8
956	Poly[bis(4,4â€²-bipyridine)(Î¼3-4,4â€²-dicarboxybiphenyl-3,3â€²-dicarboxylato)cobalt(II)]. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, m2477-m2479.	0.2	7
957	Theoretical studies on one- and two-photon absorption properties of rubrene and its derivatives. Synthetic Metals, 2006, 156, 1218-1224.	3.9	7
958	Design and synthesis of 1,4-bis[4-(1,1-dicyanovinyl)styryl]-2,5-bis(alkoxy)benzenes as red organic electroluminescent PPV analogs. Polymer, 2007, 48, 4028-4033.	3.8	7
959	Structure and second-order NLO property of the molecules bridged through n-vertex bis-substituted carborane (n=5, 6, 7). Science Bulletin, 2007, 52, 2326-2330.	1.7	7
960	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
961	Generalized Fabrication of Surfactant-Stabilized Anisotropic Metal Nanoparticles to Amino-Functionalized Surfaces: Application to Surface-Enhanced Raman Spectroscopy. Journal of Nanoscience and Nanotechnology, 2008, 8, 5887-5895.	0.9	7
962	Theoretical investigation of electronic structures and excitation energies of hexaphyrin and its group 11 transition metal (III) complexes. Journal of Organometallic Chemistry, 2009, 694, 3012-3018.	1.8	7
963	A new (3,4,7)-connected topology framework based on [Cd2(CO2)3O4N2] second building unit. Inorganic Chemistry Communication, 2009, 12, 1024-1026.	3.9	7
964	Isophorone-based analogues with A-Ï€-D-Ï€-A structure for red organic light emitting devices. Synthetic Metals, 2009, 159, 401-405.	3.9	7
965	Auxiliary aromatic-acid effect on the structures of a series of ZnII coordination polymers: Syntheses, crystal structures, and photoluminescence properties. Journal of Solid State Chemistry, 2010, 183, 849-857.	2.9	7
966	A theoretical study of ambipolar organic transport material: 1,4-Bis(pentafluorobenzyl)[60]-fullerene. Chemical Physics Letters, 2011, 506, 255-259.	2.6	7
967	Building blocks and formation thermodynamics of Î±-Keggin-type [PW12O40]3â¯ anion. Computational and Theoretical Chemistry, 2012, 999, 66-73.	2.5	7
968	Synthesis, crystal structures, and luminescent properties of Cd(II) coordination polymers assembled from semi-rigid multi-dentate N-containing ligand. Journal of Solid State Chemistry, 2012, 196, 87-92.	2.9	7
969	Quantum chemical investigation on the structure and first hyperpolarizability for Nâ€substituted [n]cyclacene. Journal of Physical Organic Chemistry, 2012, 25, 176-180.	1.9	7
970	Synthesis and property investigation of two hexa-cobalt cluster based porous coordination polymers. CrystEngComm, 2013, 15, 7402.	2.6	7
971	Solvothermal synthesis and structural characterization of a Cd-triazole-benzenedicarboxylate framework. Inorganic Chemistry Communication, 2014, 40, 8-10.	3.9	7
972	Hydrothermal synthesis, crystal structure and properties of a 3D inorganicâ€“organic hybrid based on Keggin-type polyanion and silver-pyrazine circles. Inorganic Chemistry Communication, 2014, 47, 48-51.	3.9	7

#	Article	IF	Citations
973	Facile assembly of 1D multinuclear Ag_n(nÂ= 11, 11, 12) alkynyl chains with CF₃COO^{â^'}/CH₃COO^{â^'}as the auxiliary ligand. RSC Advances, 2014, 4, 60451-60459.	3.6	7
974	Redox and acidic properties of chalcogenido-substituted mixed-metal polyoxoanions: a DFT study of Î±-[PW₁₁O₃₉ME]^{4â^'} (M = Nb, Ta; E = O, S, Se). Inorganic Chemistry Frontiers, 2015, 2, 246-253.	6.0	7
975	Theoretical investigation of armchair silicene nanoribbons with application in stretchable electronics. Journal of Materials Chemistry C, 2015, 3, 10085-10090.	5.5	7
976	Quantum Chemical Insight into the LiF Interlayer Effects in Organic Electronics: Reactions between Al Atom and LiF Clusters. Journal of Physical Chemistry Letters, 2015, 6, 2950-2958.	4.6	7
977	Theoretical studies on tricarbonyl metal derivatives of Lindqvist-type polyoxometalate complexes: electronic structures and nonlinear optical properties. Inorganic Chemistry Frontiers, 2015, 2, 544-549.	6.0	7
978	Two-electron/24-center (2e/24c) bonding in novel diradical Ï€-dimers. Physical Chemistry Chemical Physics, 2016, 18, 29041-29044.	2.8	7
979	Low efficiency roll-off and high performance OLEDs employing alkyl group modified iridium(<scp>iii</scp>) complexes as emitters. RSC Advances, 2016, 6, 111556-111563.	3.6	7
980	Multifunctional Dicyandiamide Blowing-Induced Formation of Electrocatalysts for the Hydrogen Evolution Reaction. ACS Omega, 2019, 4, 10347-10353.	3.5	7
981	How do transition-metal-substituted POMs modify the photoanode of dye-sensitized solar cells? A DFT study. Inorganic Chemistry Frontiers, 2019, 6, 969-974.	6.0	7
982	Self-assembly of zirconocene-based metalâ€“organic capsules: the structure, luminescence sensing of Fe³⁺ and iodine capture. New Journal of Chemistry, 2020, 44, 21255-21260.	2.8	7
983	The Structure and Liquid Flow Effect of Melt during NaCl Crystal Growth. Crystal Research and Technology, 2020, 55, 1900229.	1.3	7
984	Structural Extension from 0D to 3D Pillared Heterometallic 3d-4f Polyoxometalate Hybrids. Crystal Growth and Design, 2020, 20, 2706-2712.	3.0	7
985	Computational Study of sp^x(x=1â€“3)â€Hybridized Beâ^'Be Bonds Stabilized by Amidinate Ligands. Chemistry - A European Journal, 2020, 26, 10891-10895.	3.3	7
986	Synthesis, characterization of mechanochromic luminescent-active mono-/dinuclear iridium(III) complexes with near-infrared emission. Journal of Organometallic Chemistry, 2021, 931, 121628.	1.8	7
987	Near-infrared (NIR-II) luminescence for the detection of cyclotetramethylene tetranitramine based on stable Nd-MOF. Journal of Solid State Chemistry, 2021, 294, 121789.	2.9	7
988	Closeâ€packed storage of potassium metallic clusters achieved through nanostructure engineering of ultrafine hollow nanoparticlesâ€based carbon nanoclusters. EcoMat, 2021, 3, e12105.	11.9	7
989	Cu/Cu_xSâ€Embedded N,Sâ€Doped Porous Carbon Derived in Situ from a MOF Designed for Efficient Catalysis. Chemistry - A European Journal, 2021, 27, 11468-11476.	3.3	7
990	Switching of second-order nonlinear response effected by different acceptors: The impacts of environment and frequency dispersion. Dyes and Pigments, 2021, 193, 109502.	3.7	7

#	Article	IF	Citations
991	Springboard Role for Iridium Photocatalyst: Theoretical Insight of C(sp³)â^'N Crossâ€Coupling by Photoredoxâ€Mediated Iridium/Copper Dual Catalysis versus Singleâ€Copper Catalysis. ChemCatChem, 2022, 14, .	3.7	7
992	A multifunctional anionic metalâ€“organic framework for high proton conductivity and photoreduction of CO₂ induced by cation exchange. Dalton Transactions, 2022, 51, 4798-4805.	3.3	7
993	Two-dimensional conductive Ï€-conjugated metal-organic frameworks as promising electrocatalysts for highly efficient hydrogen evolution reaction. Applied Surface Science, 2022, 601, 154241.	6.1	7
994	{Î¼-1,4-Bis[2-(2-pyridyl)imidazol-1-yl]butane}bis[dichlorocopper(II)]. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, m2586-m2587.	0.2	6
995	cis-Dichlorobis[2-(2-pyridyl)-1H-imidazole-ÎºN3]zinc(II) hemihydrate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, m3479-m3480.	0.2	6
996	Effect of water on zinc (II), cadmium (II) complexes with pyridylimidazole: Theoretical study of stability and electronic spectrum. International Journal of Quantum Chemistry, 2006, 106, 490-500.	2.0	6
997	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
998	Stabilities, electronic properties of exohedral fluorine and trifluoromethyl derivatives for T_d C₂₈ fullerene C₂₈F_{4â€“n}(CF₃)_n (n = 0,1,2,3,4). International Journal of Quantum Chemistry, 2008, 108, 1391-1399.	2.0	6
999	Soluble dendrimers europium(III) Î²-diketonate complex for organic memory devices. Thin Solid Films, 2008, 516, 3123-3127.	1.8	6
1000	Two new octamolybdate-based metalâ€“organic polymers: Structures, semiconducting and photoluminescent properties. Journal of Molecular Structure, 2009, 935, 69-74.	3.6	6
1001	Syntheses and characterizations of five coordination polymers constructed by 3,5-bis(pyridin-3-ylmethoxy)benzoic acid ligand. Polyhedron, 2009, 28, 3155-3161.	2.2	6
1002	Photophysical and charge-transport properties of hole-blocking material-TAZ: A theoretical study. Synthetic Metals, 2009, 159, 1767-1771.	3.9	6
1003	Fabrication of fluorescent mesoporous silica nanoparticles with confined 8-hydroxyquinoline functionalized ZnS nanoparticles and their transparent polymer nanocomposites. Microporous and Mesoporous Materials, 2010, 130, 122-129.	4.4	6
1004	Two new extended structures built from condensed Keggin-type polyoxotungstates and copper(II)-organic units. Solid State Sciences, 2010, 12, 128-133.	3.2	6
1005	Computational studies on the mechanism and kinetics of Cl reaction with C₂H₅I. Journal of Computational Chemistry, 2010, 31, 2263-2272.	3.3	6
1006	A peanut-like Keggin-type POM-incorporated metal-organic framework. Inorganic Chemistry Communication, 2010, 13, 1473-1475.	3.9	6
1007	The effect of multiple weak interactions on the charge transport ability in polymorphs. Synthetic Metals, 2011, 161, 1073-1078.	3.9	6
1008	One-pot synthesized polyurethane-based nanocomposites filled by original rectorite with enhanced strength and elongation. Journal Wuhan University of Technology, Materials Science Edition, 2011, 26, 483-490.	1.0	6

#	Article	IF	Citations
1009	Structure-dependent optical properties of single-walled silicon nanotubes. Physical Chemistry Chemical Physics, 2012, 14, 4695.	2.8	6
1010	TD-DFT studies on electronic and spectral properties of platinum(II) complexes with phenol and pyridine groups. Chemical Research in Chinese Universities, 2013, 29, 361-365.	2.6	6
1011	A DFT study on NLO response of push-pull hybrid porphyrin-polyoxometalate complexes. Russian Journal of Physical Chemistry A, 2014, 88, 970-977.	0.6	6
1012	Isomeric thiophene-fused benzocarborane moleculesâ€"different lithium doping effect on the nonlinear optical property. Dalton Transactions, 2014, 43, 2656-2660.	3.3	6
1013	Photosensitive polyoxometalate-induced formation of thermotropic liquid crystal nanomaterial and its photovoltaic effect. RSC Advances, 2015, 5, 8194-8198.	3.6	6
1014	A novel [4 + 3] interpenetrated net containing 7-fold interlocking pseudo-helical chains and exceptional catenane-like motifs. Dalton Transactions, 2015, 44, 2844-2851.	3.3	6
1015	The interaction between Boron-carbon-nitride heteronanotubes and lithium atoms: Role of composition proportion. Chemical Physics Letters, 2016, 658, 230-233.	2.6	6
1016	Theoretical studies on lindqvist polyoxometalates [M₆O19]ⁿ^{â^'}(MÂ=ÂMo, W, n=2; MÂ=ÂV, Nb, Ta, n=8) and derivatives: Electronic structures, stability and bonding. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750054.	1.8	6
1017	Dimethyltin-functionalized cyclic selenotungstates based on {Se₂W₁₂} units. Dalton Transactions, 2018, 47, 1393-1397.	3.3	6
1018	Steam-assisted assemblies of {Ni₆PW₉}-based inorganicâ€"organic hybrid chains: synthesis, crystal structures and properties. CrystEngComm, 2018, 20, 7507-7512.	2.6	6
1019	Constructing Stable Ï€â€Đimers: Two Parallel Pancake Ï€â€"Ï€ Bonds. Chemistry - A European Journal, 2018, 24, 16919-16924.	3.3	6
1020	Organometallic Ir(III) Phosphors Decorated by Carbazole/Diphenylphosphoryl Units for Efficient Solution-Processable OLEDs with Low Efficiency Roll-Offs. Inorganic Chemistry, 2019, 58, 13807-13814.	4.0	6
1021	Faceâ€Directed Assembly of Molecular Cubes: In Situ Substitution of a Predetermined Concave Cluster. Angewandte Chemie, 2020, 132, 22218-22222.	2.0	6
1022	Exploring Charge Dissociation in a Statistical Sample of Active-Layer Models of an Organic Solar Cell. Journal of Physical Chemistry C, 2020, 124, 18840-18846.	3.1	6
1023	Heteroatom-doped C₃N as a promising metal-free catalyst for a high-efficiency carbon dioxide reduction reaction. New Journal of Chemistry, 2020, 44, 11824-11828.	2.8	6
1024	Metal-free C₅N₂ doped with a boron atom as an efficient electrocatalyst for the nitrogen reduction reaction. New Journal of Chemistry, 2022, 46, 2282-2289.	2.8	6
1025	Polymers and polyoxometalate induced Co/WC@NC for electrocatalytic hydrogen production. Journal of Solid State Chemistry, 2022, 308, 122879.	2.9	6
1026	Face-Directed Construction of a Metalâ€"Organic Isohedral Tetrahedron for the Highly Efficient Capture of Environmentally Toxic Oxoanions and Iodine. Inorganic Chemistry, 2022, 61, 7103-7110.	4.0	6

#	Article	IF	Citations
1027	Theoretical studies of ground and excited electronic states of OLED material bis(2-methyl-8-quinolinolato)gallium(iii) chlorine. Computational and Theoretical Chemistry, 2005, 722, 161-168.	1.5	5
1028	Theoretical study on geometrical structure and electronic spectrum properties of two stable conformers of boron hydroxyphenylpyridine excimers. Computational and Theoretical Chemistry, 2005, 731, 123-126.	1.5	5
1029	Bis[2-(2-oxidophenyl)-1H-benzimidazole-Î²2N3,O]zinc(II) dimethylformamide disolvate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, m2361-m2362.	0.2	5
1030	A novel large heteropolytungstate constructed from two types of lacunary Keggin anions: K7Na13[(PW11O39)2(PW9O34)2(W2O3)2]Â·25H2O. Inorganica Chimica Acta, 2007, 360, 3376-3379.	2.4	5
1031	Theoretical study on the structures, isomerization and stability of SiC3H isomers. Theoretical Chemistry Accounts, 2008, 119, 501-509.	1.4	5
1032	Investigation on fluorescence properties of ultrafine PVA fiber matsâ€contained polyoxometalate with different molecular structure. Journal of Applied Polymer Science, 2009, 113, 1369-1374.	2.6	5
1033	DFT study on second-order nonlinear optical properties of Pt(II) complexes with different chromophores. Science in China Series B: Chemistry, 2009, 52, 144-152.	0.8	5
1034	Synthesis and characterization of two novel coordination polymers based on the rigid 1H-1,2,3-triazole-4,5-dicarboxylic acid ligand. Science China Chemistry, 2010, 53, 2177-2182.	8.2	5
1035	DFT STUDIES ON ELECTRONIC STRUCTURES AND THIRD-ORDER NONLINEAR OPTICAL PROPERTIES OF A SERIES OF Ptâ€“Pt BOND-CONTAINING METAL COMPLEXES. Journal of Theoretical and Computational Chemistry, 2012, 11, 403-419.	1.8	5
1036	Hydrothermal synthesis and structural characterization of a new 2D inorganicâ€“organic hybrid compound based on {Ni6PW9}2 subunit. Inorganic Chemistry Communication, 2012, 23, 21-24.	3.9	5
1037	The origin of the unusual broad and intense visible absorption of tetrathiafulvalene-annulated zinc porphyrazine: A density functional theory study. Journal of Molecular Graphics and Modelling, 2012, 33, 26-34.	2.4	5
1038	Structural and Bonding Analyses on a Homologous Metalâ€“Metal Bond Guestâ€“Host Series M₂@C₅₀X₁₀ (M = Zn, Cd, Hg; X = CH, N, B). European Journal of Inorganic Chemistry, 2013, 2013, 2220-2230.	2.0	5
1039	Theoretical study on the gas phase reaction of allyl chloride with hydroxyl radical. Journal of Chemical Physics, 2014, 140, 084309.	3.0	5
1040	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
1041	Electron transport via phenylâ€“perfluorophenyl interaction in crystals of fluorine-substituted dibenzalacetones. RSC Advances, 2014, 4, 50188-50194.	3.6	5
1042	Theoretical characterization and design of highly efficient iridium (III) complexes bearing guanidinate ancillary ligand. Journal of Molecular Graphics and Modelling, 2014, 51, 149-157.	2.4	5
1043	Towards an efficient blue emission cationic Ir(<scp>iii</scp>) complex with azole-type ancillary ligands: a joint theoretical and experimental study. New Journal of Chemistry, 2016, 40, 4635-4642.	2.8	5
1044	Aromaticity of graphene nanoflakes in a new way: fragment analysis by combination of the nucleus-independent chemical shifts and the anisotropy of current induced density. Journal of Molecular Modeling, 2017, 23, 231.	1.8	5

#	Article	IF	Citations
1045	A theorectical design of performant chlorinated benzothiadiazole-based polymers as donor for organic photovoltaic devices. Organic Electronics, 2018, 61, 46-55.	2.6	5
1046	Self-assembly and photocatalytic properties of three nanosized polyoxometalates based on the {SiNb3W9O40} cluster and transition-metal cations. Journal of Solid State Chemistry, 2019, 277, 618-623.	2.9	5
1047	Syntheses, structure and properties of an especially stable Cd metal-organic framework driven by benzotriazole-5-carboxylic acid. Inorganic Chemistry Communication, 2020, 112, 107726.	3.9	5
1048	Theoretical Simulations of Thermochromic and Aggregationâ€Induced Emission Behaviors of a Series of Redâ€Light Anthraceneâ€oâ€carborane Derivatives. Chemistry - A European Journal, 2021, 27, 9571-9579.	3.3	5
1049	Fine-tuning emission color of aggregation-induced emission-active Ir(III) phosphors through simple ligand modification. Dyes and Pigments, 2021, 192, 109439.	3.7	5
1050	A thiol-functionalized zirconium metalâ€“organic cage for the effective removal of Hg²⁺ from aqueous solution. Nanotechnology, 2021, 32, 075602.	2.6	5
1051	CO2 electroreduction performance of transition metals supported on g-C(CN)3 monolayer with specific TMN3 active sites. Applied Surface Science, 2022, 573, 151544.	6.1	5
1052	Theoretical mechanistic study of 4CzIPN/Ni0-metallaphotoredox catalyzed enantioselective desymmetrization of cyclic meso-anhydrides. Dalton Transactions, 2021, 50, 17675-17687.	3.3	5
1053	Axially Chiral Dodecanuclear Lanthanide Clusters Constructed by â€œ<scp>Bottomâ€Up</scp>â€• Selfâ€assembly for Enantioselective Sensing. Chinese Journal of Chemistry, 2022, 40, 1165-1170.	4.9	5
1054	Stable zinc metal-organic framework as efficient bifunctional fluorescent probe for selective detection of nitrobenzene and Fe(â…¢). Journal of Solid State Chemistry, 2022, 310, 123093.	2.9	5
1055	Ground-state reduced density matrices, effective Hamiltonians, and optical properties of Schiff bases of retinal. Chemical Physics, 1999, 247, 185-192.	1.9	4
1056	A novel two-dimensional zinc(II) coordination polymer with 6-mercaptonicotinic acid. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, m70-m72.	0.4	4
1057	Secondary ligand-directed assembly of ZnII and CdII coordination architectures: From 1D to 3D compounds based on pyridine carboxylate ligands. Journal of Molecular Structure, 2010, 983, 93-98.	3.6	4
1058	Hydrothermal syntheses of two novel coordination polymers based on tetranuclear metal cluster constructed by 1,3,5-Tris(2H-tetrazol-5-yl)benzene ligand. Inorganic Chemistry Communication, 2010, 13, 1203-1206.	3.9	4
1059	Theoretical studies on electronic and electron blocking properties of iridium complexes with phenylpyrazolato ligands. Synthetic Metals, 2010, 160, 1015-1021.	3.9	4
1060	A novel luminescent 3D metalâ€“organic framework possessing 3-fold interpenetrating (3,5)-connected net. Inorganic Chemistry Communication, 2012, 26, 42-45.	3.9	4
1061	Toward design of high-performance optoelectronic materials: comparative theoretical studies on the photophysical and charge transport properties of fluorene-based compounds. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	4
1062	The effect of boron nitride nanotubes size on the <scp>HArF</scp> interaction by <scp>NBO</scp> and <scp>AIM</scp> analysis. International Journal of Quantum Chemistry, 2014, 114, 1692-1696.	2.0	4

#	Article	IF	Citations
1063	Unveiling photophysical properties of cyclometalated iridium(iii) complexes with azadipyrromethene and dipyrromethene ancillary: a theoretical perspective. RSC Advances, 2014, 4, 62197-62208.	3.6	4
1064	A comparative DFT study on the mechanism of olefin epoxidation catalyzed by substituted binuclear peroxotungstates ([SeO₄WO(O₂)₂MO(O₂)₂]ⁿ^{â^'}) Tj E	2.0	4
1065	458-462. Suitable helical cavity, suitable alkali metal, larger first hyperpolarizability. Chemical Physics Letters, 2014, 600, 123-127.	2.6	4
1066	Structures and electro-optical properties of MÃ¶bius [n]Cyclacenes[13â€“18]: a theoretical study. Journal of Molecular Modeling, 2014, 20, 2201.	1.8	4
1067	Simple Copper(II) Schiff Base Complex as Efficient Heterogeneous Photo-Fenton-like Catalyst. Chemistry Letters, 2014, 43, 1158-1160.	1.3	4
1068	Exploration of charge transfer and absorption spectra of porphyrinâ€“polyoxometalate hybrids to search for high performance sensitizers. RSC Advances, 2015, 5, 93659-93665.	3.6	4
1069	Metal-organic fameworks based on multi-carboxylate ligands with threefold symmetries and luminescence properties. Inorganic Chemistry Communication, 2017, 79, 69-73.	3.9	4
1070	Two metal-organic frameworks based on a flexible dithioether spacer with luminescence and sensing properties. Inorganic Chemistry Communication, 2017, 86, 271-275.	3.9	4
1071	NICS values scan in three-dimensional space of the hoop-shaped Ï€-conjugated molecules [6]₈cyclacene and [16]trannulene. New Journal of Chemistry, 2018, 42, 1987-1994.	2.8	4
1072	Structure-property relationships of coronene in external electric field. Organic Electronics, 2018, 59, 196-201.	2.6	4
1073	Metal ions doped into merocyanine form of coumarin derivatives: nonlinear optical molecular switches. Journal of Molecular Modeling, 2019, 25, 212.	1.8	4
1074	Polyoxovanadateâ€Based Metalâ^'Organic Octahedron Based on 1,4â€Naphthalenedicarboxylic Acid. Israel Journal of Chemistry, 2019, 59, 306-310.	2.3	4
1075	A theoretical exploration on why the replacement of hexyl group by alkoxycarbonyl in P3HT could greatly improve the performance of non-fullerene organic solar cell. Journal of the Taiwan Institute of Chemical Engineers, 2019, 100, 160-167.	5.3	4
1076	Metal-free catalysis for the Markovnikov hydrosilylation of styrene. New Journal of Chemistry, 2019, 43, 18339-18344.	2.8	4
1077	The directions of an external electric field control the catalysis of the hydroboration of Câ€“O unsaturated compounds. RSC Advances, 2019, 9, 29331-29336.	3.6	4
1078	Dinuclear Ir(<scp>iii</scp>) complexes with asymmetrical bridging ligands as highly efficient phosphors for single-layer electroluminescent devices. Journal of Materials Chemistry C, 2019, 7, 13461-13467.	5.5	4
1079	The Alî€,Al triple bond in Al₂X₅⁺ and Al₂X₆²⁺ (X = Li, Na) clusters with multiple alkali metal coordination. New Journal of Chemistry, 2020, 44, 21119-21124.	2.8	4
1080	Ultrafast Absorption of Polysulfides through Electrostatic Confinement by Protonated Molecules for Highly Efficient Liâ€“S Batteries. ACS Applied Materials & Interfaces, 2020, 12, 36220-36227.	8.0	4

#	Article	IF	Citations
1081	A simple synthesis of highly ordered microporous carbon nanospheres for high performance potassium-ion batteries. Journal of Power Sources, 2020, 479, 229113.	7.8	4
1082	Two anthracene chromophore based metalâ€“organic frameworks for gas adsorption and promising nitro aromatic sensing. New Journal of Chemistry, 2020, 44, 12496-12502.	2.8	4
1083	Sulfur-doping polyoxometallate-metal-organic intercalation compound with PPy coating as highly efficient photocatalyst for visible light degradation. Polyhedron, 2020, 179, 114350.	2.2	4
1084	An octahedral polyoxomolybdateâ€“organic molecular cage. Chemical Communications, 2021, 57, 1042-1045.	4.1	4
1085	Tunable Dual-Color Emission Perovskites via Post-Synthetic Modification Strategy for Near-Unity Photoluminescence Quantum Yield. ACS Applied Materials & Interfaces, 2021, 13, 21645-21652.	8.0	4
1086	Temperature sensitive properties and preparation of europium complexes with double ligands. Luminescence, 2021, 36, 1476-1482.	2.9	4
1087	Co2P@C derived from metal-organic coordinate interactions using polyaniline as soft template for electrocatalytic hydrogen production. Journal of Solid State Chemistry, 2021, 299, 122184.	2.9	4
1088	Near-infrared luminescence investigation of Cr4+ ions doped Li2TiGeO5. Journal of Materials Science: Materials in Electronics, 2021, 32, 18544-18550.	2.2	4
1089	Activation of Peroxymonosulfate by Co-Metalâ€“Organic Frameworks as Catalysts for Degradation of Organic Pollutants. Industrial & Engineering Chemistry Research, 2021, 60, 13223-13232.	3.7	4
1090	Sulphur-Bridged BAl5S5+ with 17 Counting Electrons: A Regular Planar Pentacoordinate Boron System. Molecules, 2021, 26, 5205.	3.8	4
1091	The synthesis of Cu nanoclusters and their dual mode colorimetric and fluorescent sensing for 2, 4-dinitrophenol. Nanotechnology, 2021, 33, .	2.6	4
1092	Synthesis of ultrafine Co/CoO nanoparticle-embedded N-doped carbon framework magnetic material and application for 4-nitrophenol catalytic reduction. New Journal of Chemistry, 2021, 45, 13751-13754.	2.8	4
1093	Metal-Free Z-Scheme aza-CMP/C₂N Heterostructure to Facilitate Photocatalytic CO₂ Reduction: A Computational Study. Journal of Physical Chemistry C, 2021, 125, 23133-23141.	3.1	4
1094	Coordination Environment Regulation of Cucurbit[6]uril-Based Metalâ€“Organic Rotaxane Networks for Proton Conduction. Crystal Growth and Design, 2022, 22, 2793-2798.	3.0	4
1095	Post-decorated synthesis of metal-organic frameworks derived Ni/Ni3S2@CN electrocatalyst for efficient hydrogen evolution. Journal of Solid State Chemistry, 2022, 313, 123287.	2.9	4
1096	Electronic Properties and Stability of DititaniumIV Substituted ?-Keggin Polyoxotungstate with Heteroatom Phosphorus by DFT. ChemInform, 2005, 36, no.	0.0	3
1097	Synthesis and characterization of three Cu(II), Zn(II), Cd(II) supramolecular complexes bridged by biphenyl 2,2â€²-dicarboxylate. Solid State Sciences, 2007, 9, 1006-1011.	3.2	3
1098	Theoretical study on the structures, isomerization and stability of SiC4 isomers. Theoretical Chemistry Accounts, 2010, 126, 15-25.	1.4	3

#	Article	IF	Citations
1099	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.	2.4	3
1100	Theoretical studies on electronic spectra and second-order nonlinear optical properties of barbituric acid derivatives substituted with schiff base. Chinese Journal of Chemistry, 2010, 22, 425-429.	4.9	3
1101	A new 2D 5-connected coordination polymer based on 3,4-bis(pyridin-4-ylmethoxy)benzoic acid ligand. Inorganic Chemistry Communication, 2010, 13, 932-934.	3.9	3
1102	DFT STUDY ON SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF THE DERIVATIVES OF DISUBSTITUTED SEVEN-VERTEX COBALTACARBORANE METALLOCENYL. Journal of Theoretical and Computational Chemistry, 2010, 09, 219-231.	1.8	3
1103	Theoretical investigation of electronic properties and redox properties for purely inorganic and aryloxide substituted Ti-containing POM derivatives. Molecular Physics, 2010, 108, 1553-1560.	1.7	3
1104	DFT studies on the electronic properties of organometallic-polyoxomolybdate anions [<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>Cp</mml:mtext></mml:mrow><mml:mrow><mml:mi>n</mml:mi></mml:mrow> (n= 1 or 2): Revealing bonding features of Cpâ^—â€“Mo. Computational and Theoretical Chemistry, 2011, 976, 1-7.	2.5	3
1105	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.	1.4	3
1106	Synthesis, Characterization, and Luminescence of Two New Zinc(II) Coordination Polymers Constructed by 5â€(4â€Carboxybenzyloxy)Isophthalic Acid Ligand. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 1414-1418.	1.2	3
1107	TDDFT study on the second-order nonlinear optical properties of a series of mono- and di-nuclear [60]fullerene complexes. Computational and Theoretical Chemistry, 2011, 963, 98-103.	2.5	3
1108	Density functional theory studies on structures and absorption spectra of [Au(tpy)Cl]²⁺ and its derivatives: Role of basis set, functional, solvent effect, and spin orbit effect. International Journal of Quantum Chemistry, 2012, 112, 1642-1653.	2.0	3
1109	A DFT study on the second-order nonlinear optical properties of the plenary mixed-metal polyoxometalate. Molecular Simulation, 2012, 38, 518-524.	2.0	3
1110	Probe the accumulation modes of the Auâ€“C22H14dimer on the structure and NLO properties. Molecular Physics, 2014, 112, 1918-1923.	1.7	3
1111	Cancer Therapy: Facile and Scalable Synthesis of Novel Spherical Au Nanocluster Assemblies@Polyacrylic Acid/Calcium Phosphate Nanoparticles for Dual-Modal Imaging-Guided Cancer Chemotherapy (Small 26/2015). Small, 2015, 11, 3082-3082.	10.0	3
1112	â€œDancing inside the ballâ€• the structures and nonlinear optical properties of three Sc2S@C3v(8)-C82 isomers. Journal of Molecular Modeling, 2015, 21, 259.	1.8	3
1113	The inner-induced effects of YCN in C76 on the structures and nonlinear optical properties. Journal of Molecular Modeling, 2016, 22, 174.	1.8	3
1114	Theoretical studies on oxidation-switchable second-order nonlinear optical responses of Metallosalen-Keggin polyoxometalate derivatives. RSC Advances, 2016, 6, 53438-53443.	3.6	3
1115	Theoretical investigation on the effect of fluorine and carboxylate substitutions on the performance of benzodithiophene-diketopyrrolopyrrole-based polymer solar cells. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	3
1116	Single step synthesized three dimensional spindle-like nanoclusters as lithium-ion battery anodes. CrystEngComm, 2018, 20, 3043-3048.	2.6	3

#	Article	IF	Citations
1117	Strong Pancake 2e/12c Bond in Ï€â€Stacking Phenalenyl Derivatives Avoiding Bond Conversion. ChemPhysChem, 2019, 20, 1879-1884.	2.1	3
1118	Manipulating charge carrier transporting of disubstituted phenylbenzoimidazole-based host materials for efficient full-color PhOLEDs. Organic Electronics, 2020, 77, 105513.	2.6	3
1119	A theoretical exploration of charge transfer dynamics in PTB7Ir/PC71BM triplet-material-based organic photovoltaics. Organic Electronics, 2020, 87, 105956.	2.6	3
1120	Synthesis, characterization, photo-and-electrochemical properties of cationic iridium(III) complexes by using 1,3,4-oxadiazole cyclometallating ligand. Inorganic Chemistry Communication, 2020, 118, 107980.	3.9	3
1121	Configuration effect in polyoxometalate-based dyes on the performance of DSSCs: an insight from a theoretical perspective. Physical Chemistry Chemical Physics, 2020, 22, 16032-16039.	2.8	3
1122	Superiority of Iridium Photocatalyst and Role of Quinuclidine in Selective Î±-C(sp³)â€“H Alkylation: Theoretical Insights. Journal of Organic Chemistry, 2021, 86, 484-492.	3.2	3
1123	Periodic B- and N-doped phenalenyl Ï€-aggregates: unexpected nonlinear optical properties by tuning pancake Ï€â€“Ï€ bonding. Physical Chemistry Chemical Physics, 2021, 23, 23998-24003.	2.8	3
1124	Second-order nonlinear optical property of carbonâ€“boronâ€“nitride heterostructure: Vertical carbon-segment into the BN nanosheet. Computational and Theoretical Chemistry, 2021, 1198, 113177.	2.5	3
1125	A typical 2D covalent organic polymer as multifunctional sensor and assemble a WLED. Journal of Solid State Chemistry, 2021, 297, 122101.	2.9	3
1126	Novel acetyleneâ€terminated thermosetting polyisoimides with excellent solubility and performed as efficient heat shields composites. Journal of Applied Polymer Science, 2022, 139, 51559.	2.6	3
1127	Cubic Ba2LaF7:Yb3+/Ln(Lnâ€‰=â€‰Er3+,Ho3+) up-conversion submicron particles controllable synthesis and luminescence properties. Journal of Materials Science: Materials in Electronics, 2021, 32, 24856-24870.	2.2	3
1128	Metalâ€“free C2N doped with sp2â€“hybridized B atom as highâ€“efficiency photocatalyst for nitrobenzene reduction reaction: A density functional theory study. Molecular Catalysis, 2022, 518, 112080.	2.0	3
1129	N-Donor flexible ligands for constructing polyoxometalate-based metalâ€“organic frameworks as multifunctional electrocatalysts. CrystEngComm, 2022, 24, 2705-2708.	2.6	3
1130	Mixed-Linker Strategy for the Construction of Metalâ€“Organic Framework Combined with Dyes toward Alcohol Detection. Inorganic Chemistry, 2022, 61, 5318-5325.	4.0	3
1131	Theoretical insight into decatungstate photocatalyzed alkylation of N-tosylimine via hydrogen atom transfer and proton-coupled electron transfer. Dalton Transactions, 2022, , .	3.3	3
1132	An anthracene-based microporous metalâ€“organic framework for adsorbing CO₂ and detecting TNP sensitivity. New Journal of Chemistry, 2022, 46, 11377-11381.	2.8	3
1133	Ir^{III}/Ni^{II}-Metallaphotoredox-Catalyzed Enantioselective Decarboxylative Arylation of Î±-Amino Acids: Theoretical Insight of Enantio-Determining Outer-Sphere Reductive Elimination. Inorganic Chemistry, 0, , .	4.0	3
1134	The effect of conformational dependent properties of radical cations on poly(N,N-dimethylaniline). Macromolecular Chemistry and Physics, 2000, 201, 1774-1779.	2.2	2

#	Article	IF	Citations
1135	Density functional theory study on isomerization reactions of pyridazine derivatives bearingN,N-dialkylaminoethyl group. International Journal of Quantum Chemistry, 2004, 98, 515-521.	2.0	2
1136	Tetraaqua(2,2â€²-bipyridine)zinc(II) terephthalate. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, m142-m144.	0.2	2
1137	Theoretical Studies on Proton Transfer Reactions of 8-Hydroxyquinoline Monomers and Dimers. Chinese Journal of Chemistry, 2006, 24, 724-730.	4.9	2
1138	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
1139	Bis[2,2â€²-(butane-1,4-diyl)bis(1H-benzimidazolium)] Î±-octamolybdate(VI). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, m584-m586.	0.2	2
1140	Theoretical study on secondâ€order nonlinear optical properties of spin crossover Fe(III) phenolateâ€pyridyl Schiff base complexes. International Journal of Quantum Chemistry, 2010, 110, 1863-1870.	2.0	2
1141	A Facile Method for Preparation of Dye-Doped Silica-Based Raspberry-Like Microspheres and Fluorescent Films. Journal of Nanoscience and Nanotechnology, 2009, 9, 6594-6599.	0.9	2
1142	Theoretical investigation on structures, electronic spectra and nonlinear optical properties of gold compounds [X-â€œAu(PMe3)â€2]. Science China Chemistry, 2010, 53, 1149-1154.	8.2	2
1143	Molecular simulation study of the binding mechanism of [Î±-PTi2W10O40]7â^' for its promising broad-spectrum inhibitory activity to FluV-A neuraminidase. Science Bulletin, 2010, 55, 2497-2504.	1.7	2
1144	Quantum chemical study on the reaction mechanism of OBrO radical with OH radical. Chinese Journal of Chemistry, 2004, 22, 611-615.	4.9	2
1145	Theoretical study of the impact factor on redox property and second-order nonlinear response for organoimido derivatives of [Mo6O19]2â^': Electron donors with magnitude of conjugated groups or length of conjugated chain. Computational and Theoretical Chemistry, 2010, 947, 9-15.	1.5	2
1146	Theoretical investigation of second-order nonlinear optical responseâ€‰â€”â€‰Hexamolybdate as a superior donor over metal carbonyl complexes in the Dâ€“Ïâ€“A model. Canadian Journal of Chemistry, 2011, 89, 61-67.	1.1	2
1147	A novel route for designing C60 derivatives with large first hyperpolarizability: Cage-opened cases. Synthetic Metals, 2011, 161, 2185-2191.	3.9	2
1148	Theoretical study on stability and nonlinear optical properties of tetrahydropyrrole diradical and its isoelectronic systems in different electronic states. Science China Chemistry, 2011, 54, 1086-1093.	8.2	2
1149	Synthesis and Luminescent Properties of Two Zinc(II) Coordination Polymers Constructed by 4â€(Pyridinâ€4â€ylmethoxy)benzolic Acid Ligand. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 1419-1422.	1.2	2
1150	Synthesis, Crystal Structure, and Fluorescent Property of A Chiral 2D Polymer Based on Bis(2-benzimidazoles) and Aromatic Carboxylate Ligands. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 2211-2214.	1.2	2
1151	Electronic properties and stabilities of methoxy-substituted Lindqvist polyoxometalates [Nb2W4O19CH3]3â^' by DFT. Science Bulletin, 2012, 57, 976-982.	1.7	2
1152	A TiO2@{Mo368} composite: synthesis, characterization, and application in dye-sensitized solar cells. Journal of Coordination Chemistry, 2014, 67, 3873-3883.	2.2	2

#	Article	IF	Citations
1153	Rational modifications on ruthenium terpyridine sensitizers with large J_{sc} for dye-sensitized solar cells: combined DFT and relativistic TDDFT studies. RSC Advances, 2015, 5, 100169-100175.	3.6	2
1154	Theoretical exploration to the cation effect on the second-order nonlinear optical properties of Strandberg-type polyoxometalates. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550007.	1.8	2
1155	Exploring the electronic properties and cation complexation of polyoxoaurates [AuIII4X4Om]nâ^'(X =) Tj ETQq1 1 0.784314 rgBT /Ove Physics, 2015, 17, 11521-11526.	2.8	2
1156	TDDFT studies on the chiroptical properties of a chiral inorganic polythioanion MÃ¶bius strip. Inorganic Chemistry Frontiers, 2016, 3, 86-91.	6.0	2
1157	Two Novel Lanthanide Metalâ€Organic Frameworks Constructed by Tetracarboxylate Ligands: Synthesis, Structures; and Luminescent Properties. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2019, 645, 940-943.	1.2	2
1158	Demulsification-induced Fast Solidification: a Novel Strategy for Preparation of Polymer Encapsulations. Chemical Research in Chinese Universities, 2019, 35, 1082-1088.	2.6	2
1159	Insight into spinâ€“orbital interaction using MCSCF method: A special analysis of the 1 Î£ g + electronic state in C 2 and the linear polyacetylenic C 4 and C 6. Journal of Computational Chemistry, 2019, 40, 1338-1343.	3.3	2
1160	External Electric Fieldâ€”Phenyl interaction boosts hydrosilylation of substituted alkynes to Î±â€vinylsilane. International Journal of Quantum Chemistry, 2020, 120, e26134.	2.0	2
1161	ZIF-8 and polyaniline modified coconut gel to fabricate composite aerogel for efficient removal of tetracycline. E3S Web of Conferences, 2020, 185, 04055.	0.5	2
1162	Synthesis and proton-conducting performance of crystalline hydrogen-bonded organic networks. Journal of Solid State Chemistry, 2020, 290, 121550.	2.9	2
1163	The nonlinear optics property of heterodinuclear (Li and Na) sexipyridine helix: A density functional theory study. International Journal of Quantum Chemistry, 2021, 121, e26478.	2.0	2
1164	Theoretical investigation of the influence of different electric field directions and strengths on a POM-based dye for dye-sensitized solar cells. Materials Chemistry Frontiers, 2021, 5, 929-936.	5.9	2
1165	A fluorescent porous covalent-organic polymer (COP-3) for highly selective and sensitive detection of Fe³⁺ in aqueous solution. New Journal of Chemistry, 2021, 45, 2370-2373.	2.8	2
1166	Tuning the NLO response of bis-cyclometalated iridium(iii) complexes by modifying ligands: experimental and structural DFT analysis. New Journal of Chemistry, 2021, 45, 5491-5496.	2.8	2
1167	Synthesis and CO₂ photoreduction of two 3dâ€“4f heterometalâ€“organic frameworks. New Journal of Chemistry, 2021, 45, 18790-18795.	2.8	2
1168	High performance doping-free WOLEDs based on rationally designed asymmetric orange-red Ir(III) emitter with balanced charge mobility. Organic Electronics, 2021, 89, 106022.	2.6	2
1169	Enhanced Fluorescence of La 3+ , Gd 3+ doped EuW 10 for Temperature sensing performance. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 1221-1226.	1.2	2
1170	Two functional hybrids based on polyoxometalate coordination polymers: Synthesis, electrochemical and photocatalytic properties. Inorganic Chemistry Communication, 2021, 130, 108673.	3.9	2

#	Article	IF	Citations
1171	A stable Cd metalâ€“organic framework as efficient fluorescent probe for sensing Fe3+ in water. Inorganica Chimica Acta, 2021, 528, 120635.	2.4	2
1172	Hexanuclear nickel-based [P4Mo11O50] with photocatalytic reduction of CO2 activity. Inorganic Chemistry Communication, 2021, 134, 109009.	3.9	2
1173	Study on the photoluminescence properties and magnetization performance of Lu3+, Tb3+: CeF3 nanoparticles. Journal of Materials Science: Materials in Electronics, 2021, 32, 28098-28107.	2.2	2
1174	Organic Supramolecular Zippers with Ultralong Organic Phosphorescence by a Dexter Energy Transfer Mechanism. Angewandte Chemie, 2022, 134, .	2.0	2
1175	Surface modification strategy based on molecular engineering of an organic cation toward spectrally stable deep-blue emission perovskites. Journal of Materials Chemistry C, 2022, 10, 2067-2072.	5.5	2
1176	Green Catalytic Method for Hydrothiolation of Allylamines: An External Electric Field. ACS Omega, 2022, 7, 5782-5790.	3.5	2
1177	Theoretical study of Ni^Iâ€“Ni^{III} cycle mediated by heterogeneous zinc in Câ€“N cross-coupling reaction. Physical Chemistry Chemical Physics, 2022, 24, 7617-7623.	2.8	2
1178	Rational design of an AIE-active metal-organic framework for highly sensitive and portable sensing nitroaromatic explosives. Chinese Chemical Letters, 2023, 34, 107291.	9.0	2
1179	Improved ablation resistance and thermal insulation performances of polyimide composites by introducing albite/glass powder composition. Polymers and Polymer Composites, 2022, 30, 096739112210878.	1.9	2
1180	Anisotropic conductivity of undoped and [FeCl 4] â^' -doped trans -polyacetylene. Computational and Theoretical Chemistry, 2001, 540, 1-4.	1.5	1
1181	Bis{4,4â€²-[(2,2â€²-bi-1H-imidazole-1,1â€²-diyl)dimethylene]dipyridinium} Î²-octamolybdate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, m2817-m2817.	0.2	1
1182	THEORETICAL STUDIES ON THE FORMATION MECHANISM AND STRUCTURE OF PENTAFULVENONE AND AZAFULVENONE. Journal of Theoretical and Computational Chemistry, 2008, 07, 233-246.	1.8	1
1183	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.	4.9	1
1184	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.	2.0	1
1185	Theoretical study on the second-order nonlinear optical properties of gold (III) alkyl complexes. Synthetic Metals, 2009, 159, 2406-2409.	3.9	1
1186	Theoretical studies on the structures and absorption spectra ofâ€“CnR2n+1(R = H, F;n= 1, 2) substituted 5-(2-pyridyl) pyrazolate boron complexes. Molecular Physics, 2009, 107, 2511-2520.	1.7	1
1187	Aspects of the Nonlinear Optical Properties as a Guide to Protonation Sites: A Theoretical Study upon Î±-Keggin [SiW12O40]4â^' and [SiV3W9O40]7â^'. Chemistry Letters, 2010, 39, 580-581.	1.3	1
1188	A theoretical study of ground and excited state proton transfer and rotamerim in salicylanilide and its 1:1 complex with methanol. Computational and Theoretical Chemistry, 2010, 945, 110-115.	1.5	1

#	Article	IF	Citations
1189	Two inorganicâ€“organic hybrid compounds based on [Ni2(V3O9)2]2â¯ cluster and {Co2V2} cage subunits. Inorganic Chemistry Communication, 2010, 13, 981-984.	3.9	1
1190	QUANTUM CHEMISTRY STUDIES ON THE Fe-Hg INTERACTIONS AND 31P NMR IN [Fe(CO)3(RPhPpy)2 (HgCl2)] (R = Me, Et, Ph). Journal of Theoretical and Computational Chemistry, 2011, 10, 53-63.	1.8	1
1191	Molecular dynamic and quantum mechanics study of drug recognition for the extremity of DNA G-quadruplex groove. Medicinal Chemistry Research, 2012, 21, 4010-4016.	2.4	1
1192	Reply to â€œComment on â€˜How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Grapheneâ€™â€•. Journal of Physical Chemistry C, 2013, 117, 725-728.	3.1	1
1193	Recent Theoretical Advances in Understanding the Mechanism of Aggregation-Induced Emission for Small Organic Molecules. , 2013, , 399-418.		1
1194	TDDFT studies on electronic structures, chiroptical properties and solvent effect on the CD spectra of diphosphonate-functionalized polyoxomolybdates. Journal of Molecular Graphics and Modelling, 2013, 44, 26-32.	2.4	1
1195	Structure and mechanical properties of waterborne polyurethane-based composites filled with self-assembled supramolecular nanoplatelets. Journal Wuhan University of Technology, Materials Science Edition, 2013, 28, 773-780.	1.0	1
1196	Hydrothermal synthesis and structure characterization of two six-connected metalâ€“organic frameworks based on the mixed ligands. Solid State Sciences, 2014, 34, 8-11.	3.2	1
1197	A novel nitrogen-containing compound with D-Ï€-A structure: theoretical and experimental study. Canadian Journal of Chemistry, 2014, 92, 411-416.	1.1	1
1198	Probing the relationship between spin contamination and first hyperpolarizability: Openâ€shell MÃ¶bius anion. International Journal of Quantum Chemistry, 2014, 114, 720-724.	2.0	1
1199	Theoretical design of organic-inorganic hybrids based on hexamolybdate toward high performance dye-sensitized solar cells. Molecular Simulation, 2016, 42, 688-692.	2.0	1
1200	A comparative computational analysis on the photophysical and charge transport properties of three 5,5-bis(2,2-diphenylvinyl)-biheterocyclic compounds. Chemical Physics Letters, 2020, 748, 137348.	2.6	1
1201	Regioisomeric BODIPY derivatives: second-order nonlinear optical properties under an external electric field. New Journal of Chemistry, 2021, 45, 4335-4339.	2.8	1
1202	Efficient catalytic reduction of 4-nitrophenol by Cu1.96S/NSC hybrid material derived from metal-organic framework. E3S Web of Conferences, 2021, 252, 02065.	0.5	1
1203	Carbon nitride derivatives as photocatalysts for the CO2 reduction reaction: computational study. Physical Chemistry Chemical Physics, 2021, 23, 3401-3406.	2.8	1
1204	Interior surface (confinement effect) and exterior (odd-even effect) of Fe-BNNTs (n, 0) for CO oxidation: A computational view. Applied Surface Science, 2021, 549, 149314.	6.1	1
1205	Doping alkali metal ions and introducing electron donor groups to fulleropyrrolidine derivatives: Large second-order nonlinear optical responses. Computational and Theoretical Chemistry, 2021, 1201, 113254.	2.5	1
1206	Machine Learning Corrections for DFT Noncovalent Interactions. Springer Series in Materials Science, 2021, , 183-212.	0.6	1

#	Article	IF	Citations
1207	Synthesis, Crystal Structure, and Luminescent Properties of a New Holmium(III) Coordination Polymer Involving 2,5-Dihydroxy-1,4-terephthalic Acid Dianion as Ligand. Crystals, 2021, 11, 1294.	2.2	1
1208	The interesting luminescence behavior and rare nonlinear optical properties of the {Ag₅₅Mo₆} nanocluster. RSC Advances, 2021, 11, 38814-38819.	3.6	1
1209	A low-dimensional N-rich coordination polymer as an effective fluorescence sensor for 2,4,6-trinitrophenol detection in an aqueous medium. New Journal of Chemistry, 0, , .	2.8	1
1210	A supported Crâ€“Cr sextuple bond in an all-metal cluster. Dalton Transactions, 2022, 51, 2664-2668.	3.3	1
1211	Anthraceneâ€Modified Cadmium Metalâ€Organic Framework as an Excellent Sensor for the Detection of 2,4,6â€Trinitrophenol and Nitrofurantoin. European Journal of Inorganic Chemistry, 2022, 2022, .	2.0	1
1212	Theoretical design and characterization of new terpolymer donors based on PTB7Ir for high-efficiency triplet-material-based organic photovoltaics. RSC Advances, 2022, 12, 8578-8587.	3.6	1
1213	Electric Field and Ion Diffusion Triggered Precisely Regulated Construction of Micron-scale Water-based Polymer Films: a Detailed Mechanistic Exploration. Chemical Research in Chinese Universities, 2022, 38, 1435-1445.	2.6	1
1214	Facile construction of a highly proton-conductive matrix-mixed membrane based on a â€“SO₃H functionalized polyamide. Soft Matter, 0, , .	2.7	1
1215	Electronic Properties Of The Model Organometallic Polymer [M-C=C(N)]n (M = Cu(I), Ag(I), Au(I)). Materials Research Society Symposia Proceedings, 1999, 576, 389.	0.1	0
1216	Electrical anisotropy of orientedtrans-polyacetylene undoped and doped with SO3. Science Bulletin, 2000, 45, 893-896.	1.7	0
1217	Ab initio and DFT study on [Si(O2Ph)n]mÂ± (n=1â€“3, m=0,Â±2). Computational and Theoretical Chemistry, 2002, 578, 159-167.	1.5	0
1218	Quantum chemical study on ferromagnetic property on theN,N-dimethylaniline dimer radical cation. International Journal of Quantum Chemistry, 2002, 89, 484-488.	2.0	0
1219	A one-dimensional nickel(II) coordination polymer with pyridine and isophthalate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, m322-m324.	0.2	0
1220	catena-Poly[[diaquabis(2-methoxymethyl-1H-benzimidazole-ÎºN3)cadmium(II)]-Î¼-terephthalato-ÎºO:Oâ€²]. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, m292-m293.	0.2	0
1221	A tetranuclear copper(II) complex constructed from the salen ligand with alkoxo groups. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, m2932-m2932.	0.2	0
1222	Theoretical study on the mechanism for the reaction of pentafulvenone with HNC in singlet and triplet states, interconversions and solvation effect. Molecular Physics, 2008, 106, 1767-1776.	1.7	0
1223	NOVEL ANODE Li-ION SECONDARY BATTERIES DERIVED FROM NANOCRYSTALLINE Li4Ti5O12/POLYACENE MATERIALS. International Journal of Nanoscience, 2009, 08, 333-336.	0.7	0
1224	Syntheses and Characterization of Two Coordination Polymers Constructed by the Ligand 3,5-Bis(pyridin-4-ylmethoxy)benzoic Acid. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, NA-NA.	1.2	0

#	Article	IF	Citations
1225	Mechanism and Kinetics for the Reaction of NCS and OH Radicals. Chinese Journal of Chemistry, 2004, 22, 590-593.	4.9	0
1226	Density functional study on the mechanism of collision reaction among protons, N₂ and water vapor. Chinese Journal of Chemistry, 2004, 22, 594-598.	4.9	0
1227	Accurate Prediction of the Optical Absorption Energies by Neural Network Ensemble Approach. , 2010, , .		0
1228	Improving the Accuracy of Low Level Density Functional Theory Calculation for Absorption Energies: The Least Squares Support Vector Machine. , 2010, , .		0
1229	Accurate Prediction of Transition Energies in Organic Molecules. , 2010, , .		0
1230	Combined Density Functional Theory and Ensembled Elman Network Correction Approach for Electronic Excitation Energies. , 2011, , .		0
1231	Inside Cover: Spiral Intramolecular Charge Transfer and Large First Hyperpolarizability in MÃ¶bius Cyclacenes: New Insight into the Localized Ï€ Electrons (ChemPhysChem 9/2012). ChemPhysChem, 2012, 13, 2222-2222.	2.1	0
1232	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
1233	The Effect of the different spin multiplicity on nonlinear optical properties of lithium decahydroborate dimers. Journal of Molecular Modeling, 2014, 20, 2415.	1.8	0
1234	Syntheses, Structures, and Photophysical Properties of Two Coordination Polymers Based on 2,3â€Dioxoâ€1,2,3,4â€tetrahydroquinoxalineâ€6â€carboxylic Acid. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 531-535.	1.2	0
1235	Theoretical studies on the chiral polyoxoanions [P₂Mo₁₈O₆₂]^{6â^'} and [PMo₉O₃₁(OH₂)₃]^{3â^'} with histidine: chiral inversion and chiral induction. Inorganic Chemistry Frontiers, 2018, 5, 1992-1997.	6.0	0
1236	Synthesis and characterization of two isostructural 3dâ€“4f coordination compounds based on pyridine-2,6-dicarboxylic acid and 4,4â€²-bipyridine. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 723-727.	0.5	0
1237	A new polyniobotungstate based on {GeW9Nb3O40} clusters and nickel cation with photocatalytic properties. Inorganic Chemistry Communication, 2020, 120, 108151.	3.9	0
1238	An efficient strategy for improving the water stability of a nearinfrared- emissive lanthanide MOF. E3S Web of Conferences, 2020, 185, 04070.	0.5	0
1239	A new covalent organic polymer used to highly selective detection of Fe3+ ions. E3S Web of Conferences, 2020, 213, 01008.	0.5	0
1240	Synthesis, structure and properties of a new Sm(III) rare-earth metal coordination complex with 2,5-dihydroxy-terephthalic acid ligand. Journal of Coordination Chemistry, 2021, 74, 1907-1918.	2.2	0
1241	Tetraaquabis(2-oxo-1,2-dihydroquinoline-4-carboxylato-Î²O4)nickel(II). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, m389-m390.	0.2	0
1242	Synthesis and multifunctional sensing ability of axially chiral tetranuclear europium clusters. CrystEngComm, 0, , .	2.6	0

#	Article	IF	Citations
1243	Demonstration of temperature-sensitive paints with rigorously controlled thickness applied to variously shaped metal substrates with a highly stable connection based on a demulsification-induced fast solidification strategy. New Journal of Chemistry, 2022, 46, 3623-3630.	2.8	0
1244	Synthesis, crystal structure and characterisation of the complex {Ln(DHTA)1.5(H2O)3]Â·H2O}n (Ln = La,) Tj ETQq0 0 0 rgBT /Overlock 10 0.9		0
1245	Study on Luminescence Properties of TbÂ³âº, YbÂ³âº Doped CeFâ‚ƒ Nanoparticles. , 2021, , .		0
1246	Preparation and Characterization of Silica Fiber Reinforced Boron Modified Methyl Phenolic Resin Matrix Composites. , 2021, , .		0
1247	Study on Luminescence Properties of EuÂ³âº/TbÂ³âº Doped Gadolinium Barium Borosilicate Glass. , 2021, , .		0