

# Zhongmin Su

## List of Publications by Citations

**Source:** <https://exaly.com/author-pdf/3996021/zhongmin-su-publications-by-citations.pdf>

**Version:** 2024-04-20

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

1,206  
papers

42,581  
citations

94  
h-index

152  
g-index

1,275  
ext. papers

46,965  
ext. citations

5.2  
avg, IF

7.73  
L-index

#	Paper	IF	Citations
1206	Highly stable crystalline catalysts based on a microporous metal-organic framework and polyoxometalates. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 1883-8	16.4	798
1205	Recent advances in porous polyoxometalate-based metal-organic framework materials. <i>Chemical Society Reviews</i> , <b>2014</b> , 43, 4615-32	58.5	709
1204	Chiral 3D architectures with helical channels constructed from polyoxometalate clusters and copper-amino acid complexes. <i>Angewandte Chemie - International Edition</i> , <b>2006</b> , 45, 904-8	16.4	552
1203	Metal nuclearity modulated four-, six-, and eight-connected entangled frameworks based on mono-, bi-, and trimetallic cores as nodes. <i>Chemistry - A European Journal</i> , <b>2006</b> , 12, 2680-91	4.8	471
1202	Ultrastable Polymolybdate-Based Metal-Organic Frameworks as Highly Active Electrocatalysts for Hydrogen Generation from Water. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 7169-77	16.4	469
1201	Efficient and tunable white-light emission of metal-organic frameworks by iridium-complex encapsulation. <i>Nature Communications</i> , <b>2013</b> , 4, 2717	17.4	454
1200	Interlocked and interdigitated architectures from self-assembly of long flexible ligands and cadmium salts. <i>Angewandte Chemie - International Edition</i> , <b>2004</b> , 43, 5036-40	16.4	434
1199	Zeolitic Imidazolate framework-8 as efficient pH-sensitive drug delivery vehicle. <i>Dalton Transactions</i> , <b>2012</b> , 41, 6906-9	4.3	408
1198	Entangled coordination networks with inherent features of polycatenation, polythreading, and polyknotting. <i>Angewandte Chemie - International Edition</i> , <b>2005</b> , 44, 5824-7	16.4	405
1197	A sodalite-type porous metal-organic framework with polyoxometalate templates: adsorption and decomposition of dimethyl methylphosphonate. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 4178-81	16.4	372
1196	Self-assembly of nanometer-scale [Cu <sub>24</sub> I <sub>10</sub> L <sub>12</sub> ] <sup>14+</sup> cages and ball-shaped Keggin clusters into a (4,12)-connected 3D framework with photoluminescent and electrochemical properties. <i>Angewandte Chemie - International Edition</i> , <b>2006</b> , 45, 7411-4	16.4	371
1195	Polyoxometalate-based cobalt-phosphate molecular catalysts for visible light-driven water oxidation. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 5359-66	16.4	366
1194	Chiral nanoporous metal-organic frameworks with high porosity as materials for drug delivery. <i>Advanced Materials</i> , <b>2011</b> , 23, 5629-32	24	331
1193	Effect of Imidazole Arrangements on Proton-Conductivity in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 6183-6189	16.4	315
1192	An exceptional 54-fold interpenetrated coordination polymer with 10(3)-srs network topology. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 11406-9	16.4	314
1191	Syntheses and characterization of six coordination polymers of zinc(II) and cobalt(II) with 1,3,5-benzenetricarboxylate anion and bis(imidazole) ligands. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 3027-37	5.1	300
1190	Colorimetric detection of Pb <sup>2+</sup> using glutathione functionalized gold nanoparticles. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2010</b> , 2, 1466-70	9.5	298

1189	Density functional theory characterization and design of high-performance diarylamine-fluorene dyes with different $\beta$ spacers for dye-sensitized solar cells. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 568-576		291
1188	N-rich zeolite-like metal-organic framework with sodalite topology: high CO <sub>2</sub> uptake, selective gas adsorption and efficient drug delivery. <i>Chemical Science</i> , <b>2012</b> , 3, 2114	9.4	252
1187	A fluorescent sensor for highly selective detection of nitroaromatic explosives based on a 2D, extremely stable, metal-organic framework. <i>Chemistry - A European Journal</i> , <b>2014</b> , 20, 3589-94	4.8	247
1186	A bridge between pillared-layer and helical structures: a series of three-dimensional pillared coordination polymers with multiform helical chains. <i>Chemistry - A European Journal</i> , <b>2006</b> , 12, 6528-41	4.8	229
1185	A series of three-dimensional lanthanide coordination polymers with rutile and unprecedented rutile-related topologies. <i>Inorganic Chemistry</i> , <b>2005</b> , 44, 7122-9	5.1	220
1184	Assembly of the highest connectivity Wells-Dawson polyoxometalate coordination polymer: the use of organic ligand flexibility. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 3274-83	5.1	219
1183	Quantum mechanical design and structure of the Li@B10H14 basket with a remarkably enhanced electro-optical response. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 11833-40	16.4	218
1182	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. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 8179-87	5.1	209
1181	Self-assembly and photocatalytic properties of polyoxoniobates: {Nb <sub>24</sub> O <sub>72</sub> }, {Nb <sub>32</sub> O <sub>96</sub> }, and {K <sub>12</sub> Nb <sub>96</sub> O <sub>288</sub> } clusters. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 14004-10	16.4	205
1180	An unprecedented eight-connected self-penetrating network based on pentanuclear zinc cluster building blocks. <i>Chemical Communications</i> , <b>2005</b> , 4789-91	5.8	203
1179	Tailored Synthesis of Octopus-type Janus Nanoparticles for Synergistic Actively-Targeted and Chemo-Photothermal Therapy. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 2118-21	16.4	199
1178	Chiral polyoxometalate-based materials: From design syntheses to functional applications. <i>Coordination Chemistry Reviews</i> , <b>2013</b> , 257, 702-717	23.2	197
1177	Solvatochromic behavior of chiral mesoporous metal-organic frameworks and their applications for sensing small molecules and separating cationic dyes. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 3639-45	4.8	189
1176	Tuning the Dimensionality of the Coordination Polymer Based on Polyoxometalate by Changing the Spacer Length of Ligands. <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 3717-3724	3.5	188
1175	Structures and Luminescent Properties of Seven Coordination Polymers of Zinc(II) and Cadmium(II) with 3,3',4,4'-Benzophenone Tetracarboxylate Anion and Bis(imidazole). <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 675-684	3.5	186
1174	Unusual parallel and inclined interlocking modes in polyrotaxane-like metal-organic frameworks. <i>Chemical Communications</i> , <b>2008</b> , 2233-5	5.8	181
1173	Assemblies of copper bis(triazole) coordination polymers using the same kegglin polyoxometalate template. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 100-10	5.1	179
1172	Stable luminescent metal-organic frameworks as dual-functional materials to encapsulate Ln(3+) ions for white-light emission and to detect nitroaromatic explosives. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 3290-5	5.1	178

- 1171 Bottom-up synthesis of porous coordination frameworks: apical substitution of a pentanuclear tetrahedral precursor. *Angewandte Chemie - International Edition*, **2009**, 48, 5291-5 16.4 176
- 1170 Highly efficient visible-light-driven CO<sub>2</sub> reduction to formate by a new anthracene-based zirconium MOF via dual catalytic routes. *Journal of Materials Chemistry A*, **2016**, 4, 2657-2662 13 174
- 1169 How to design proper spacer order of the D-πA dyes for DSSCs? A density functional response. *Dyes and Pigments*, **2012**, 95, 313-321 4.6 169
- 1168 Chiral polyoxometalate-induced enantiomerically 3D architectures: a new route for synthesis of high-dimensional chiral compounds. *Journal of the American Chemical Society*, **2007**, 129, 10066-7 16.4 168
- 1167 Polyoxometalates in dye-sensitized solar cells. *Chemical Society Reviews*, **2019**, 48, 260-284 58.5 168
- 1166 Thermally Induced Reversible Phase Transformations Accompanied by Emission Switching Between Different Colors of Two Aromatic-Amine Compounds. *Advanced Materials*, **2009**, 21, 3165-3169 24 166
- 1165 Exceptional self-penetrating networks containing unprecedented quintuple-stranded molecular braid, 9-fold meso helices, and 17-fold interwoven helices. *Inorganic Chemistry*, **2007**, 46, 4158-66 5.1 164
- 1164 Spontaneous resolution of a 3D chiral polyoxometalate-based polythreaded framework consisting of an achiral ligand. *Chemical Communications*, **2008**, 58-60 5.8 163
- 1163 Self-assembly of 2D→2D interpenetrating coordination polymers showing polyrotaxane- and polycatenane-like motifs: influence of various ligands on topological structural diversity. *Inorganic Chemistry*, **2008**, 47, 10600-10 5.1 159
- 1162 An ionothermal synthetic approach to porous polyoxometalate-based metal-organic frameworks. *Angewandte Chemie - International Edition*, **2012**, 51, 7985-9 16.4 155
- 1161 pH-dependent assembly of hybrids based on Wells-Dawson POM/Ag chemistry. *Inorganic Chemistry*, **2008**, 47, 5145-53 5.1 155
- 1160 Stepwise assembly of metal-organic framework based on a metal-organic polyhedron precursor for drug delivery. *Chemical Communications*, **2011**, 47, 7128-30 5.8 154
- 1159 Controllable fabrication of carbon nanotube and nanobelt with a polyoxometalate-assisted mild hydrothermal process. *Journal of the American Chemical Society*, **2005**, 127, 6534-5 16.4 153
- 1158 An unusual polyoxometalate-encapsulating 3D polyrotaxane framework formed by molecular squares threading on a twofold interpenetrated diamondoid skeleton. *Chemical Communications*, **2007**, 4245-7 5.8 147
- 1157 Supramolecular isomerism with polythreaded topology based on [Mo<sub>8</sub>O<sub>26</sub>]<sup>4-</sup> isomers. *Inorganic Chemistry*, **2008**, 47, 529-34 5.1 144
- 1156 Transesterification of Vegetable Oil to Biodiesel using a Heteropolyacid Solid Catalyst. *Advanced Synthesis and Catalysis*, **2007**, 349, 1057-1065 5.6 144
- 1155 A microporous anionic metal-organic framework for sensing luminescence of lanthanide(III) ions and selective absorption of dyes by ionic exchange. *Chemistry - A European Journal*, **2014**, 20, 5625-30 4.8 143
- 1154 Influence of neutral ligands on the structures of silver(I) sulfonates. *Inorganic Chemistry*, **2005**, 44, 9374-83 14.3 143

1153	An unprecedented fivefold interpenetrated lvt network containing the exceptional racemic motifs originated from nine interwoven helices. <i>Chemical Communications</i> , <b>2005</b> , 5450-2	5.8	143
1152	Role of Excess Electrons in Nonlinear Optical Response. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 612-9	6.4	140
1151	L-cysteine functionalized gold nanoparticles for the colorimetric detection of Hg <sup>2+</sup> induced by ultraviolet light. <i>Nanotechnology</i> , <b>2010</b> , 21, 025501	3.4	138
1150	Carbon nanodots@zeolitic imidazolate framework-8 nanoparticles for simultaneous pH-responsive drug delivery and fluorescence imaging. <i>CrystEngComm</i> , <b>2014</b> , 16, 3259	3.3	129
1149	Two Dawson-templated three-dimensional metal-organic frameworks based on oxalate-bridged binuclear cobalt(II)/Nickel(II) SBUs and Bpy linkers. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 7133-8	5.1	128
1148	Rationally designed, polymeric, extended metal-ciprofloxacin complexes. <i>Chemistry - A European Journal</i> , <b>2005</b> , 11, 6673-86	4.8	126
1147	Protein-sized chiral Fe(168) cages with NbO-type topology. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 14600-1	16.4	121
1146	A Practicable Li/Na-Ion Hybrid Full Battery Assembled by a High-Voltage Cathode and Commercial Graphite Anode: Superior Energy Storage Performance and Working Mechanism. <i>Advanced Energy Materials</i> , <b>2018</b> , 8, 1702504	21.8	120
1145	An Interpenetrating Architecture Based on the WellsDawson Polyoxometalate and AgI⋯AgI Interactions. <i>Crystal Growth and Design</i> , <b>2011</b> , 11, 2736-2742	3.5	120
1144	Spontaneous resolution of chiral polyoxometalate-based compounds consisting of 3D chiral inorganic skeletons assembled from different helical units. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 9999-10006	4.8	119
1143	A three-dimensional porous metal-organic framework with the rutile topology constructed from triangular and distorted octahedral building blocks. <i>Chemical Communications</i> , <b>2005</b> , 2402-4	5.8	118
1142	DFT Study on Sulfur-Doped g-C <sub>3</sub> N <sub>4</sub> Nanosheets as a Photocatalyst for CO <sub>2</sub> Reduction Reaction. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 7712-7719	3.8	116
1141	Quantum chemical design of nonlinear optical materials by sp <sup>2</sup> -hybridized carbon nanomaterials: issues and opportunities. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 5439	7.1	116
1140	A Series of Lead(II)-Organic Frameworks Based on Pyridyl Carboxylate Acid N-Oxide Derivatives: Syntheses, Structures, and Luminescent Properties. <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 3566-3576	3.5	116
1139	Two multi-copper-containing heteropolyoxotungstates constructed from the lacunary Keggin polyoxoanion and the high-nuclear spin cluster. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 8162-9	5.1	116
1138	Using Flexible and Rigid Organic Ligands to Tune Topology Structures Based on Keggin Polyoxometalates. <i>Crystal Growth and Design</i> , <b>2010</b> , 10, 1104-1110	3.5	115
1137	A mixed-valence tin-oxygen cluster containing six peripheral ferrocene units. <i>Angewandte Chemie - International Edition</i> , <b>2004</b> , 43, 2409-11	16.4	112
1136	Enhanced proton and electron reservoir abilities of polyoxometalate grafted on graphene for high-performance hydrogen evolution. <i>Energy and Environmental Science</i> , <b>2016</b> , 9, 1012-1023	35.4	109

1135	Polyoxometalate-based materials for sustainable and clean energy conversion and storage. <i>EnergyChem</i> , <b>2019</b> , 1, 100021	36.9	109
1134	Highly sensitive oxygen sensors based on Cu(I) complex-polystyrene composite nanofibrous membranes prepared by electrospinning. <i>Chemical Communications</i> , <b>2009</b> , 5868-70	5.8	109
1133	Assembly of Multitrack Cu <sup>II</sup> Coordination Polymeric Chain-Modified Polyoxometalates Influenced by Polyoxoanion Cluster and Ligand. <i>Crystal Growth and Design</i> , <b>2007</b> , 7, 2535-2541	3.5	109
1132	Multifunctional hollow mesoporous silica nanocages for cancer cell detection and the combined chemotherapy and photodynamic therapy. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2011</b> , 3, 2479-86	9.5	108
1131	Silver/Polyaniline Composite Nanotubes: One-Step Synthesis and Electrocatalytic Activity for Neurotransmitter Dopamine. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 15175-15181	3.8	108
1130	Theoretical characterization and design of small molecule donor material containing naphthodithiophene central unit for efficient organic solar cells. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 1611-9	3.5	105
1129	Biorecognition-Driven Self-Assembly of Gold Nanorods: A Rapid and Sensitive Approach toward Antibody Sensing. <i>Chemistry of Materials</i> , <b>2007</b> , 19, 5809-5811	9.6	105
1128	Structures and Luminescent Properties of a Series of Zinc(II) and Cadmium(II) 4,4'-Oxydipthalate Coordination Polymers with Various Ligands Based on Bis(pyridyl imidazole) under Hydrothermal Conditions. <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 1610-1616	3.5	104
1127	Syntheses, Characterization, and Luminescent Properties of Three 3D Lead <sup>II</sup> Organic Frameworks with 1D Channels. <i>Crystal Growth and Design</i> , <b>2007</b> , 7, 513-520	3.5	104
1126	Mixed-valence iron(II, III) trimesates with open frameworks modulated by solvents. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 7782-8	5.1	104
1125	A multifunctional microporous anionic metal-organic framework for column-chromatographic dye separation and selective detection and adsorption of Cr <sup>3+</sup> . <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 23426-23434	13	102
1124	Controllable synthesis of iridium(III)-based aggregation-induced emission and/or piezochromic luminescence phosphors by simply adjusting the substitution on ancillary ligands. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 1440	7.1	102
1123	A cationic iridium(III) complex with aggregation-induced emission (AIE) properties for highly selective detection of explosives. <i>Chemical Communications</i> , <b>2014</b> , 50, 6031-4	5.8	101
1122	A polyoxometalate-encapsulated 3D porous metal-organic pseudo-rotaxane framework. <i>Chemical Communications</i> , <b>2010</b> , 46, 5097-9	5.8	100
1121	Building block approach to nanostructures: step-by-step assembly of large lanthanide-containing polytungstoarsenate aggregates. <i>Dalton Transactions</i> , <b>2007</b> , 4293-301	4.3	99
1120	Uniform hollow mesoporous silica nanocages for drug delivery in vitro and in vivo for liver cancer therapy. <i>Journal of Materials Chemistry</i> , <b>2011</b> , 21, 5299		97
1119	An unprecedented (6,8)-connected self-penetrating network based on two distinct zinc clusters. <i>Chemical Communications</i> , <b>2007</b> , 4863-5	5.8	97
1118	Catenation of loop-containing 2D layers with a 3D pcu skeleton into a new type of entangled framework having polyrotaxane and polycatenane character. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 5555-7	5.1	96

1117	An organic-inorganic hybrid material constructed from a three-dimensional coordination complex cationic framework and entrapped hexadecavanadate clusters. <i>Chemical Communications</i> , <b>2005</b> , 5023-5	5.8	95
1116	Oxidative Polyoxometalates Modified Graphitic Carbon Nitride for Visible-Light CO Reduction. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 11689-11695	9.5	94
1115	2D Cd(II)-lanthanide(III) heterometallic-organic frameworks based on metalloligands for tunable luminescence and highly selective, sensitive, and recyclable detection of nitrobenzene. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 8105-13	5.1	94
1114	Metal-organic replica of gamma-Pu: the first uninodal 10-connected coordination network based on pentanuclear cadmium clusters. <i>Chemical Communications</i> , <b>2009</b> , 410-2	5.8	94
1113	Syntheses and structures of organic-inorganic hybrid compounds based on metal-fluconazole coordination polymers and the beta-Mo8O26 anion. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 8283-90	5.1	94
1112	The stability and nonlinear optical properties: Encapsulation of an excess electron compound LiCN <sup>-</sup> Li within boron nitride nanotubes. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 2196-2202		93
1111	Precise synthesis of unique polydopamine/mesoporous calcium phosphate hollow Janus nanoparticles for imaging-guided chemo-photothermal synergistic therapy. <i>Chemical Science</i> , <b>2017</b> , 8, 8067-8077	9.4	92
1110	Utilizing d-p Bonds for Ultralong Organic Phosphorescence. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 6645-6649	16.4	90
1109	Reversible piezochromic behavior of two new cationic iridium(III) complexes. <i>Chemical Communications</i> , <b>2012</b> , 48, 2000-2	5.8	90
1108	Design and syntheses of blue luminescent zinc(II) and cadmium(II) complexes with bidentate or tridentate pyridyl-imidazole ligands. <i>Polyhedron</i> , <b>2006</b> , 25, 635-644	2.7	90
1107	Unusual microporous polycatenane-like metal-organic frameworks for the luminescent sensing of Ln <sup>3+</sup> cations and rapid adsorption of iodine. <i>Chemical Communications</i> , <b>2012</b> , 48, 5919-21	5.8	88
1106	Iodine-templated assembly of unprecedented 3d-4f metal-organic frameworks as photocatalysts for hydrogen generation. <i>Chemical Communications</i> , <b>2013</b> , 49, 3564-6	5.8	87
1105	Realization of High-Energy Emission from [Cu(N <sub>3</sub> )(P <sub>3</sub> ) <sup>+</sup> Complexes for Organic Light-Emitting Diode Applications. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 13968-13973	3.8	87
1104	Entangled structures in polyoxometalate-based coordination polymers. <i>Coordination Chemistry Reviews</i> , <b>2014</b> , 279, 141-160	23.2	86
1103	A 2D bilayered metal-organic framework as a fluorescent sensor for highly selective sensing of nitro explosives. <i>Dalton Transactions</i> , <b>2015</b> , 44, 7822-7	4.3	85
1102	Redox-switchable second-order nonlinear optical responses of push-pull monotetraphialfulvalene-metalloporphyrins. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 6548-54	5.1	85
1101	Polyoxometalate-based crystalline tubular microreactor: redox-active inorganic-organic hybrid materials producing gold nanoparticles and catalytic properties. <i>Chemical Science</i> , <b>2012</b> , 3, 705-710	9.4	84
1100	Quantum chemical study of benzimidazole derivatives to tune the second-order nonlinear optical molecular switching by proton abstraction. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 4791-9	3.6	84

1099	A new molybdenum-oxide-based organic-inorganic hybrid framework templated by double-Keggin anions. <i>Chemical Communications</i> , <b>2007</b> , 2593-5	5.8	84
1098	Two Highly Water-Stable Imidazole-Based Ln-MOFs for Sensing Fe,CrO/CrO in a Water Environment. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 2005-2010	5.1	83
1097	Theoretical discussions on electron transport properties of perylene bisimide derivatives with different molecular packings and intermolecular interactions. <i>Journal of Materials Chemistry</i> , <b>2011</b> , 21, 134-143		83
1096	Chiral 3D Architectures with Helical Channels Constructed from Polyoxometalate Clusters and Copper@Amino Acid Complexes. <i>Angewandte Chemie</i> , <b>2006</b> , 118, 918-922	3.6	83
1095	Novel butterfly pyrene-based organic semiconductors for field effect transistors. <i>Chemical Communications</i> , <b>2006</b> , 755-7	5.8	83
1094	Spectroscopic and Excited-State Properties of Luminescent Rhenium(I) N-Heterocyclic Carbene Complexes Containing Aromatic Diimine Ligands. <i>Organometallics</i> , <b>1998</b> , 17, 1622-1630	3.8	83
1093	A hexanuclear cobalt metal@organic framework for efficient CO <sub>2</sub> reduction under visible light. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 12498-12505	13	82
1092	A DFT Study on The Two-Dimensional Second-Order Nonlinear Optical (NLO) Response of Terpyridine-Substituted Hexamolybdates: Physical Insight on 2D Inorganic@Organic Hybrid Functional Materials. <i>European Journal of Inorganic Chemistry</i> , <b>2012</b> , 2012, 705-711	2.3	82
1091	A luminescent dye@MOF as a dual-emitting platform for sensing explosives. <i>Chemical Communications</i> , <b>2015</b> , 51, 17521-4	5.8	81
1090	Electrical conductivity and electroluminescence of a new anthracene-based metal-organic framework with @conjugated zigzag chains. <i>Chemical Communications</i> , <b>2016</b> , 52, 2019-22	5.8	81
1089	Three neutral metal@organic frameworks with micro- and meso-pores for adsorption and separation of dyes. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 13060	13	81
1088	Theoretical study on the electronic spectrum and the origin of remarkably large third-order nonlinear optical properties of organoimide derivatives of hexamolybdates. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 23092-8	3.4	81
1087	Luminescent Metal@Organic Frameworks with Anthracene Chromophores: Small-Molecule Sensing and Highly Selective Sensing for Nitro Explosives. <i>Crystal Growth and Design</i> , <b>2016</b> , 16, 4374-4382	3.5	81
1086	Keggin POMs Modified by Bonding to Multitrack Cu(bipy) Chains through Linearly Arrayed Terminal and Bridging Oxygen Atoms of the M <sub>3</sub> O <sub>13</sub> Triad. <i>European Journal of Inorganic Chemistry</i> , <b>2007</b> , 2007, 1268-1274	2.3	80
1085	Uniform Pomegranate-Like Nanoclusters Organized by Ultrafine Transition Metal Oxide@Nitrogen-Doped Carbon Subunits with Enhanced Lithium Storage Properties. <i>Advanced Energy Materials</i> , <b>2018</b> , 8, 1702347	21.8	80
1084	Controllable synthesis of isorecticular pillared-layer MOFs: gas adsorption, iodine sorption and sensing small molecules. <i>Journal of Materials Chemistry A</i> , <b>2014</b> , 2, 14827-14834	13	79
1083	Investigation of Dibenzoboroles Having @Electrons: Toward a New Type of Two-Dimensional NLO Molecular Switch?. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 12551-12557	3.8	79
1082	Prediction of remarkably large second-order nonlinear optical properties of organoimido-substituted hexamolybdates. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 3576-87	2.8	78



1081	A stable Alq3@MOF composite for white-light emission. <i>Chemical Communications</i> , <b>2016</b> , 52, 3288-91	5.8	77
1080	Enhanced CO <sub>2</sub> photoreduction via tuning halides in perovskites. <i>Journal of Catalysis</i> , <b>2019</b> , 369, 201-208	7.3	77
1079	Redox and Photoisomerization Switching the Second-Order Nonlinear Optical Properties of a Tetrathiafulvalene Derivative Across Six States: A DFT Study. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 23946-23954	3.8	76
1078	A (3,12)-Connected 3D Metal-Organic Framework Based on Nanosized Octanuclear Zinc Clusters. <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 3490-3492	3.5	76
1077	Versatile frameworks constructed from divalent metals and 1,2,3,4-butanetetracarboxylate anion: syntheses, crystal structures, luminescence and magnetic properties. <i>CrystEngComm</i> , <b>2008</b> , 10, 894	3.3	75
1076	A stable luminescent anionic porous metal-organic framework for moderate adsorption of CO <sub>2</sub> and selective detection of nitro explosives. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 7224-7228	1.3	74
1075	A stable porous anionic metal-organic framework for luminescence sensing of Ln(3+) ions and detection of nitrobenzene. <i>Chemistry - an Asian Journal</i> , <b>2014</b> , 9, 749-53	4.5	73
1074	pH-dependent self-assembly of divalent metals with a new ligand containing polycarboxylate: syntheses, crystal structures, luminescent and magnetic properties. <i>CrystEngComm</i> , <b>2010</b> , 12, 2157	3.3	73
1073	Derivation and Decoration of Nets with Trigonal-Prismatic Nodes: A Unique Route to Reticular Synthesis of Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 5299-307	16.4	73
1072	Dinuclear metal complexes: multifunctional properties and applications. <i>Chemical Society Reviews</i> , <b>2020</b> , 49, 765-838	58.5	72
1071	A new type of organic-inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. <i>Dalton Transactions</i> , <b>2013</b> , 42, 15053-62	4.3	72
1070	Assembly of a luminescent core-shell nanocluster featuring a Ag <sub>34</sub> S <sub>26</sub> shell and a W <sub>6</sub> O <sub>21</sub> (6-) polyoxoanion core. <i>Chemical Communications</i> , <b>2012</b> , 48, 5844-6	5.8	72
1069	The excess electron in a boron nitride nanotube: pyramidal NBO charge distribution and remarkable first hyperpolarizability. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 11350-5	4.8	72
1068	Construction and property investigation of transition-metal complexes modified octamolybdate hybrid materials based on V-shaped organic ligands. <i>CrystEngComm</i> , <b>2010</b> , 12, 434-445	3.3	72
1067	Obtaining carbon nanotubes from grass. <i>Nanotechnology</i> , <b>2005</b> , 16, 1192-1195	3.4	72
1066	Ternary hybrids as efficient bifunctional electrocatalysts derived from bimetallic metal-organic-frameworks for overall water splitting. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 5789-5796	1.3	71
1065	Creation of cationic iridium(III) complexes with aggregation-induced phosphorescent emission (AIPE) properties by increasing rotation groups on carbazole peripheries. <i>Dalton Transactions</i> , <b>2011</b> , 40, 2947-53	4.3	71
1064	Capturing a synergistic effect of a conical push and an inward pull in fluoro derivatives of Li@B <sub>10</sub> H <sub>14</sub> basket: toward a higher vertical ionization potential and nonlinear optical response. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 923-31	2.8	71

1063	A polyoxometalate-based single-molecule magnet with a mixed-valent {Mn(IV)2Mn(III)6Mn(II)4} core. <i>Chemical Communications</i> , <b>2013</b> , 49, 2515-7	5.8	70
1062	Novel rare-earth(III)-based water soluble emitters for Fe(III) detection. <i>Sensors and Actuators B: Chemical</i> , <b>2010</b> , 143, 595-599	8.5	70
1061	A novel carboxyethyltin functionalized sandwich-type germanotungstate: synthesis, crystal structure, photosensitivity, and application in dye-sensitized solar cells. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2014</b> , 6, 7876-84	9.5	69
1060	A stable metal-organic framework with suitable pore sizes and rich uncoordinated nitrogen atoms on the internal surface of micropores for highly efficient CO <sub>2</sub> capture. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 7361-7367	13	69
1059	Assembly of organic-inorganic hybrid materials constructed from polyoxometalate and metal-1,2,4-triazole units: synthesis, structures, magnetic, electrochemical and photocatalytic properties. <i>CrystEngComm</i> , <b>2015</b> , 17, 2176-2189	3.3	69
1058	Selected-control synthesis of monodisperse Fe <sub>3</sub> O <sub>4</sub> @C core-shell spheres, chains, and rings as high-performance anode materials for lithium-ion batteries. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 11417-22	4.8	69
1057	Diamondoid-structured polymolybdate-based metal-organic frameworks as high-capacity anodes for lithium-ion batteries. <i>Chemical Communications</i> , <b>2017</b> , 53, 5204-5207	5.8	68
1056	Selective sensing of 2,4,6-trinitrophenol (TNP) in aqueous media with "aggregation-induced emission enhancement" (AIEE)-active iridium(III) complexes. <i>Chemical Communications</i> , <b>2018</b> , 54, 1730-1733	5.8	68
1055	Iridium(III) complexes adopting 1,2-diphenyl-1H-benzimidazole ligands for highly efficient organic light-emitting diodes with low efficiency roll-off and non-doped feature. <i>Journal of Materials Chemistry C</i> , <b>2014</b> , 2, 2150	7.1	67
1054	Theoretical studies on organoimido-substituted hexamolybdates dyes for dye-sensitized solar cells (DSSC). <i>Dyes and Pigments</i> , <b>2013</b> , 99, 440-446	4.6	67
1053	Construction of different dimensional inorganic-organic hybrid materials based on polyoxometalates and metal-organic units via changing metal ions: from non-covalent interactions to covalent connections. <i>Dalton Transactions</i> , <b>2008</b> , 3824-35	4.3	67
1052	Controllable colours and shapes of silver nanostructures based on pH: application to surface-enhanced Raman scattering. <i>Nanotechnology</i> , <b>2007</b> , 18, 325602	3.4	67
1051	Assembly of cerium(III)-stabilized polyoxotungstate nanoclusters with SeO <sub>3</sub> (2-)/TeO <sub>3</sub> (2-) templates: from single polyoxoanions to inorganic hollow spheres in dilute solution. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 11007-15	4.8	66
1050	Remarkable solvent-size effects in constructing novel porous 1,3,5-benzenetricarboxylate metal-organic frameworks. <i>CrystEngComm</i> , <b>2012</b> , 14, 5596	3.3	66
1049	Designed fabrication of unique eccentric mesoporous silica nanocluster-based core-shell nanostructures for pH-responsive drug delivery. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2013</b> , 5, 7282-90	9.5	66
1048	Fluorescent hollow/rattle-type mesoporous Au@SiO <sub>2</sub> nanocapsules for drug delivery and fluorescence imaging of cancer cells. <i>Journal of Colloid and Interface Science</i> , <b>2011</b> , 358, 109-15	9.3	66
1047	Two Heterometallic Aggregates Constructed from the {P <sub>2</sub> W <sub>12</sub> }-Based Trimeric Polyoxotungstates and 3d-4f Heterometals. <i>Crystal Growth and Design</i> , <b>2010</b> , 10, 135-139	3.5	65
1046	Two eight-connected self-penetrating porous metal-organic frameworks: configurational isomers caused by different linking modes between terephthalate and binuclear nickel building units. <i>CrystEngComm</i> , <b>2009</b> , 11, 274-277	3.3	65

1045	Preparation and Formation Mechanism of Different $\beta$ -Fe <sub>2</sub> O <sub>3</sub> Morphologies from Snowflake to Paired Microplates, Dumbbell, and Spindle Microstructures. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 9049-9054	3.8	65
1044	Controllable synthesis of a non-interpenetrating microporous metal-organic framework based on octahedral cage-like building units for highly efficient reversible adsorption of iodine. <i>Chemical Communications</i> , <b>2012</b> , 48, 10001-3	5.8	64
1043	Boron/nitrogen substitution of the central carbon atoms of the biphenalenyl diradical dimer: a novel 2e-12c bond and large NLO responses. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 11773-9	4.8	64
1042	Charge Carrier Transporting, Photoluminescent, and Electroluminescent Properties of Zinc(II)-2-(2-hydroxyphenyl)benzothiazolate Complex. <i>Chemistry of Materials</i> , <b>2007</b> , 19, 1740-1748	9.6	64
1041	Modulation on charge recombination and light harvesting toward high-performance benzothiadiazole-based sensitizers in dye-sensitized solar cells: A theoretical investigation. <i>Journal of Power Sources</i> , <b>2014</b> , 267, 300-308	8.9	63
1040	Control of interpenetration in S-containing metal-organic frameworks for selective separation of transition metal ions. <i>Chemical Communications</i> , <b>2013</b> , 49, 1088-90	5.8	63
1039	Quantum chemical research on structures, linear and nonlinear optical properties of the Li@n-acenes salt (n = 1, 2, 3, and 4). <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 2035-40	2.8	63
1038	Influence of anionic sulfonate-containing co-ligands on the solid structures of silver complexes supported by 4,4'-bipyridine bridges. <i>Dalton Transactions</i> , <b>2008</b> , 5331-41	4.3	63
1037	Structural study of silver(I) sulfonate complexes with pyrazine derivatives. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 7299-311	5.1	63
1036	Graphene-coated hybrid electrocatalysts derived from bimetallic metal-organic frameworks for efficient hydrogen generation. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 5000-5006	13	62
1035	Pillared metal organic frameworks for the luminescence sensing of small molecules and metal ions in aqueous solutions. <i>Dalton Transactions</i> , <b>2015</b> , 44, 1754-60	4.3	62
1034	How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 19792-19798	3.8	62
1033	Fac-Alq <sub>3</sub> and mer-Alq <sub>3</sub> nano/microcrystals with different emission and charge-transporting properties. <i>Advanced Materials</i> , <b>2010</b> , 22, 1631-4	24	62
1032	Polyaniline Nanotubes Prepared Using Fiber Mats Membrane as the Template and their Gas-response Behavior. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 8215-8222	3.8	62
1031	d(10)-Metal coordination polymers based on analogue di(pyridyl)imidazole derivatives and 4,4'-oxydibenzoic acid: influence of flexible and angular characters of neutral ligands on structural diversity. <i>Dalton Transactions</i> , <b>2008</b> , 6796-807	4.3	62
1030	A Ligand Exchange Route to Highly Luminescent Surface-Functionalized ZnS Nanoparticles and Their Transparent Polymer Nanocomposites. <i>Advanced Functional Materials</i> , <b>2008</b> , 18, 3070-3079	15.6	62
1029	Tailored Surfaces on 2D Material: UFO-Like Cyclodextrin-Pd Nanosheet/Metal Organic Framework Janus Nanoparticles for Synergistic Cancer Therapy. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1803815	15.6	62
1028	Encapsulating Red Phosphorus in Ultralarge Pore Volume Hierarchical Porous Carbon Nanospheres for Lithium/Sodium-Ion Half/Full Batteries. <i>ACS Nano</i> , <b>2019</b> , 13, 13513-13523	16.7	61

1027	pH-Dependent Binary Metal-Organic Compounds Assembled from Different Helical Units: Structural Variation and Supramolecular Isomers. <i>Crystal Growth and Design</i> , <b>2010</b> , 10, 1699-1705	3.5	61
1026	Metal-Organic Frameworks Based on Different Benzimidazole Derivatives: Effect of Length and Substituent Groups of the Ligands on the Structures. <i>Crystal Growth and Design</i> , <b>2010</b> , 10, 1161-1170	3.5	61
1025	Electronic structures and chemical bonding in transition metal monosilicides MSi (M = 3d, 4d, 5d elements). <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 184306	3.9	61
1024	An Anionic Interpenetrated Zeolite-Like Metal-Organic Framework Composite As a Tunable Dual-Emission Luminescent Switch for Detecting Volatile Organic Molecules. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 17298-17304	4.8	61
1023	Self-organization towards complex multi-fold meso-helices in the structures of Wells-Dawson polyoxometalate-based hybrid materials for lithium-ion batteries. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 3371-3376	13	60
1022	Intramolecular $\pi$ -stacking in cationic iridium(III) complexes with a triazole-pyridine type ancillary ligand: synthesis, photophysics, electrochemistry properties and piezochromic behavior. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 12736		60
1021	A series of pillar-layer metal-organic frameworks based on 5-aminoisophthalic acid and 4,4'-bipyridine. <i>Dalton Transactions</i> , <b>2012</b> , 41, 1047-53	4.3	60
1020	Hetero-metallic active sites coupled with strongly reductive polyoxometalate for selective photocatalytic CO-to-CH conversion in water. <i>Chemical Science</i> , <b>2019</b> , 10, 185-190	9.4	59
1019	Enhanced Visible Photovoltaic Response of TiO <sub>2</sub> Thin Film with an All-Inorganic Donor-Acceptor Type Polyoxometalate. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 13714-21	9.5	59
1018	A Stable Polyoxometalate-Pillared Metal-Organic Framework for Proton-Conducting and Colorimetric Biosensing. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 11894-8	4.8	59
1017	High-Performance Metal-Organic Framework-Based Single Ion Conducting Solid-State Electrolytes for Low-Temperature Lithium Metal Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 43206-43213	9.5	59
1016	Heterogeneous hydroxylation catalyzed by multi-walled carbon nanotubes at low temperature. <i>Applied Catalysis A: General</i> , <b>2006</b> , 299, 212-217	5.1	59
1015	Three-dimensional mesomeric networks assembled from helix-linked sheets: syntheses, structures, and magnetisms. <i>Dalton Transactions</i> , <b>2005</b> , 2609-14	4.3	59
1014	Self-assembled arrays of polyoxometalate-based metal-organic nanotubes for proton conduction and magnetism. <i>Chemical Communications</i> , <b>2015</b> , 51, 11313-6	5.8	58
1013	Piezochromic luminescent (PCL) behavior and aggregation-induced emission (AIE) property of a new cationic iridium(III) complex. <i>Dalton Transactions</i> , <b>2012</b> , 41, 9590-3	4.3	58
1012	Theoretical interpretation of different nanotube morphologies among Group III (B, Al, Ga) nitrides. <i>Chemical Physics Letters</i> , <b>2005</b> , 408, 145-149	2.5	58
1011	First principles study for the key electronic, optical and nonlinear optical properties of novel donor-acceptor chalcones. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 72, 58-69	2.8	57
1010	Facile and Scalable Synthesis of Novel Spherical Au Nanocluster Assemblies@Polyacrylic Acid/Calcium Phosphate Nanoparticles for Dual-Modal Imaging-Guided Cancer Chemotherapy. <i>Small</i> , <b>2015</b> , 11, 3162-73	11	57

1009	Solid-state structural transformation doubly triggered by reaction temperature and time in 3D metal-organic frameworks: great enhancement of stability and gas adsorption. <i>Chemical Science</i> , <b>2014</b> , 5, 1368	9.4	57
1008	An unprecedented organic-inorganic hybrid based on the first $\{Nb_{10}V_{40}O_{40}(OH)_2\}(12-)$ clusters and copper cations. <i>Chemical Communications</i> , <b>2012</b> , 48, 103-5	5.8	57
1007	Adsorption of volatile organic compounds in porous metal-organic frameworks functionalized by polyoxometalates. <i>Journal of Solid State Chemistry</i> , <b>2011</b> , 184, 3034-3039	3.3	57
1006	A 3D chiral nanoporous coordination framework consisting of homochiral nanotubes assembled from octuple helices. <i>Chemical Communications</i> , <b>2007</b> , 4620-2	5.8	57
1005	Density functional theory study on the first hyperpolarizabilities of organoimido derivatives of hexamolybdates. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 22332-6	3.4	57
1004	A neutral dinuclear Ir(III) complex for anti-counterfeiting and data encryption. <i>Chemical Communications</i> , <b>2017</b> , 53, 3022-3025	5.8	56
1003	AIE Multinuclear Ir(III) Complexes for Biocompatible Organic Nanoparticles with Highly Enhanced Photodynamic Performance. <i>Advanced Science</i> , <b>2019</b> , 6, 1802050	13.6	56
1002	New AIE-active dinuclear Ir(III) complexes with reversible piezochromic phosphorescence behaviour. <i>Chemical Communications</i> , <b>2015</b> , 51, 13036-9	5.8	56
1001	Self-Assembly of Goldberg Polyhedra from a Concave $[WVO(RCO)(SO)]$ Building Block with 5-Fold Symmetry. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 17365-17368	16.4	56
1000	The preparation of new covalent organic framework embedded with silver nanoparticles and its applications in degradation of organic pollutants from waste water. <i>Dalton Transactions</i> , <b>2019</b> , 48, 1051-1059	4.3	55
999	New ionic dinuclear Ir(III) Schiff base complexes with aggregation-induced phosphorescent emission (AIPE). <i>Chemical Communications</i> , <b>2014</b> , 50, 6977-80	5.8	55
998	The interplay of intermolecular interactions, packing motifs and electron transport properties in perylene diimide related materials: a theoretical perspective. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 20840		55
997	Second-Order Nonlinear Optical Properties of Transition-Metal-Trisubstituted Polyoxometalate-Diphosphate Complexes: A Donor-Conjugated Bridge-Acceptor Paradigm for Totally Inorganic Nonlinear Optical Materials. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 19672-19676	3.8	55
996	Two Novel One-Dimensional $\mu$ -Keggin-Based Coordination Polymers with Argentophilic $\{Ag_3\}^{3+}/\{Ag_4\}^{4+}$ Clusters. <i>Crystal Growth and Design</i> , <b>2009</b> , 9, 2110-2116	3.5	55
995	Theoretical study on the second-order nonlinear optical properties of asymmetric spiro-silabifluorene derivatives. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 4817-21	2.8	55
994	Interlocked and Interdigitated Architectures from Self-Assembly of Long Flexible Ligands and Cadmium Salts. <i>Angewandte Chemie</i> , <b>2004</b> , 116, 5146-5150	3.6	55
993	Theoretical insight into the origin of large Stokes shift and photophysical properties of anilido-pyridine boron difluoride dyes. <i>ChemPhysChem</i> , <b>2012</b> , 13, 3714-22	3.2	54
992	Chirality and magnetism of an open-framework cobalt phosphite containing helical channels from achiral materials. <i>Chemical Communications</i> , <b>2010</b> , 46, 2614-6	5.8	54

991	Effects of starch nanocrystals on structure and properties of waterborne polyurethane-based composites. <i>Carbohydrate Polymers</i> , <b>2011</b> , 85, 824-831	10.3	54
990	Fluorescent Gold Nanoprobes for the Sensitive and Selective Detection for Hg. <i>Nanoscale Research Letters</i> , <b>2010</b> , 5, 1856-1860	5	54
989	pH-tuned synthesis of gold nanostructures from gold nanorods with different aspect ratios. <i>Nanotechnology</i> , <b>2005</b> , 16, 2555-2560	3.4	54
988	Anderson-like alkoxo-polyoxovanadate clusters serving as unprecedented second building units to construct metal-organic polyhedra. <i>Chemical Communications</i> , <b>2016</b> , 52, 9632-5	5.8	53
987	Polyoxometalate-anatase TiO <sub>2</sub> composites are introduced into the photoanode of dye-sensitized solar cells to retard the recombination and increase the electron lifetime. <i>Dalton Transactions</i> , <b>2013</b> , 42, 2691-5	4.3	53
986	Self-assembly versus stepwise synthesis: heterometal-organic frameworks based on metalloligands with tunable luminescence properties. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 11279-86	4.8	53
985	Study of a hydrothermal reaction system of copper, imidazole and polyoxometalates: selective assembly of a 3D porous metal-organic pseudo-rotaxane framework and encapsulation of polyoxometalate clusters. <i>CrystEngComm</i> , <b>2011</b> , 13, 7079	3.3	53
984	A theoretical discussion on the relationships among molecular packings, intermolecular interactions, and electron transport properties for naphthalene tetracarboxylic diimide derivatives. <i>Journal of Materials Chemistry</i> , <b>2011</b> , 21, 15558		53
983	Quasi-Solid-State Sodium-Ion Full Battery with High-Power/Energy Densities. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 17903-17910	9.5	52
982	Two carboxyethyltin functionalized polyoxometalates for assembly on carbon nanotubes as efficient counter electrode materials in dye-sensitized solar cells. <i>Chemical Communications</i> , <b>2014</b> , 50, 14678-81	5.8	52
981	Assembly of Fe-substituted Dawson-type nanoscale selenotungstate clusters with photocatalytic H <sub>2</sub> evolution activity. <i>Chemical Communications</i> , <b>2014</b> , 50, 13265-7	5.8	52
980	A highly stable polyoxometalate-based metal-organic framework with an ABW zeolite-like structure. <i>Chemical Communications</i> , <b>2017</b> , 53, 10054-10057	5.8	52
979	Electronic properties and stability of dititanium(IV) substituted alpha-Keggin polyoxotungstate with heteroatom phosphorus by DFT. <i>Inorganic Chemistry</i> , <b>2005</b> , 44, 100-7	5.1	52
978	Bottom-Up Construction and Reversible Structural Transformation of Supramolecular Isomers based on Large Truncated Tetrahedra. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 780-784	16.4	52
977	Three novel 3D (3,8)-connected metal-organic frameworks constructed from flexible-rigid mixed ligands. <i>CrystEngComm</i> , <b>2009</b> , 11, 1842	3.3	51
976	Assembly of Organic-Inorganic Hybrid Materials Based on Dawson-Type Polyoxometalate and Multinuclear Copper-phen Complexes with Unique Magnetic Properties. <i>Crystal Growth and Design</i> , <b>2009</b> , 9, 3655-3660	3.5	51
975	Inorganic-organic hybrid materials with different dimensions constructed from copper-fluconazole metal-organic units and Keggin polyanion clusters. <i>Dalton Transactions</i> , <b>2008</b> , 2015-25	4.3	51
974	A luminescent metal organic framework with high sensitivity for detecting and removing copper ions from simulated biological fluids. <i>Dalton Transactions</i> , <b>2017</b> , 46, 2456-2461	4.3	50

973	A promising anchor group for efficient organic dye sensitized solar cells with iodine-free redox shuttles: a theoretical evaluation. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 14000	13	50
972	An orange iridium(III) complex with wide-bandwidth in electroluminescence for fabrication of high-quality white organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 7371	7.1	49
971	Facile preparation of fluorescent Au nanoclusters-based test papers for recyclable detection of Hg <sup>2+</sup> and Pb <sup>2+</sup> . <i>Sensors and Actuators B: Chemical</i> , <b>2017</b> , 241, 592-600	8.5	49
970	Complex-surfactant-assisted hydrothermal synthesis and properties of hierarchical worm-like cobalt sulfide microtubes assembled by hexagonal nanoplates. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 6625-31	4.8	49
969	Theoretical characterization of a typical hole/exciton-blocking material bathocuproine and its analogues. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 9097-103	2.8	49
968	The facile synthesis of hollow Au nanoflowers for synergistic chemo-photothermal cancer therapy. <i>Chemical Communications</i> , <b>2015</b> , 51, 14338-41	5.8	48
967	Facile and fast synthesis of urchin-shaped Fe <sub>3</sub> O <sub>4</sub> @Bi <sub>2</sub> S <sub>3</sub> core-shell hierarchical structures and their magnetically recyclable photocatalytic activity. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 4832		48
966	White light emission from Mn <sup>2+</sup> doped ZnS nanocrystals through the surface chelating of 8-hydroxyquinoline-5-sulfonic acid. <i>Nanotechnology</i> , <b>2010</b> , 21, 115702	3.4	48
965	Effect of pi-conjugated length of bridging ligand on the optoelectronic properties of platinum(II) dimers. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 2347-55	5.1	48
964	Metal-organic framework composites with luminescent gold(III) complexes. Strongly emissive and long-lived excited states in open air and photo-catalysis. <i>Chemical Science</i> , <b>2015</b> , 6, 7105-7111	9.4	47
963	Theoretical study on charge transport properties of cyanovinyl-substituted oligothiophenes. <i>Organic Electronics</i> , <b>2012</b> , 13, 1213-1222	3.5	47
962	A new electrodeposition approach for preparing polyoxometalates-based electrochromic smart windows. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 216-220	13	47
961	Knot-Isomers of Möbius Cyclacene: How Does the Number of Knots Influence the Structure and First Hyperpolarizability?. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 15380-15383	3.8	47
960	Syntheses, Structures, and Luminescent Properties of Zinc(II) and Cadmium(II) Coordination Complexes Based on Different (Pyridyl)imidazole Derivatives and 1,4-Benzenedicarboxylate. <i>Crystal Growth and Design</i> , <b>2009</b> , 9, 1353-1360	3.5	47
959	How does hybrid bridging core modification enhance the nonlinear optical properties in donor-acceptor configuration? A case study of dinitrophenol derivatives. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 118-28	3.5	46
958	A cationic iridium(III) complex showing aggregation-induced phosphorescent emission (AIPE) in the solid state: synthesis, characterization and properties. <i>Dalton Transactions</i> , <b>2012</b> , 41, 523-30	4.3	46
957	Theoretical study of the bridging effect on the charge carrier transport properties of cyclooctatetrathiophene and its derivatives. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 6907		46
956	Modification on C219 by coumarin donor toward efficient sensitizer for dye sensitized solar cells: A theoretical study. <i>Dyes and Pigments</i> , <b>2013</b> , 99, 127-135	4.6	46

955	Widening or Lengthening? Enhancing the First Hyperpolarizability of Tubiform Multilithium Salts. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 16340-16346	3.8	46
954	Second-order nonlinear optical properties of trisubstituted Keggin and Wells-Dawson polyoxometalates: density functional theory investigation of the inorganic donor-conjugated bridge-acceptor structure. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 8115-9	5.1	46
953	Directed Copper-Catalyzed Intermolecular Aminative Difunctionalization of Unactivated Alkenes. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 18475-18485	16.4	45
952	Theoretical study and design of triphenylamine-malononitrile-based p-type organic dyes with different linkers for dyes-sensitized solar cells. <i>Dyes and Pigments</i> , <b>2014</b> , 108, 106-114	4.6	45
951	Conformational Supramolecular Isomerism in Two-Dimensional Fluorescent Coordination Polymers Based on Flexible Tetracarboxylate Ligand. <i>Crystal Growth and Design</i> , <b>2013</b> , 13, 4092-4099	3.5	45
950	A Highly Energetic N-Rich Zeolite-Like Metal-Organic Framework with Excellent Air Stability and Insensitivity. <i>Advanced Science</i> , <b>2015</b> , 2, 1500150	13.6	45
949	A designed bithiopheneimide-based conjugated polymer for organic photovoltaic with ultrafast charge transfer at donor/PC(71)BM interface: theoretical study and characterization. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 25799-808	3.6	45
948	Theoretical investigation of structural and electronic properties of [PW12O40]3- on graphene layer. <i>Dalton Transactions</i> , <b>2012</b> , 41, 4602-7	4.3	45
947	Computational Study on Redox-Switchable 2D Second-Order Nonlinear Optical Properties of PushPull Mono-tetrathiafulvalene-Bis(Salicylaldehyde) Zn(II) Schiff Base Complexes. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 6024-6032	3.8	45
946	Construction of a three-dimensional polynuclear zinc compound based on unique metallophthalocyanine-like subunits. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 10-2	5.1	45
945	A (4,8)-Connected Fluorite Topology Framework Based on Mononuclear and Dinuclear Metal Centers. <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 2055-2057	3.5	45
944	A novel class of Zn(II) Schiff base complexes with aggregation-induced emission enhancement (AIEE) properties: Synthesis, characterization and photophysical/electrochemical properties. <i>Dyes and Pigments</i> , <b>2013</b> , 96, 467-474	4.6	44
943	Chiral salen-metal derivatives of polyoxometalates with asymmetric catalytic and photocatalytic activities. <i>Dalton Transactions</i> , <b>2011</b> , 40, 9964-6	4.3	44
942	Prediction of second-order optical nonlinearity of porphyrin-metal-polyoxometalate sandwich compounds. <i>Dalton Transactions</i> , <b>2010</b> , 39, 7645-9	4.3	44
941	Ligand-Directed Assembly of Polyoxovanadate-Based Metal-Organic Polyhedra. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 8770-5	5.1	44
940	Effect of alkyl chain length on piezochromic luminescence of iridium(III)-based phosphors adopting 2-phenyl-1H-benzimidazole type ligands. <i>Journal of Materials Chemistry C</i> , <b>2014</b> , 2, 7648-7655	7.1	43
939	Forward molecular design for highly efficient OLED emitters: a theoretical analysis of photophysical properties of platinum(II) complexes with N-heterocyclic carbene ligands. <i>Dalton Transactions</i> , <b>2011</b> , 40, 4480-8	4.3	43
938	Reversible redox-switchable second-order optical nonlinearity in polyoxometalate: a quantum chemical study of [PW11O39(ReN)]n- (n = 3-7). <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 5245-52	5.1	43



937	Theoretical study on the considerable second-order nonlinear optical properties of naphthylimido-substituted hexamolybdates. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 9919-23	2.8	43
936	HKUST-1 Derived Hollow C-Cu S Nanotube/g-C N Composites for Visible-Light CO Photoreduction with H O Vapor. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 379-385	4.8	43
935	An ultrastable {Ag <sub>55</sub> Mo <sub>6</sub> } nanocluster with a Ag-centered multishell structure. <i>Chemical Communications</i> , <b>2014</b> , 50, 11934-7	5.8	42
934	The influence of the diphenylphosphoryl moiety on the phosphorescent properties of heteroleptic iridium(III) complexes and the OLED performance: a theoretical study. <i>Journal of Materials Chemistry C</i> , <b>2014</b> , 2, 2859	7.1	42
933	Secondary ligand-directed assembly of metal-organic coordination polymers based on a 2-(pyridin-4-yl)-1H-imidazole-4,5-dicarboxylic acid ligand: Syntheses, structures and photoluminescent properties. <i>CrystEngComm</i> , <b>2012</b> , 14, 1865	3.3	42
932	DFT/TD-DFT study on the electronic structures and optoelectronic properties of several blue-emitting iridium(III) complexes. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 6559-64	2.8	42
931	Molecular tectonics of metal-organic frameworks based on ligand-modulated polynuclear zinc SBUs and aromatic multicarboxylic acids. <i>CrystEngComm</i> , <b>2011</b> , 13, 889-896	3.3	42
930	A novel (4,8)-connected 3D polyoxometalate-based metal-organic framework containing an in situ ligand. <i>CrystEngComm</i> , <b>2008</b> , 10, 1129	3.3	42
929	Synthesis of an Organotin Oligomer Containing a Heptanuclear Tin Phosphonate Cluster by Debenzylation Reactions: X-ray Crystal Structure of {Na <sub>6</sub> (CH <sub>3</sub> OH) <sub>2</sub> (H <sub>2</sub> O)}-[(BzSn) <sub>3</sub> (PhPO <sub>3</sub> ) <sub>5</sub> ( $\beta$ -O)(CH <sub>3</sub> O)] <sub>2</sub> Bz <sub>2</sub> Sn}·[CH <sub>3</sub> OH. <i>Organometallics</i> , <b>2007</b> , 26, 2125-2128	3.8	42
928	Prediction of second-order optical nonlinearity of trisorganotin-substituted beta-Keggin polyoxotungstate. <i>Inorganic Chemistry</i> , <b>2006</b> , 45, 7864-8	5.1	42
927	A new triazine-based covalent organic polymer for efficient photodegradation of both acidic and basic dyes under visible light. <i>Dalton Transactions</i> , <b>2018</b> , 47, 4191-4197	4.3	41
926	Tuning Emission of AIE-Active Organometallic Ir(III) Complexes by Simple Modulation of Strength of Donor/Acceptor on Ancillary Ligands. <i>Organometallics</i> , <b>2016</b> , 35, 3996-4001	3.8	41
925	Alkylene-Chain Effect on Microwire Growth and Crystal Packing of $\beta$ Moieties. <i>Chemistry of Materials</i> , <b>2012</b> , 24, 1944-1949	9.6	41
924	Three-propeller-blade-shaped electride: remarkable alkali-metal-doped effect on the first hyperpolarizability. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 128, 241-248	1.9	41
923	Electronic Structures of 5d Transition Metal Monoxides by Density Functional Theory. <i>Theoretical Chemistry Accounts</i> , <b>2006</b> , 117, 115-122	1.9	41
922	Anion-specific aggregation induced phosphorescence emission (AIPE) in an ionic iridium complex in aqueous media. <i>Chemical Communications</i> , <b>2015</b> , 51, 16924-7	5.8	40
921	Nitrogen-doped carbon dots for the detection of mercury ions in living cells and visualization of latent fingerprints. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 6824-6830	3.6	40
920	Alkali Metals-Substituted Adamantanes Lead to Visible Light Absorption: Large First Hyperpolarizability. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 6952-6958	3.8	40

919	Theoretical study on photophysical and charge transport properties of 1,6-bis(2-hydroxyphenol)pyridylboron bis(4-n-butylphenyl)phenyleneamine compound. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 8758-62	2.8	40
918	A stable mixed lanthanide metal-organic framework for highly sensitive thermometry. <i>Dalton Transactions</i> , <b>2019</b> , 48, 3723-3729	4.3	40
917	Recent progress in phosphorescent Ir(III) complexes for nondoped organic light-emitting diodes. <i>Coordination Chemistry Reviews</i> , <b>2020</b> , 413, 213283	23.2	40
916	Spontaneous chiral resolution of a rare 3D self-penetration coordination polymer for sensitive aqueous-phase detection of picric acid. <i>Dalton Transactions</i> , <b>2015</b> , 44, 18386-94	4.3	39
915	Facile one-pot synthesis of carbon/calcium phosphate/Fe <sub>3</sub> O <sub>4</sub> composite nanoparticles for simultaneous imaging and pH/NIR-responsive drug delivery. <i>Chemical Communications</i> , <b>2016</b> , 52, 11068-71	5.8	39
914	NIR-responsive NaYF <sub>4</sub> :Yb,Er,Gd fluorescent upconversion nanorods for the highly sensitive detection of blood fingerprints. <i>Dyes and Pigments</i> , <b>2016</b> , 134, 178-185	4.6	39
913	Supercapacitor with high cycling stability through electrochemical deposition of metal-organic frameworks/polypyrrole positive electrode. <i>Dalton Transactions</i> , <b>2018</b> , 47, 13472-13478	4.3	39
912	An AIE-active phosphorescent Ir(III) complex with piezochromic luminescence (PCL) and its application for monitoring volatile organic compounds (VOCs). <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 12189-12193	7.1	39
911	In situ assembly of monodispersed Ag nanoparticles in the channels of ordered mesopolymers as a highly active and reusable hydrogenation catalyst. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 4307-4313	13	39
910	Generalized approach to the synthesis of reversible concentric and eccentric polymer-coated nanostructures. <i>Small</i> , <b>2013</b> , 9, 825-30	11	39
909	Two unprecedented porous anionic frameworks: organoammonium templating effects and structural diversification. <i>Dalton Transactions</i> , <b>2009</b> , 8562-6	4.3	39
908	Density Functional Studies of Diatomic LaO to LuO. <i>Journal of Cluster Science</i> , <b>2007</b> , 18, 444-458	3	39
907	One-pot controllable synthesis of CoFe <sub>2</sub> O <sub>4</sub> solid, hollow and multi-shell hollow nanospheres as superior anode materials for lithium ion batteries. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 21994-22003	13	38
906	Ultrafast and Noninvasive Long-Term Bioimaging with Highly Stable Red Aggregation-Induced Emission Nanoparticles. <i>Analytical Chemistry</i> , <b>2019</b> , 91, 3467-3474	7.8	38
905	Two-State Reactivity Mechanism of Benzene C-C Activation by Trinuclear Titanium Hydride. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 11069-72	16.4	38
904	Polyoxovanadate-based organic-inorganic hybrids: from {V <sub>5</sub> O <sub>9</sub> Cl} clusters to nanosized octahedral cages. <i>Dalton Transactions</i> , <b>2016</b> , 45, 3698-701	4.3	38
903	Quantum chemical studies on high-valent metal nitrido derivatives of Keggin-type polyoxometalates ([PW <sub>11</sub> O <sub>39</sub> {M(VI)N}] <sub>4</sub> <sup>-</sup> (M = Ru, Os, Re)): M(VI)-N bonding and electronic structures. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 541-8	5.1	38
902	Hydrogen Adsorption in Polyoxometalate Hybrid Compounds Based on Porous Metal-Organic Frameworks. <i>European Journal of Inorganic Chemistry</i> , <b>2010</b> , 2010, 3756-3761	2.3	38

8901	Metal-Organic Frameworks Containing Flexible Bis(benzimidazole) Ligands. <i>European Journal of Inorganic Chemistry</i> , <b>2008</b> , 2008, 745-755	2.3	38
8900	Syntheses and characterizations of four metal coordination polymers constructed by the pyridine-3,5-dicarboxylate ligand. <i>Polyhedron</i> , <b>2008</b> , 27, 583-592	2.7	38
899	Improving the Accuracy of Density-Functional Theory Calculation: The Statistical Correction Approach. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 8514-8525	2.8	38
898	Theoretical Design of Perylene Diimide Dimers with Different Linkers and Bridged Positions as Promising Non-Fullerene Acceptors for Organic Photovoltaic Cells. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 2125-2134	3.8	37
897	Control of bulk homochirality and proton conductivity in isostructural chiral metal-organic frameworks. <i>Chemical Communications</i> , <b>2017</b> , 53, 1892-1895	5.8	37
896	Controllable synthesis of microporous, nanotubular and mesocage-like metal-organic frameworks by adjusting the reactant ratio and modulated luminescence properties of Alq3@MOF composites. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 17947		37
895	Synthesis and characterization of two {Mo6}-based/templated metal-organic frameworks. <i>CrystEngComm</i> , <b>2011</b> , 13, 1461-1466	3.3	37
894	Polyoxometalate-Based Porous Framework with Perovskite Topology. <i>Crystal Growth and Design</i> , <b>2010</b> , 10, 4227-4230	3.5	37
893	A series of novel chiral lanthanide coordination polymers with channels constructed from 16Ln-based cage-like building units. <i>CrystEngComm</i> , <b>2010</b> , 12, 1147-1152	3.3	37
892	Inorganic-organic hybrid compounds based on the co-existence of different isomers or forms of polymolybdate. <i>CrystEngComm</i> , <b>2010</b> , 12, 3684	3.3	37
891	Assembly of a Chiral Bikitaite Zeolite Metal-Organic Framework Based on the Asymmetrical Tetrahedral Building Blocks. <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 2986-2989	3.5	37
890	A comparative study of a fluorene-based non-fullerene electron acceptor and PC61BM in an organic solar cell at a quantum chemical level. <i>RSC Advances</i> , <b>2016</b> , 6, 81164-81173	3.7	37
889	Theoretical design and characterization of pyridalthiadiazole-based chromophores with fast charge transfer at donor/acceptor interface toward small molecule organic photovoltaics. <i>RSC Advances</i> , <b>2015</b> , 5, 29401-29411	3.7	36
888	Improved Photoreduction of CO with Water by Tuning the Valence Band of Covalent Organic Frameworks. <i>ChemSusChem</i> , <b>2020</b> , 13, 2973-2980	8.3	36
887	pH-controlled and sulfite anion-directed assembly of a family of cerium(III)-containing polyoxotungstates clusters. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 9486-97	5.1	36
886	A Rational Design for Dye Sensitizer: Density Functional Theory Study on the Electronic Absorption Spectra of Organoimido-Substituted Hexamolybdates. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 2245-2251	3.8	36
885	Schiff-base as highly sensitive and reversible chemosensors for HCl gas. <i>Sensors and Actuators B: Chemical</i> , <b>2013</b> , 177, 41-49	8.5	36
884	Synthesis, Characterization, and Crystal Structures of Double-Cubane-Substituted and Asymmetric Penta-Ni-Substituted Dimeric Polyoxometalates. <i>Crystal Growth and Design</i> , <b>2007</b> , 7, 1305-1311	3.5	36

883	Intercalation and photophysical properties of the tetra-(8-hydroxyquinolato) boron complex and 3,3',4,4'-benzophenone tetracarboxylic anion into Mg-Al layered double hydroxides. <i>Inorganic Chemistry</i> , <b>2006</b> , 45, 4364-71	5.1	36
882	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. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 17337-17343	3.4	36
881	Keplerate-type polyoxometalate/semiconductor composite electrodes with light-enhanced conductivity towards highly efficient photoelectronic devices. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 14025-14032	13	36
880	From Octahedral to Icosahedral Metal-Organic Polyhedra Assembled from Two Types of Polyoxovanadate Clusters. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 4649-4653	16.4	35
879	Photoreduction of carbon dioxide under visible light by ultra-small Ag nanoparticles doped into Co-ZIF-9. <i>Nanotechnology</i> , <b>2018</b> , 29, 284003	3.4	35
878	Introduction of Molecular Building Blocks to Improve the Stability of Metal-Organic Frameworks for Efficient Mercury Removal. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 6118-6123	5.1	35
877	Theoretical studies on the hole transport property of tetrathienoarene derivatives: The influence of the position of sulfur atom, substituent and $\pi$ -conjugated core. <i>Organic Electronics</i> , <b>2014</b> , 15, 602-613	3.5	35
876	A novel 3D inorganic heteropoly blue as visible light responsive photocatalyst. <i>Dalton Transactions</i> , <b>2014</b> , 43, 10005-12	4.3	35
875	ZIF-8 templated fabrication of rhombic dodecahedron-shaped ZnO@SiO <sub>2</sub> , ZIF-8@SiO <sub>2</sub> yolk-shell and SiO <sub>2</sub> hollow nanoparticles. <i>CrystEngComm</i> , <b>2014</b> , 16, 6534	3.3	35
874	Theoretical study on photophysical properties of phenolpyridyl boron complexes. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 2739-44	2.8	35
873	Two-dimensional lanthanide heteropolyvanadates of manganese(IV) and nickel(IV) containing two types of heteropoly anions with 1:13 and 1:12 stoichiometry. <i>Inorganic Chemistry</i> , <b>2006</b> , 45, 8036-40	5.1	35
872	Expediting the Conversion of LiS to Li <sub>2</sub> S Enables High-Performance Li-S Batteries. <i>ACS Nano</i> , <b>2021</b> , 15, 7318-7327	16.7	35
871	The Enhancement on Proton Conductivity of Stable Polyoxometalate-Based Coordination Polymers by the Synergistic Effect of MultiProton Units. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 9299-304	4.8	35
870	Carbon/Binder-Free NiO@NiO/NF with In Situ Formed Interlayer for High-Areal-Capacity Lithium Storage. <i>Advanced Energy Materials</i> , <b>2019</b> , 9, 1803690	21.8	35
869	A cascaded QSAR model for efficient prediction of overall power conversion efficiency of all-organic dye-sensitized solar cells. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 1036-46	3.5	34
868	The substitution effect of heterocyclic rings to tune the optical and nonlinear optical properties of hybrid chalcones: A comparative study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2018</b> , 81, 25-31	2.8	34
867	Efficient Light-Emitting Electrochemical Cells (LECs) Based on Ionic Iridium(III) Complexes with 1,3,4-Oxadiazole Ligands. <i>Advanced Functional Materials</i> , <b>2013</b> , 23, n/a-n/a	15.6	34
866	Rational molecular design of aggregation-induced emission cationic Ir(III) phosphors achieving supersensitive and selective detection of nitroaromatic explosives. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 10847-10854	7.1	34

865	An unprecedented (3,4,24)-connected heteropolyoxozincate organic framework as heterogeneous crystalline Lewis acid catalyst for biodiesel production. <i>Scientific Reports</i> , <b>2013</b> , 3, 2616	4.9	34
864	Electronic structures of 4d transition metal monoxides by density functional theory. <i>Theoretical Chemistry Accounts</i> , <b>2007</b> , 117, 407-415	1.9	34
863	Ultrasmall C-TiO <sub>2</sub> nanoparticle/g-C <sub>3</sub> N <sub>4</sub> composite for CO <sub>2</sub> photoreduction with high efficiency and selectivity. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 21596-21604	13	34
862	Spadix-Bract Structured Nanobowls for Bimodal Imaging-Guided Multidrug Chemo-Photothermal Synergistic Therapy. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 3722-3733	9.6	34
861	Evidence of Amine-CO <sub>2</sub> Interactions in Two Pillared-Layer MOFs Probed by X-ray Crystallography. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 7238-44	4.8	33
860	3D Racemic Microporous Frameworks and 3D Chiral Supramolecular Architectures Based on Evans-Showell-Type Polyoxometalates Controlled by the Temperature. <i>Crystal Growth and Design</i> , <b>2015</b> , 15, 164-175	3.5	33
859	Pure inorganic D <sub>3h</sub> type polyoxometalate/reduced graphene oxide nanocomposite for the photoanode of dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 3297-3303	13	33
858	Flexible blue-green and white light-emitting electrochemical cells based on cationic iridium complex. <i>Organic Electronics</i> , <b>2016</b> , 28, 314-318	3.5	33
857	Assembly of Keggin-/Dawson-type Polyoxotungstate Clusters with Different Metal Units and SeO <sub>3</sub> <sup>2-</sup> Heteroanion Templates. <i>Crystal Growth and Design</i> , <b>2014</b> , 14, 5099-5110	3.5	33
856	Thermally Activated Delayed Fluorescence in Cu Complexes Originating from Restricted Molecular Vibrations. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 11761-11766	4.8	33
855	From racemic compound to spontaneous resolution: a linker-imposed evolution of chiral [MnMo(9)O(32)](6-)-based polyoxometalate compounds. <i>Chemistry - A European Journal</i> , <b>2009</b> , 15, 10940-7	4.8	33
854	Quantum Chemical Study of Structures, Electronic Spectrum, and Nonlinear Optical Properties of GoldPentacene Complexes. <i>Organometallics</i> , <b>2007</b> , 26, 2082-2087	3.8	33
853	Two novel lead-carboxylate complexes based on nicotinic acid N-oxide: Synthesis, crystal structures and luminescent properties. <i>Inorganic Chemistry Communication</i> , <b>2007</b> , 10, 410-414	3.1	33
852	Synthesis and characterization of one- to three-dimensional compounds composed of paradodecatungstate-B cluster and transition metals as linkers. <i>Journal of Solid State Chemistry</i> , <b>2006</b> , 179, 2093-2100	3.3	33
851	An Amine-Functionalized Zirconium Metal-Organic Polyhedron Photocatalyst with High Visible-Light Activity for Hydrogen Production. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 2824-2830	4.8	33
850	Encapsulation of an iridium complex in a metal-organic framework to give a composite with efficient white light emission. <i>Inorganic Chemistry Frontiers</i> , <b>2017</b> , 4, 547-552	6.8	32
849	Cluster-based metal-organic frameworks as sensitive and selective luminescent probes for sensing nitro explosives. <i>New Journal of Chemistry</i> , <b>2015</b> , 39, 7858-7862	3.6	32
848	Polyaniline as interface layers promoting the in-situ growth of zeolite imidazole skeleton on regenerated cellulose aerogel for efficient removal of tetracycline. <i>Journal of Colloid and Interface Science</i> , <b>2020</b> , 579, 119-127	9.3	32

- 847 Unexpected 1D self-assembly of carbonate-templated sandwich-like macrocycle-based Ag<sub>20</sub>S<sub>10</sub> luminescent nanoclusters. *CrystEngComm*, **2014**, 16, 7860 3.3 32
- 846 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 7.1 32
- 845 High-performance oxygen sensors based on Eu(III) complex/polystyrene composite nanofibrous membranes prepared by electrospinning. *ChemPhysChem*, **2011**, 12, 349-55 3.2 32
- 844 Theoretical investigation of the reactions of CF<sub>3</sub>CHFOCF<sub>3</sub> with the OH radical and Cl atom. *Journal of Physical Chemistry A*, **2010**, 114, 417-24 2.8 32
- 843 Electronic structures and chemical bonding in diatomic ScX to ZnX (X = S, Se, Te). *Journal of Computational Chemistry*, **2007**, 28, 703-14 3.5 32
- 842 Self-Assembly of Nanometer-Scale [Cu<sub>24</sub>I<sub>10</sub>L<sub>12</sub>]<sup>14+</sup> Cages and Ball-Shaped Keggin Clusters into a (4,12)-Connected 3D Framework with Photoluminescent and Electrochemical Properties. *Angewandte Chemie*, **2006**, 118, 7571-7574 3.6 32
- 841 Orange emissive carbon dots for colorimetric and fluorescent sensing of 2,4,6-trinitrophenol by fluorescence conversion.. *RSC Advances*, **2018**, 8, 16095-16102 3.7 31
- 840 A novel strategy to fabricate multifunctional Fe<sub>3</sub>O<sub>4</sub>@C@TiO<sub>2</sub> yolk-shell structures as magnetically recyclable photocatalysts. *Nanoscale*, **2014**, 6, 6603-8 7.7 31
- 839 Stepwise modulation of the electron-donating strength of ancillary ligands: understanding the AIE mechanism of cationic iridium(III) complexes. *Chemical Communications*, **2014**, 50, 10986-9 5.8 31
- 838 Polyoxometalate/TiO<sub>2</sub> 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 3.9 31
- 837 Three cobalt(II)-linked {P<sub>8</sub>W<sub>48</sub>} network assemblies: syntheses, structures, and magnetic and photocatalysis properties. *Chemistry - an Asian Journal*, **2014**, 9, 470-8 4.5 31
- 836 An Ionothermal Synthetic Approach to Porous Polyoxometalate-Based Metal-Organic Frameworks. *Angewandte Chemie*, **2012**, 124, 8109-8113 3.6 31
- 835 Theoretical study on the relationship between spin multiplicity effects and nonlinear optical properties of the pyrrole radical (C<sub>4</sub>H<sub>4</sub>N). *Journal of Physical Chemistry A*, **2008**, 112, 83-8 2.8 31
- 834 DFT study on second-order nonlinear optical properties of a series of mono Schiff-base M(II) (M=Ni, Pd, Pt) complexes. *Chemical Physics Letters*, **2006**, 429, 570-574 2.5 31
- 833 Recent advances in luminescent dinuclear iridium(III) complexes and their application in organic electroluminescent devices. *Polyhedron*, **2018**, 140, 146-157 2.7 31
- 832 Polyurethane derivatives for highly sensitive and selective fluorescence detection of 2,4,6-trinitrophenol (TNP). *Journal of Materials Chemistry C*, **2018**, 6, 11287-11291 7.1 31
- 831 Bright red aggregation-induced emission nanoparticles for multifunctional applications in cancer therapy. *Chemical Science*, **2020**, 11, 2369-2374 9.4 30
- 830 Metal-Organic Framework with Aromatic Rings Tentacles: High Sulfur Storage in Li-S Batteries and Efficient Benzene Homologues Distinction. *ACS Applied Materials & Interfaces*, **2016**, 8, 33183-33188 9.5 30

829	Switchable NLO response induced by rotation of metallocarboranes [Ni(III/IV)(C <sub>2</sub> B <sub>9</sub> H <sub>11</sub> ) <sub>2</sub> ](-/0) and C-,B-functionalized derivatives. <i>Dalton Transactions</i> , <b>2014</b> , 43, 5069-75	4.3	30
828	New heteropolyniobates based on a bicapped Keggin-type {VNb <sub>14</sub> } cluster with selective adsorption and photocatalytic properties. <i>CrystEngComm</i> , <b>2014</b> , 16, 9582-9585	3.3	30
827	Theoretical study on the electron transfer and phosphorescent properties of iridium(III) complexes with 2-phenylpyridyl and 8-hydroxyquinolate ligands. <i>Dalton Transactions</i> , <b>2010</b> , 39, 7733-40	4.3	30
826	An unprecedented 3D 8-connected pure inorganic framework based on nanosized {[Na <sub>12</sub> PO <sub>16</sub> H <sub>24</sub> ] <sup>7-</sup> [P <sub>4</sub> Mo <sub>6</sub> O <sub>31</sub> H <sub>6</sub> ] <sub>4</sub> }] <sub>15</sub> - clusters and zinc cations. <i>Chemical Communications</i> , <b>2011</b> , 47, 2832-4	5.8	30
825	Bottom-Up Synthesis of Porous Coordination Frameworks: Apical Substitution of a Pentanuclear Tetrahedral Precursor. <i>Angewandte Chemie</i> , <b>2009</b> , 121, 5395-5399	3.6	30
824	How Do the Different Defect Structures and Element Substitutions Affect the Nonlinear Optical Properties of Lacunary Keggin Polyoxometalates? A DFT Study. <i>European Journal of Inorganic Chemistry</i> , <b>2006</b> , 2006, 4179-4183	2.3	30
823	A novel strong fluorescent three-dimensional supramolecular coordination polymer based on bridging terephthalate. <i>Inorganic Chemistry Communication</i> , <b>2004</b> , 7, 260-263	3.1	30
822	HKUST-1 modified ultrastability cellulose/chitosan composite aerogel for highly efficient removal of methylene blue. <i>Carbohydrate Polymers</i> , <b>2021</b> , 255, 117402	10.3	30
821	Theoretical studies on POM-based organic-inorganic hybrids containing double D-A1- $\pi$ A2 chains for high-performance p-type, dye-sensitized solar cells (DSSCs). <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 5459-65	3.6	29
820	Theoretical study and design of multifunctional phosphorescent platinum(II) complexes containing triarylboron moieties for efficient OLED emitters. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 2438-46	3.6	29
819	Modification of iridium(III) complexes for fabrication of high-performance non-doped organic light-emitting diode. <i>Dyes and Pigments</i> , <b>2015</b> , 112, 8-16	4.6	29
818	A carbon-free polyoxometalate molecular catalyst with a cobalt-arsenic core for visible light-driven water oxidation. <i>Chemical Communications</i> , <b>2016</b> , 52, 9514-7	5.8	29
817	Metal ion directed metal-organic rotaxane frameworks with intrinsic features of self-penetration and interpenetration. <i>Chemical Communications</i> , <b>2013</b> , 49, 8555-7	5.8	29
816	Steam-Assisted Synthesis of an Extra-Stable Polyoxometalate-Encapsulating Metal Azolate Framework: Applications in Reagent Purification and Proton Conduction. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 13058-64	4.8	29
815	A long-term stable Pt counter electrode modified by POM-based multilayer film for high conversion efficiency dye-sensitized solar cells. <i>Dalton Transactions</i> , <b>2012</b> , 41, 2227-30	4.3	29
814	Step-wise synthesis of inorganic-organic hybrid based on Ectamolybdate-based tectons. <i>Dalton Transactions</i> , <b>2011</b> , 40, 3176-82	4.3	29
813	Anion-directed genuine meso-helical supramolecular isomers of two 1D Ag(I) complexes based on arene-linked bis(pyrazolyl)methane ligands. <i>CrystEngComm</i> , <b>2010</b> , 12, 3458	3.3	29
812	3d - 4f Heterometallic Complexes for the Construction of POM-based Inorganic - Organic Hybrid Compounds: from Nanoclusters to One-Dimensional Ladder-Like Chains. <i>Australian Journal of Chemistry</i> , <b>2010</b> , 63, 1389	1.2	29

811	A theoretical investigation of intermolecular interaction of a phthalimide based $\text{Cu}^{\text{II}}$ sensor with different halide ions: tuning its efficiency and electro-optical properties. <i>Theoretical Chemistry Accounts</i> , <b>2009</b> , 122, 77-86	1.9	29
810	Computational Study on Second-Order Nonlinear Response of a Series of Two-Dimensional Carbazole-Cored Chromophores. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 7021-7028	3.8	29
809	DFT Studies on second-order nonlinear optical properties of mono (salicylaldiminato) Nickel(II) polyenyl Schiff base metal complexes. <i>Chemical Physics Letters</i> , <b>2007</b> , 443, 163-168	2.5	29
808	A chiral 3D polymer with right- and left-helices based on 2,2'-biimidazole: Synthesis, crystal structure and fluorescent property. <i>Inorganic Chemistry Communication</i> , <b>2007</b> , 10, 720-723	3.1	29
807	Synthesis, Structure, Electronic State, and Luminescent Properties of Novel Blue-Light-Emitting Aryl-Substituted 9,9-Di(4-(di-p-tolyl)aminophenyl)fluorenes. <i>Advanced Functional Materials</i> , <b>2008</b> , 18, 2335-2347	15.6	29
806	Improving the accuracy of density-functional theory calculation: the genetic algorithm and neural network approach. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 144101	3.9	29
805	Covalently crosslinked zirconium-based metal-organic framework aerogel monolith with ultralow-density and highly efficient Pb(II) removal. <i>Journal of Colloid and Interface Science</i> , <b>2020</b> , 561, 211-219	9.3	29
804	Assembly of two novel 3D organic-inorganic hybrids based on Keggin-type polyoxometalates: syntheses, crystal structures and properties. <i>CrystEngComm</i> , <b>2016</b> , 18, 6370-6377	3.3	29
803	A dual-emitting mixed-lanthanide MOF with high water-stability for ratiometric fluorescence sensing of $\text{Fe}^{3+}$ and ascorbic acid. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 562-568	7.1	29
802	Metal-organic frameworks constructed from tib and carboxylate acid ligands: selective sensing of nitro explosives and magnetic properties. <i>Dalton Transactions</i> , <b>2017</b> , 46, 7567-7576	4.3	28
801	A stable pillared-layer Cu(II) metal-organic framework with magnetic properties for dye adsorption and separation. <i>New Journal of Chemistry</i> , <b>2017</b> , 41, 3661-3666	3.6	28
800	Utilizing d $\pi$ -p $\pi$ Bonds for Ultralong Organic Phosphorescence. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 6717-6721	3.6	28
799	Assembly of Zn-metal organic frameworks based on a N-rich ligand: selective sorption for $\text{CO}_2$ and luminescence sensing of nitro explosives. <i>RSC Advances</i> , <b>2015</b> , 5, 49606-49613	3.7	28
798	Metal-Organic Rotaxane Frameworks Assembly by Cucurbit[6]uril-Based Pseudorotaxanes and Mixed Ligands. <i>Crystal Growth and Design</i> , <b>2015</b> , 15, 4311-4317	3.5	28
797	Nitrogen and Sulfur-Codoped Porous Carbon Nanospheres with Hierarchical Micromesoporous Structures and an Ultralarge Pore Volume for High-Performance Supercapacitors. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 8225-8232	9.5	28
796	A machine learning correction for DFT non-covalent interactions based on the S22, S66 and X40 benchmark databases. <i>Journal of Cheminformatics</i> , <b>2016</b> , 8, 24	8.6	28
795	Nitrogen- and sulfur-doped carbon dots as peroxidase mimetics: colorimetric determination of hydrogen peroxide and glutathione, and fluorimetric determination of lead(II). <i>Mikrochimica Acta</i> , <b>2019</b> , 186, 604	5.8	28
794	Facile synthesis of conjugated microporous polymer-based porphyrin units for adsorption of $\text{CO}_2$ and organic vapors. <i>Polymer Chemistry</i> , <b>2019</b> , 10, 819-822	4.9	28



793	Enhancing the luminescence properties and stability of cationic iridium(III) complexes based on phenylbenzoimidazole ligand: a combined experimental and theoretical study. <i>Dalton Transactions</i> , <b>2013</b> , 42, 11056-65	4.3	28
792	Designed preparation of polyacrylic acid/calcium carbonate nanoparticles with high doxorubicin payload for liver cancer chemotherapy. <i>CrystEngComm</i> , <b>2015</b> , 17, 4768-4773	3.3	28
791	Inorganic crown ethers: sulfate-based Preyssler polyoxometalates. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 9184-8	4.8	28
790	Syntheses and characterizations of three coordination polymers based on dipyritylbenzoates and 1,4-benzenedicarboxylate. <i>Polyhedron</i> , <b>2009</b> , 28, 975-979	2.7	28
789	Unprecedented interweaving of single-helical chains into a chiral metal-organic framework based on a flexible ligand. <i>CrystEngComm</i> , <b>2009</b> , 11, 1711	3.3	28
788	Tuning the Excited-State Properties of Luminescent Rhenium(V) Benzylidyne Complexes Containing Phosphorus and Nitrogen Donor Ligands. <i>Organometallics</i> , <b>1998</b> , 17, 1946-1955	3.8	28
787	Electronic structures and chemical bonding in 4d transition metal monohalides. <i>Journal of Computational Chemistry</i> , <b>2007</b> , 28, 2190-202	3.5	28
786	Aggregation-Induced Long-Lived Phosphorescence in Nonconjugated Polyurethane Derivatives at 77 K. <i>Macromolecules</i> , <b>2018</b> , 51, 4178-4184	5.5	28
785	The assembly of vanadium(IV)-substituted Keggin-type polyoxometalate/graphene nanocomposite and its application in photovoltaic system. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 10174-10178	13	27
784	Metal-organic framework composites with luminescent pincer platinum(ii) complexes: MMLCT emission and photoinduced dehydrogenation catalysis. <i>Chemical Science</i> , <b>2018</b> , 9, 2357-2364	9.4	27
783	Multilithiation Effect on the First Hyperpolarizability of Carbon-Boron-Nitride Heteronanotubes: Activating Segment versus Connecting Pattern. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 14185-14191	3.8	27
782	A pillar-layer MOF for detection of small molecule acetone and metal ions in dilute solution. <i>RSC Advances</i> , <b>2015</b> , 5, 48881-48884	3.7	27
781	Li doped effect of through novel noncovalent charge transfer on nonlinear optical properties. <i>Dyes and Pigments</i> , <b>2014</b> , 106, 7-13	4.6	27
780	Chiroptical, linear, and second-order nonlinear optical properties of binaphthol derivatives. <i>Organic and Biomolecular Chemistry</i> , <b>2012</b> , 10, 8418-25	3.9	27
779	Auxiliary ligand induced structural allomorphism in nanotubular microporous metal-organic frameworks based on discrete magnesium clusters. <i>Dalton Transactions</i> , <b>2012</b> , 41, 2231-3	4.3	27
778	On the origin of the relative stability of Wells-Dawson isomers: a DFT study of $\text{H}_2\text{W}_{12}\text{O}_{42}^{10-}$ , $\text{H}_2\text{W}_{12}\text{O}_{42}^{8-}$ , and $\text{H}_2\text{W}_{12}\text{O}_{42}^{6-}$ anions. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 4967-77	5.1	27
777	Synthesis and characterization of new bifunctional nanocomposites possessing upconversion and oxygen-sensing properties. <i>Nanotechnology</i> , <b>2010</b> , 21, 285701	3.4	27
776	Novel Trumpet-Shaped Conjugation Bridge (Carbon Nanocone) for Nonlinear Optical Materials. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 18545-18551	3.8	27

775	Tin-oxo clusters based on aryl arsonate anions. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 4093-103	4.8	27
774	A fluorescent sensor for highly selective sensing of nitro explosives and Hg(II) ions based on a 3D porous layer metal-organic framework. <i>CrystEngComm</i> , <b>2016</b> , 18, 4765-4771	3.3	27
773	Two-dimensional $\pi$ -conjugated metal bis(dithiolene) nanosheets as promising electrocatalysts for carbon dioxide reduction: a computational study. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 15341-15346 <sup>13</sup>		26
772	Exploring the influence of electron donating/withdrawing groups on hexamolybdate-based derivatives for efficient p-type dye-sensitized solar cells (DSSCs). <i>RSC Advances</i> , <b>2015</b> , 5, 39821-39827	3.7	26
771	Theoretical investigation on redox-switchable second-order nonlinear optical responses of push-pull Cp*CoEt <sub>2</sub> C <sub>2</sub> B <sub>4</sub> H <sub>3</sub> -expanded (metallo)porphyrins. <i>Journal of Computational Chemistry</i> , <b>2012</b> , 33, 211-9	3.5	26
770	An efficient strategy for improving carrier transport performance $\square$ Introducing fluorine into aryl substituted tetracene. <i>Organic Electronics</i> , <b>2013</b> , 14, 1359-1369	3.5	26
769	Cyano or o-nitrophenyl? Which is the optimal electron-withdrawing group for the acrylic acid acceptor of D- $\pi$ A sensitizers in DSSCs? A density functional evaluation. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 1597-604	2	26
768	A photovoltaic system composed of a keplerate-type polyoxometalate and a water-soluble poly(p-phenylenevinylene) derivative. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 6727	13	26
767	Rational design of a highly sensitive and selective "turn-on" fluorescent sensor for PO <sub>4</sub> (3-) detection. <i>Dalton Transactions</i> , <b>2015</b> , 44, 20830-3	4.3	26
766	Theoretical investigation on electronic structure and second-order nonlinear optical properties of novel hexamolybdate-organoimido-(car)borane hybrid. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 5605-12	3.6	26
765	Functional heterometallic coordination polymers with metalloligands as tunable luminescent crystalline materials. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 19673		26
764	The influence of thienyl-S,S-dioxidation on the photoluminescence and charge transport properties of dithienothiophenes: a theoretical study. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 129, 247-255	1.9	26
763	Mechanistic and kinetic study of CH <sub>2</sub> O+O <sub>3</sub> reaction. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 3516-22	2.8	26
762	Tuning Second-Order Non-linear (NLO) Optical Response of Organoimido-Substituted Hexamolybdates through Halogens: Quantum Design of Novel Organic-Inorganic Hybrid NLO Materials. <i>Australian Journal of Chemistry</i> , <b>2010</b> , 63, 836	1.2	26
761	Theoretical study on the chiroptical optical properties of chiral fullerene C <sub>60</sub> derivative. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 13356-63	2.8	26
760	Studies on the interactions of Ti-containing polyoxometalates (POMs) with SARS-CoV 3CLpro by molecular modeling. <i>Journal of Inorganic Biochemistry</i> , <b>2007</b> , 101, 89-94	4.2	26
759	Facile method to detect oligonucleotides with functionalized polydiacetylene vesicles. <i>Sensors and Actuators B: Chemical</i> , <b>2006</b> , 113, 510-515	8.5	26
758	New cationic Ir(III) complexes without $\pi$ -ny soft substituents $\square$ aggregation-induced emission and piezochromic luminescence. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 12217-12223	7.1	26

757	A bimetallic-MOF catalyst for efficient CO <sub>2</sub> photoreduction from simulated flue gas to value-added formate. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 11712-11718	13	25
756	A water-stable terbium metal-organic framework with functionalized ligands for the detection of Fe <sup>3+</sup> and CrO <sub>7</sub> <sup>2-</sup> ions in water and picric acid in seawater. <i>CrystEngComm</i> , <b>2020</b> , 22, 3638-3643	3.3	25
755	Synthesis, structures, and magnetic properties of metal-organic polyhedra based on unprecedented {V} isopolyoxometalate clusters. <i>Dalton Transactions</i> , <b>2016</b> , 45, 14898-14901	4.3	25
754	Aggregation-induced emission (AIE) active iridium complexes toward highly efficient single-layer non-doped electroluminescent devices. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 10464-10470	7.1	25
753	Continuous detection of HCl and NH <sub>3</sub> gases with a high-performance fluorescent polymer sensor. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 13367-13374	3.6	25
752	Hydrothermal synthesis and structural characterization of a new inorganic-organic hybrid compound with photocatalytic activity based on Keggin-type polyanion and cadmium-1, 2, 4-triazolate units. <i>Inorganic Chemistry Communication</i> , <b>2012</b> , 20, 273-276	3.1	25
751	Self-assembly of metal-organic frameworks based on N-donor ligand and flexible tricarboxylic acids with different angular characters. <i>CrystEngComm</i> , <b>2013</b> , 15, 8214	3.3	25
750	Exploring what prompts ITIC to become a superior acceptor in organic solar cell by combining molecular dynamics simulation with quantum chemistry calculation. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 31227-31235	3.6	25
749	Assembly of Sandwich-Like Supermolecules Li Salts CpLi-C60: Structures, Stabilities, and Nonlinear Optical Properties. <i>Organometallics</i> , <b>2012</b> , 31, 4409-4414	3.8	25
748	Selected-control fabrication of multifunctional fluorescent-magnetic core-shell and yolk-shell hybrid nanostructures. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 3745-52	4.8	25
747	DFT characterization on the mechanism of water splitting catalyzed by single-Ru-substituted polyoxometalates. <i>Dalton Transactions</i> , <b>2013</b> , 42, 10617-25	4.3	25
746	Combination of POMs and deliberately designed macrocations: a rational approach for synthesis of POM-pillared metal-organic framework. <i>Dalton Transactions</i> , <b>2009</b> , 940-7	4.3	25
745	Prediction of robustly large molecular second-order nonlinear optical properties of terpyridine-substituted hexamolybdates: structural modelling towards a rational entry to NLO materials. <i>Journal of Molecular Graphics and Modelling</i> , <b>2010</b> , 28, 735-45	2.8	25
744	Synthesis of a Magnetic 2D Co@NC-600 Material by Designing a MOF Precursor for Efficient Catalytic Reduction of Water Pollutants. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 12672-12680	5.1	25
743	Promoted Photocharge Separation in 2D Lateral Epitaxial Heterostructure for Visible-Light-Driven CO Photoreduction. <i>Advanced Materials</i> , <b>2020</b> , 32, e2004311	24	25
742	Precise Molecular-Level Modification of Nafion with Bismuth Oxide Clusters for High-performance Proton-Exchange Membranes. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 6076-6085	16.4	25
741	Changes of coordination modes of Cu-based coordination complexes as tuneable proton-conducting solid electrolytes. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 1085-1093	13	24
740	Rational design of well-dispersed ultrafine CoS <sub>2</sub> nanocrystals in micro-mesoporous carbon spheres with a synergistic effect for high-performance lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 10885-10890	13	24

- 739 Ir/Ni-Metallaphotoredox catalysis: the oxidation state modulation mechanism versus the radical mechanism. *Chemical Communications*, **2018**, 54, 5968-5971 5.8 24
- 738 Beryllium-beryllium double-bonds in the octahedral cluster of Be( $\text{BX}$ ) ( $\text{X} = \text{Li}, \text{Cu}, \text{BeF}$ ). *Physical Chemistry Chemical Physics*, **2018**, 20, 23898-23902 3.6 24
- 737 All-inorganic perovskite/graphitic carbon nitride composites for CO photoreduction into C1 compounds under low concentrations of CO. *Dalton Transactions*, **2019**, 48, 14115-14121 4.3 24
- 736 A polyrotaxane-like metal-organic framework exhibiting luminescent sensing of  $\text{Eu}^{3+}$  cations and proton conductivity. *CrystEngComm*, **2014**, 16, 6882-6888 3.3 24
- 735 Achieving High Performances of Nondoped OLEDs Using Carbazole and Diphenylphosphoryl-Functionalized Ir(III) Complexes as Active Components. *Inorganic Chemistry*, **2017**, 56, 9979-9987 5.1 24
- 734 Highly tuneable proton-conducting coordination polymers derived from a sulfonate-based ligand. *CrystEngComm*, **2017**, 19, 7050-7056 3.3 24
- 733 BN Segment Doped Effect on the First Hyperpolarizability of Heteronanotubes: Focused on an Effective Connecting Pattern. *Journal of Physical Chemistry C*, **2013**, 117, 10039-10044 3.8 24
- 732 Theoretical exploration to second-order nonlinear optical properties of new hybrid complexes via coordination interaction between (metallo)porphyrin and  $[\text{MSiW}_{11}\text{O}_{39}]^{3-}$  ( $\text{M} = \text{Nb}(\text{V})$  or  $\text{V}(\text{V})$ ) polyoxometalates. *Journal of Molecular Graphics and Modelling*, **2013**, 46, 59-64 2.8 24
- 731 Carbazolyl-contained phenol-pyridyl boron complexes: syntheses, structures, photoluminescent and electroluminescent properties. *Dalton Transactions*, **2010**, 39, 5123-9 4.3 24
- 730 Ionothermal synthesis of a new open-framework zinc phosphite NIS-3 with low framework density. *CrystEngComm*, **2010**, 12, 1401 3.3 24
- 729 Theoretical studies on the electronic structure and spectral properties of versatile diarylethene-containing 1,10-phenanthroline ligands and their rhenium(I) complexes. *Journal of Organometallic Chemistry*, **2007**, 692, 5368-5374 2.3 24
- 728 Improved performance of electrophosphorescent devices based on  $\text{Re}(\text{CO})_3\text{Cl}$ -dipyrido[3,2-a:2',3'-c]phenazine. *Applied Physics Letters*, **2006**, 88, 093507 3.4 24
- 727 Anion-directed assembly of two novel cadmium(II) complexes constructed by 2,2'-(1,4-butanediyl)bis(1H-benzimidazole) ligand. *Inorganic Chemistry Communication*, **2006**, 9, 1207-1211 3.1 24
- 726 Polyoxotungstates containing uranyl group: Germanotungstates with Keggin sandwich structure. *Inorganic Chemistry Communication*, **2006**, 9, 1331-1334 3.1 24
- 725 Entangled Coordination Networks with Inherent Features of Polycatenation, Polythreading, and Polyknotting. *Angewandte Chemie*, **2005**, 117, 5974-5977 3.6 24
- 724 Luminescent compounds diphenylboron analogs of  $\text{Alq}_3$  and its methyl substituents: A theoretical investigation of their electronic and spectroscopic properties. *International Journal of Quantum Chemistry*, **2005**, 103, 775-780 2.1 24
- 723 A theoretical design and investigation on Zn-porphyrin-polyoxometalate hybrids with different linkers for searching high performance sensitizers of p-type dye-sensitized solar cells. *Dyes and Pigments*, **2016**, 130, 168-175 4.6 24
- 722 Planar  $\text{NiC}_3$  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 1.3 23

7 <sup>21</sup>	A strategy for breaking the MOF template to obtain small-sized and highly dispersive polyoxometalate clusters loaded on solid films. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 14573-14577	13	23
7 <sup>20</sup>	A Well-Established POM-based Single-Crystal Proton-Conducting Model Incorporating Multiple Weak Interactions. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 2365-2369	4.8	23
7 <sup>19</sup>	Functionalized polyoxometalate-based metal-organic cuboctahedra for selective adsorption toward cationic dyes in aqueous solution. <i>Dalton Transactions</i> , <b>2018</b> , 47, 12979-12983	4.3	23
7 <sup>18</sup>	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. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 6800	7.1	23
7 <sup>17</sup>	A new organic-inorganic hybrid based on the crescent-shaped polyoxoanion [H <sub>6</sub> SiNb <sub>18</sub> O <sub>54</sub> ] <sup>8-</sup> and copper-organic cations. <i>Dalton Transactions</i> , <b>2012</b> , 41, 6075-7	4.3	23
7 <sup>16</sup>	pH variation induced construction of a series of entangled frameworks based on bi- and tri-metallic cores as nodes. <i>CrystEngComm</i> , <b>2012</b> , 14, 124-130	3.3	23
7 <sup>15</sup>	Spiral intramolecular charge transfer and large first hyperpolarizability in Möbius cyclacenes: new insight into the localized $\pi$ electrons. <i>ChemPhysChem</i> , <b>2012</b> , 13, 2349-53	3.2	23
7 <sup>14</sup>	Theoretical insights into [PMo <sub>12</sub> O <sub>40</sub> ] <sup>(3-)</sup> grafted on single-walled carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 9177-85	3.6	23
7 <sup>13</sup>	pH-Tuned self-assembly of organic/inorganic hybrids based on different vanadate chains, Zn(II) ions and flexible ligands: crystallizing in polar and centrosymmetric space group. <i>CrystEngComm</i> , <b>2011</b> , 13, 779-786	3.3	23
7 <sup>12</sup>	Preparation and application of multiple-component-doped kegglin polyoxometalate microtubes--towards a component-tunable hollow structure. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 3657-62	4.8	23
7 <sup>11</sup>	Coordination between [H <sub>2</sub> P <sub>2</sub> W <sub>12</sub> O <sub>48</sub> ] <sup>12-</sup> and antimony(III): synthesis and characterization of sandwich complex derived from the new {P <sub>2</sub> W <sub>13</sub> O <sub>51</sub> } fragment. <i>Dalton Transactions</i> , <b>2010</b> , 39, 8033-7	4.3	23
7 <sup>10</sup>	A Quantum Chemical Study of the Structure, Bonding Characteristics and Nonlinear Optical Properties of Aryloxo and Salicylaldehyde Derivatives of [XW <sub>5</sub> O <sub>18</sub> ] <sup>3-</sup> (X = Zr or Ti). <i>European Journal of Inorganic Chemistry</i> , <b>2009</b> , 2009, 2529-2535	2.3	23
7 <sup>09</sup>	Ferromagnetically coupled dimer of Cu(II)-substituted gamma-decatungstosilicate. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 10041-3	5.1	23
7 <sup>08</sup>	TiO <sub>2</sub> film decorated with highly dispersed polyoxometalate nanoparticles synthesized by micelle directed method for the efficiency enhancement of dye-sensitized solar cells. <i>Journal of Power Sources</i> , <b>2016</b> , 328, 1-7	8.9	23
7 <sup>07</sup>	Luminescent Cd(II) metal-organic frameworks with anthracene nitrogen-containing organic ligands as novel multifunctional chemosensors for the detection of picric acid, pesticides, and ferric ions. <i>Dyes and Pigments</i> , <b>2021</b> , 185, 108834	4.6	23
7 <sup>06</sup>	The composite material based on Dawson-type polyoxometalate and activated carbon as the supercapacitor electrode. <i>Inorganic Chemistry Communication</i> , <b>2015</b> , 55, 149-152	3.1	22
7 <sup>05</sup>	Controlled synthesis of mesoporous hollow SnO <sub>2</sub> nanococoons with enhanced lithium storage capability. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 22021-22025	13	22
7 <sup>04</sup>	Atomic Nb Anchoring on Graphdiyne as a New Potential Electrocatalyst for Nitrogen Fixation: A Computational View. <i>Advanced Theory and Simulations</i> , <b>2019</b> , 2, 1900132	3.5	22

- 703 Two hybrid materials assembled from transition metal mono-substituted Keggin polyoxoanions as photocatalysts under visible light. *CrystEngComm*, **2014**, 16, 9163-9167 3.3 22
- 702 Prediction of second-order nonlinear optical properties of WellsDawson polyoxometalate derivatives  $[X_6(CH_2O)_3P_2M_2M_3O_{59}]_6$  [X = NO<sub>2</sub>, NH<sub>2</sub>, and CH<sub>3</sub>, M? = V and Nb, M = W and Mo). *Inorganic Chemistry Frontiers*, **2014**, 1, 65-70 6.8 22
- 701 The research of a new polyoxometalates based photosensitizer on dye sensitized solar cell. *Inorganic Chemistry Communication*, **2013**, 38, 78-82 3.1 22
- 700 Computational Study on M/POM Single-Atom Catalysts (M = Cu, Zn, Ag, and Au; POM = [PWO]): Metal-Support Interactions and Catalytic Cycle for Alkene Epoxidation. *Inorganic Chemistry*, **2017**, 56, 10496-10504 5.1 22
- 699 Synthesis and characterization of two self-catenated networks and one case of pcu topology based on the mixed ligands. *CrystEngComm*, **2012**, 14, 4205 3.3 22
- 698 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 1.9 22
- 697 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 3.3 22
- 696 ITO electrode modified with chitosan nanofibers loading polyoxometalate by one step self-assembly method and its electrocatalysis. *Electrochemistry Communications*, **2007**, 9, 2224-2228 5.1 22
- 695 Predication of second-order optical nonlinearity of [(Bu<sub>2</sub>t Im)AuX] (X=halogen) using time-dependent density-functional theory combined with sum-over-states method. *Journal of Chemical Physics*, **2005**, 123, 134302 3.9 22
- 694 Polyoxometalates/Active Carbon Thin Separator for Improving Cycle Performance of Lithium-Sulfur Batteries. *ACS Applied Materials & Interfaces*, **2018**, 10, 35911-35918 9.5 22
- 693 Influence of Aggregation on the Structure and Fluorescent Properties of a Tetraphenylethylene Derivative: a Theoretical Study. *ChemPhysChem*, **2017**, 18, 755-762 3.2 21
- 692 A tetraphenylethylene-based covalent organic polymer for highly selective and sensitive detection of Fe and as a white light emitting diode. *Chemical Communications*, **2019**, 55, 12328-12331 5.8 21
- 691 TMC (TM = Co, Ni, and Cu) monolayers with planar pentacoordinate carbon and their potential applications. *Journal of Materials Chemistry C*, **2019**, 7, 6406-6413 7.1 21
- 690 Coordination assemblies of seven metal-organic frameworks based on a bent connector: structural diversity and properties. *CrystEngComm*, **2015**, 17, 3129-3138 3.3 21
- 689 Sulfur-containing bimetallic metal organic frameworks with multi-fold helix as anode of lithium ion batteries. *Dalton Transactions*, **2018**, 47, 4827-4832 4.3 21
- 688 A difunctional metalorganic framework with Lewis basic sites demonstrating turn-off sensing of Cu<sup>2+</sup> and sensitization of Ln<sup>3+</sup>. *Journal of Materials Chemistry C*, **2018**, 6, 7874-7879 7.1 21
- 687 Two-Dimensional Cobaltporphyrin-based CobaltOrganic Framework as an Efficient Photocatalyst for CO<sub>2</sub> Reduction Reaction: A Computational Study. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 14102-14110 8.3 21
- 686 Rational design and characterization of high-efficiency planar ADA type electron donors in small molecule organic solar cells: A quantum chemical approach. *Materials Chemistry and Physics*, **2014**, 145, 387-396 4.4 21

685	The Application of ZnO Nanoparticles Containing Polyoxometalates in Dye-Sensitized Solar Cells. <i>European Journal of Inorganic Chemistry</i> , <b>2013</b> , 2013, 1951-1959	2.3	21
684	Computational Design of Host Materials Suitable for Green-(Deep) Blue Phosphors through Effectively Tuning the Triplet Energy While Maintaining the Ambipolar Property. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 8420-8428	3.8	21
683	3D Chiral Microporous (10,3)-a Topology Metal-Organic Framework Containing Large Helical Channels. <i>Crystal Growth and Design</i> , <b>2011</b> , 11, 2510-2514	3.5	21
682	Theoretical study on a novel series of fullerene-containing organometallics $\text{Fe}(\eta^5\text{-C}_5\text{X}_5)_2$ (X = CH, N, B) and their large third-order nonlinear optical properties. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 8086-92	2.8	21
681	Two unprecedented 1D coordination polymer chains based on tetranuclear copper(II) building blocks. <i>Journal of Solid State Chemistry</i> , <b>2008</b> , 181, 2406-2411	3.3	21
680	A novel pentanuclear Zn(II) coordination polymer with double helices: Synthesis, structure and luminescent property. <i>Inorganic Chemistry Communication</i> , <b>2008</b> , 11, 1246-1249	3.1	21
679	A DFT Study on the Electronic and Redox Properties of $[\text{PW}_{11}\text{O}_{39}(\text{ReN})]_n$ (n = 3, 4, 5) and $[\text{PW}_{11}\text{O}_{39}(\text{OsN})]_2$ . <i>European Journal of Inorganic Chemistry</i> , <b>2006</b> , 2006, 5126-5129	2.3	21
678	Density functional study of protonation sites of $\beta$ -Keggin isopolyanions. <i>International Journal of Quantum Chemistry</i> , <b>2006</b> , 106, 1860-1864	2.1	21
677	Electrochemical reduction of carbon dioxide on the two-dimensional $\text{M}_3(\text{Hexaiminotriphenylene})_2$ sheet: A computational study. <i>Applied Surface Science</i> , <b>2019</b> , 467-468, 98-103	6.7	21
676	A simple strategy to achieve remarkable mechanochromism of cationic Ir(III) phosphors through subtle ligand modification. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 11686-11693	7.1	21
675	Towards red-light o-carborane derivatives with both aggregation induced emission and thermally activated delayed fluorescence combining quantum chemistry calculation with molecular dynamics simulation. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 2699-2709	7.1	20
674	How Does Iridium(III) Photocatalyst Regulate Nickel(II) Catalyst in Metallaphotoredox-Catalyzed C $\beta$ Cross-Coupling? Theoretical and Experimental Insights. <i>ACS Catalysis</i> , <b>2019</b> , 9, 3858-3865	13.1	20
673	High-Nuclear Vanadoniobate $\{\text{Nb}_{48}\text{V}_8\}$ Multiple-Strand Wheel. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 11083-7	5.1	20
672	Self-assembly and photocatalytic properties of Ta/W mixed-addendum polyoxometalate and transition-metal cations. <i>CrystEngComm</i> , <b>2016</b> , 18, 8722-8725	3.3	20
671	Self-assembly and photocatalytic H evolution activity of two unprecedented polytantalotungstates based on the largest $\{\text{Ta}\}$ and $\{\text{TaYb}\}$ clusters. <i>Chemical Communications</i> , <b>2016</b> , 52, 13787-13790	5.8	20
670	Latent harmony in dicarbon between VB and MO theories through orthogonal hybridization of $3d$ and $2p$ . <i>Chemical Science</i> , <b>2016</b> , 7, 1028-1032	9.4	20
669	Uniform NiCo $2$ O $4$ /NiFe $2$ O $4$ hollow nanospheres with excellent properties for Li-ion batteries and supercapacitors. <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 767, 223-231	5.7	20
668	Intramolecular $\pi$ -Stacking in Cationic Iridium(III) Complexes with Phenyl-Functionalized Cyclometalated Ligands: Synthesis, Structure, Photophysical Properties, and Theoretical Studies. <i>European Journal of Inorganic Chemistry</i> , <b>2014</b> , 2014, 2376-2382	2.3	20

667	The relationship between intermolecular interactions and charge transport properties of trifluoromethylated polycyclic aromatic hydrocarbons. <i>Organic Electronics</i> , <b>2014</b> , 15, 1896-1905	3.5	20
666	Multipoint interactions enhanced H <sub>2</sub> storage and organosulfur removal in a microporous metal-organic framework. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 11111	13	20
665	Influence of alkyl chain lengths on the properties of iridium(III)-based piezochromic luminescent dyes with triazole-pyridine type ancillary ligands. <i>Dyes and Pigments</i> , <b>2013</b> , 99, 1082-1090	4.6	20
664	Self-Assembly and Visible-Light Photocatalytic Properties of W/Nb Mixed-Addendum Polyoxometalate and Transition-Metal Cations. <i>ChemPlusChem</i> , <b>2013</b> , 78, 775-779	2.8	20
663	Chiroptical, linear, and second-order nonlinear optical properties of tetrathiafulvalenylallene: a multifunctional molecular material. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 1399	7.1	20
662	Controlled synthesis and magnetically separable photocatalytic properties of magnetic iron oxides@SnO <sub>2</sub> yolk-shell nanocapsules. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 13380		20
661	Metal-organic replica of chiral natural material beta-SnF(2): an enantiopure binodal (3,5)-connected net based on triangular and trigonal bipyramidal coordination. <i>Chemical Communications</i> , <b>2010</b> , 46, 604-608	5.8	20
660	Synthesis and photovoltaic properties of low-bandgap polymers based on N-arylcarbazole. <i>Polymer</i> , <b>2011</b> , 52, 1748-1754	3.9	20
659	Photoluminescent metal-organic framework with hex topology constructed from infinite rod-shaped secondary building units and single e,e-trans-1,4-cyclohexanedicarboxylic dianion. <i>Inorganica Chimica Acta</i> , <b>2007</b> , 360, 3108-3112	2.7	20
658	A two-dimensional conductive Mo-based covalent organic framework as an efficient electrocatalyst for nitrogen fixation. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 23599-23606	13	20
657	Fluorescence, Phosphorescence, or Delayed Fluorescence? A Theoretical Exploration on the Reason Why a Series of Similar Organic Molecules Exhibit Different Luminescence Types. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 23091-23101	3.8	20
656	The electronic and optical properties of carbon nitride derivatives: A first principles study. <i>Applied Surface Science</i> , <b>2018</b> , 453, 442-448	6.7	20
655	Rational design and synthesis of cationic Ir(III) complexes with triazolate cyclometalated and ancillary ligands for multi-color tuning. <i>Dyes and Pigments</i> , <b>2017</b> , 139, 524-532	4.6	19
654	Ir(III) Phosphors Modified with Fluorine Atoms in Pyridine-1,2,4-triazolyl Ligands for Efficient OLEDs Possessing Low-Efficiency Roll-off. <i>Organometallics</i> , <b>2016</b> , 35, 3870-3877	3.8	19
653	Monodisperse and Tiny Co <sub>2</sub> N <sub>0.67</sub> Nanocrystals Uniformly Embedded over Two Curving Surfaces of Hollow Carbon Microfibers as Efficient Electrocatalyst for Oxygen Evolution Reaction. <i>ACS Applied Nano Materials</i> , <b>2018</b> , 1, 4461-4473	5.6	19
652	Polyoxometalate supported complexes as effective electron-transfer mediators in dye-sensitized solar cells. <i>Dalton Transactions</i> , <b>2014</b> , 43, 1493-7	4.3	19
651	Redox-controlled Dawson {Mn <sub>2</sub> (III)W <sub>17</sub> } polyoxometalate with photocatalytic H <sub>2</sub> evolution activity. <i>Chemical Communications</i> , <b>2014</b> , 50, 5961-3	5.8	19
650	Assembly of tetrameric dimethyltin-functionalized selenotungstates: from nanoclusters to one-dimensional chains. <i>Chemical Communications</i> , <b>2015</b> , 51, 2433-6	5.8	19



649	Theoretical Studies on MetalloporphyrinPolyoxometalates Hybrid Complexes for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 29623-29628	3.8	19
648	Phenylcarbazole and phosphine oxide/sulfide hybrids as host materials for blue phosphors: effectively tuning the charge injection property without influencing the triplet energy. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 1685-93	3.6	19
647	TDDFT studies on the electronic structures and chiroptical properties of mono-tin-substituted Wells-Dawson polyoxotungstates. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 4152-8	2.8	19
646	Two unusual self-threading frameworks self-assembled from mixed ligands and cobalt/zinc ions. <i>CrystEngComm</i> , <b>2011</b> , 13, 325-329	3.3	19
645	Charge transport and electronic properties of N-heteroquinones: quadruple weak hydrogen bonds and strong $\pi$ -stacking interactions. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 128, 257-264	1.9	19
644	Macroscopic single-crystal tubes assembled with porous supramolecular architecture of water-soluble calixarene and phenanthroline. <i>Chemical Communications</i> , <b>2009</b> , 1861-3	5.8	19
643	Theoretical studies on nitrido ruthenium (VI) porphyrin and high valent ruthenium nitrido derivatives of Keggin typical polyoxometalate ([PW <sub>11</sub> O <sub>39</sub> {Ru(VI)N} <sub>4</sub> ]-): electronic structures and bonding features. <i>Dalton Transactions</i> , <b>2009</b> , 6208-13	4.3	19
642	Quantum Chemical Design for Enhanced Second-Order NLO Response of Terpyridine-Substituted Hexamolybdates. <i>European Journal of Inorganic Chemistry</i> , <b>2010</b> , 2010, 3466-3472	2.3	19
641	A series of inorganicorganic hybrid compounds constructed from bis(undecatungstophosphate) lanthanates and copper-organic units. <i>Inorganica Chimica Acta</i> , <b>2010</b> , 363, 3823-3831	2.7	19
640	Simple molecular structure design of iridium(III) complexes: Achieving highly efficient non-doped devices with low efficiency roll-off. <i>Organic Electronics</i> , <b>2016</b> , 35, 142-150	3.5	19
639	Exploring more effective polymer donors for the famous non-fullerene acceptor ITIC in organic solar cells by increasing electron-withdrawing ability. <i>Organic Electronics</i> , <b>2018</b> , 53, 308-314	3.5	19
638	A metal-organic framework based on nanosized hexagonal channels as fluorescent indicator for detection of nitroaromatic explosives. <i>Journal of Solid State Chemistry</i> , <b>2018</b> , 258, 781-785	3.3	18
637	Tailored Synthesis of Octopus-type Janus Nanoparticles for Synergistic Actively-Targeted and Chemo-Photothermal Therapy. <i>Angewandte Chemie</i> , <b>2016</b> , 128, 2158-2161	3.6	18
636	Syntheses, crystal structures and properties of inorganicorganic hybrids constructed from Keggin-type polyoxometalates and silver coordination compounds. <i>CrystEngComm</i> , <b>2014</b> , 16, 7410-7418	3.3	18
635	Flowerlike Fe <sub>2</sub> O <sub>3</sub> @NiO hierarchical core-shell nanostructures as superb capability and magnetically separable adsorbents for water treatment. <i>RSC Advances</i> , <b>2013</b> , 3, 12671	3.7	18
634	An accurate and efficient method to predict the electronic excitation energies of BODIPY fluorescent dyes. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 566-75	3.5	18
633	Design of Hexabenzocoronene Derivatives as Non-Fullerene Acceptors in Organic Photovoltaics by Bridging Dimers and Modulating Structural Twists. <i>Solar Rrl</i> , <b>2017</b> , 1, 1700060	7.1	18
632	Synthesis of cationic iridium(III) complexes with high quantum yield via enhancing the steric hindrance of ligands. <i>Journal of Organometallic Chemistry</i> , <b>2012</b> , 702, 27-35	2.3	18

- 631 After the electronic field: structure, bonding, and the first hyperpolarizability of HArF. *Journal of Computational Chemistry*, **2013**, 34, 952-7 3.5 18
- 630 Theoretical exploration of photoisomerization-switchable second-order nonlinear optical responses of two-dimensional  $\pi$  and w-shaped polyoxometalate derivatives of dithienylperfluorocyclopentene. *Journal of Physical Chemistry A*, **2013**, 117, 10783-9 2.8 18
- 629 Identification of nonplanar small molecule for G-quadruplex grooves: molecular docking and molecular dynamic study. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 6969-72 2.9 18
- 628 An accurate density functional theory calculation for electronic excitation energies: the least-squares support vector machine. *Journal of Chemical Physics*, **2009**, 130, 184104 3.9 18
- 627 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 2.3 18
- 626 Calculations of two-photon absorption cross-sections of stilbene and bis (styryl) benzene derivatives by means of TDDFT-SOS method. *Computational and Theoretical Chemistry*, **2005**, 726, 61-65 18
- 625 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 3.6 18
- 624 Water-stable lanthanide-based metal-organic gel for the detection of organic amines and white-light emission. *Journal of Materials Chemistry C*, **2020**, 8, 13648-13654 7.1 18
- 623 Three Keggin-Type Transition Metal-Substituted Polyoxometalates as Pure Inorganic Photosensitizers for p-Type Dye-Sensitized Solar Cells. *Chemistry - A European Journal*, **2016**, 22, 3234-3238 4.8 18
- 622 Designed Synthesis of Lipid-Coated Polyacrylic Acid/Calcium Phosphate Nanoparticles as Dual pH-Responsive Drug-Delivery Vehicles for Cancer Chemotherapy. *Chemistry - A European Journal*, **2017**, 23, 6586-6595 4.8 17
- 621 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 8.5 17
- 620 Self-assembly and photocatalytic H<sub>2</sub> evolution activity of two nanoscale polytantalotungstates based on unprecedented {Cr<sub>3</sub>Ta<sub>6</sub>} and {Cr<sub>4</sub>Ta<sub>12</sub>} clusters. *Journal of Materials Chemistry A*, **2017**, 5, 22970-22974 13.7 17
- 619 Self-Assembly of Nanoscale Lanthanoid-Containing Selenotungstates: Synthesis, Structures, and Magnetic Studies. *Inorganic Chemistry*, **2019**, 58, 12895-12904 5.1 17
- 618 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 4.7 17
- 617 Self-assembly and photocatalytic hydrogen evolution of a niobium-containing polyoxometalate. *Inorganic Chemistry Communication*, **2014**, 44, 195-197 3.1 17
- 616 Hydrothermal synthesis and luminescence properties of hierarchical SrF<sub>2</sub> and SrF<sub>2</sub>:Ln<sup>3+</sup> (Ln = Er, Nd, Yb, Eu, Tb) micro/nanocomposite architectures. *Materials Research Bulletin*, **2012**, 47, 328-332 5.1 17
- 615 An effective method for accurate prediction of the first hyperpolarizability of alkalides. *Journal of Computational Chemistry*, **2012**, 33, 231-6 3.5 17
- 614 The encapsulated lithium effect of Li@C<sub>60</sub>Cl<sub>8</sub> remarkably enhances the static first hyperpolarizability. *RSC Advances*, **2013**, 3, 13348 3.7 17

613	Near-infrared light and pH-responsive Au@carbon/calcium phosphate nanoparticles for imaging and chemo-photothermal cancer therapy of cancer cells. <i>Dalton Transactions</i> , <b>2017</b> , 46, 14746-14751	4.3	17
612	Synthesis, crystal structure, and application of an acenaphtho[1,2-k] fluoranthene diimide derivative. <i>Science China Chemistry</i> , <b>2015</b> , 58, 364-369	7.9	17
611	Redox-active polyoxometalate-based crystalline material-immobilized noble metal nanoparticles: spontaneous reduction and synergistic catalytic activity. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 21040		17
610	Quantum chemical characterization of the generation of high-valent oxoruthenium species of Keggin type polyoxometalates: electronic structure and bonding features. <i>Dalton Transactions</i> , <b>2011</b> , 40, 2967-74	4.3	17
609	A series of POM-based entangled frameworks with the rigid ligand 1,4-bis(1-imidazolyl)benzene and different isomers of octamolybdate. <i>Journal of Solid State Chemistry</i> , <b>2011</b> , 184, 1141-1147	3.3	17
608	Quantum chemical study of structures, electronic spectrum, and nonlinear optical properties of polynuclear lithium compounds. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 966, 14-19	2	17
607	Construction of a series of 0D, 2D and 3D inorganic-organic hybrid coordination polymers based on octamolybdate and 2-(2-pyridyl)imidazole and its derivative. <i>Inorganica Chimica Acta</i> , <b>2010</b> , 363, 118-126	2.7	17
606	An equatorial tri-iron substituted Wells-Dawson type tungstophosphate with magnetic and bifunctional electrocatalytic properties. <i>Inorganica Chimica Acta</i> , <b>2010</b> , 363, 718-722	2.7	17
605	Synthesis, structure and characterization of a new cobalt-containing germanotungstate with open Wells-Dawson structure: $K_{13}[\{Co(H_2O)\}_2\{Ge_2W_{18}O_{66}\}] \cdot 2H_2O$ . <i>Journal of Molecular Structure</i> , <b>2006</b> , 785, 170-175	3.4	17
604	Structure, stability, and aromaticity of $M_3Pc$ ( $M=B, Al, \text{ and } Ga$ ): Computational study. <i>International Journal of Quantum Chemistry</i> , <b>2005</b> , 103, 54-59	2.1	17
603	Highly Efficient Photoreduction of Low-Concentration CO to Syngas by Using a Polyoxometalates/Ru Composite. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 2735-2740	4.8	17
602	in situ engineered ultrafine NiS-ZnS heterostructures in micro-mesoporous carbon spheres accelerating polysulfide redox kinetics for high-performance lithium-sulfur batteries. <i>Nanoscale</i> , <b>2020</b> , 12, 16201-16207	7.7	17
601	Assembly of Mn-Containing Unprecedented Selenotungstate Clusters with Photocatalytic H <sub>2</sub> Evolution Activity. <i>Crystal Growth and Design</i> , <b>2016</b> , 16, 2481-2486	3.5	17
600	Visible-light CO <sub>2</sub> photoreduction of polyoxometalate-based hybrids with different cobalt clusters. <i>CrystEngComm</i> , <b>2019</b> , 21, 6423-6431	3.3	17
599	A triazine-based metal-organic framework with solvatochromic behaviour and selectively sensitive photoluminescent detection of nitrobenzene and Cu <sup>2+</sup> ions. <i>Dyes and Pigments</i> , <b>2019</b> , 163, 159-167	4.6	17
598	Effect of polyoxometalate in organic-inorganic hybrids on charge transfer and absorption spectra towards sensitizers. <i>Dyes and Pigments</i> , <b>2017</b> , 142, 379-386	4.6	16
597	POM-based inorganic-organic hybrid compounds: synthesis, structures, highly-connected topologies and photodegradation of organic dyes. <i>RSC Advances</i> , <b>2015</b> , 5, 59093-59098	3.7	16
596	An intriguing window opened by a metallic two-dimensional Lindqvist-cobaltporphyrin organic framework as an electrochemical catalyst for the CO <sub>2</sub> reduction reaction. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 14807-14814	13	16

- 595 A 3D pillared-layer metal-organic framework with fluorescence property for detection of nitroaromatic explosives. *New Journal of Chemistry*, **2019**, 43, 963-969 3.6 16
- 594 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 8.3 16
- 593 Helical Carbon Segment in Carbon-Boron-Nitride Heteronanotubes: Structure and Nonlinear Optical Properties. *ChemPlusChem*, **2014**, 79, 732-736 2.8 16
- 592 Theoretical exploration on switchable NLO response induced by photochromic properties of covalently connected unsymmetrical spiropyran-polyoxometalate complex. *Dyes and Pigments*, **2014**, 106, 105-110 4.6 16
- 591 The photovoltaic performance of dye-sensitized solar cells enhanced by using Dawson-type heteropolyacid and heteropoly blue-TiO<sub>2</sub> composite films as photoanode. *Inorganic Chemistry Communication*, **2014**, 47, 138-143 3.1 16
- 590 Nonaqueous synthesis of uniform polyaniline nanospheres Via cellulose acetate template. *Journal of Polymer Science Part A*, **2012**, 50, 912-917 2.5 16
- 589 Syntheses, structures, and photoluminescence of d10 coordination architectures: From 1D to 3D complexes based on mixed ligands. *Solid State Sciences*, **2011**, 13, 1083-1091 3.4 16
- 588 Thermochemical stabilities, electronic structures, and optical properties of C<sub>56</sub>X<sub>10</sub> (X = H, F, and Cl) fullerene compounds. *Journal of Computational Chemistry*, **2011**, 32, 658-67 3.5 16
- 587 Electronic properties of unprecedented bridging organoimido-substituted hexamolybdate: new insights from density functional theory study. *Journal of Physical Chemistry B*, **2010**, 114, 3754-8 3.4 16
- 586 Two New Helical Compounds Based on Pitch-Tunable Keggin Clusters. *European Journal of Inorganic Chemistry*, **2009**, 2009, 5175-5180 2.3 16
- 585 Quantum chemical study of redox-switchable second-order optical nonlinearity in Keggin-type organoimido derivative [PW<sub>11</sub>O<sub>39</sub>(ReNC<sub>6</sub>H<sub>5</sub>)<sub>n</sub>]<sub>n</sub> (n = 2-4). *Theoretical Chemistry Accounts*, **2009**, 122, 265-273 1.9 16
- 584 Synthesis, characterization and crystal structure of a novel Os(II)-supported tungstoarsenate [HAsW<sub>7</sub>O<sub>28</sub>Os(dmsO)<sub>3</sub>]<sub>6</sub>. *Journal of Solid State Chemistry*, **2009**, 182, 83-88 3.3 16
- 583 Synthesis, crystal structures and nonlinear optical properties of three TCF-based chromophores. *CrystEngComm*, **2009**, 11, 589-596 3.3 16
- 582 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 3.3 16
- 581 Colorimetric detection of immunoglobulin G by use of functionalized gold nanoparticles on polyethylenimine film. *Analytical and Bioanalytical Chemistry*, **2006**, 384, 1518-24 4.4 16
- 580 Construction of porous covalent organic polymer as photocatalysts for RhB degradation under visible light. *Science Bulletin*, **2017**, 62, 931-937 10.6 15
- 579 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 3.7 15
- 578 A novel Ta/W mixed-addendum polyoxometalate with photocatalytic properties. *Dalton Transactions*, **2017**, 46, 10177-10180 4.3 15

577	Intra- and Intermolecular Charge Transfer in a Novel Dimer: Cooperatively Enhancing Second-Order Optical Nonlinearity. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 25472-25478	3.8	15
576	Co-sensitization promoted light harvesting with a new mixed-addenda polyoxometalate [Cu(C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> [V <sub>2</sub> W <sub>4</sub> O <sub>19</sub> ] <sub>4</sub> ·4H <sub>2</sub> O in dye-sensitized solar cells. <i>Dalton Transactions</i> , <b>2015</b> , 44, 18553-6243	4.3	15
575	A sulfur-free iridium(III) complex for highly selective and multi-signaling mercury(II)-chemosensors. <i>Dalton Transactions</i> , <b>2015</b> , 44, 19997-20003	4.3	15
574	Theoretical design and characterization of high-efficiency organic dyes with different electron-withdrawing groups based on C <sub>275</sub> toward dye-sensitized solar cells. <i>New Journal of Chemistry</i> , <b>2016</b> , 40, 9320-9328	3.6	15
573	Syntheses, crystal structures and properties of metal-organic rotaxane frameworks with cucurbit[6]uril. <i>CrystEngComm</i> , <b>2016</b> , 18, 2327-2336	3.3	15
572	Theoretical studies on the photoisomerization-switchable second-order nonlinear optical responses of DTE-linked polyoxometalate derivatives. <i>Journal of Molecular Graphics and Modelling</i> , <b>2013</b> , 40, 110-5	2.8	15
571	Synthesis, structure and photophysical properties of cationic Ir(III) complexes with functionalized 1,10-phenanthroline ancillary ligands. <i>Journal of Organometallic Chemistry</i> , <b>2012</b> , 713, 20-26	2.3	15
570	Theoretical studies of the effect of electron-withdrawing dicyanovinyl group on the electronic and charge-transport properties of fluorene-thiophene oligomers. <i>Theoretical Chemistry Accounts</i> , <b>2012</b> , 131, 1	1.9	15
569	Probing the linear and nonlinear optical properties of nitrogen-substituted carbon nanotube. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 3219-25	2	15
568	Theoretical study on the rectifying performance of organoimido derivatives of hexamolybdates. <i>ChemPhysChem</i> , <b>2013</b> , 14, 610-7	3.2	15
567	Bonding Interactions between Nitrous Oxide (N <sub>2</sub> O) and Mono-Ruthenium Substituted Keggin-Type Polyoxometalates: Electronic Structures of Ruthenium/N <sub>2</sub> O Adducts. <i>European Journal of Inorganic Chemistry</i> , <b>2011</b> , 2011, 489-494	2.3	15
566	Self-assembly of zinc polymers based on a flexible linear ligand at different pH values: Syntheses, structures and fluorescent properties. <i>Solid State Sciences</i> , <b>2009</b> , 11, 635-642	3.4	15
565	1,2,3,4-Alternate double cone conformational extreme in the supramolecular assemblies of p-sulfonatocalix[8]arene. <i>CrystEngComm</i> , <b>2009</b> , 11, 1803	3.3	15
564	Theoretical predication of third-order optical nonlinearities of [Al <sub>4</sub> MA <sub>4</sub> ] <sub>n</sub> (n = 0, M = Ti, V and Cr) clusters. <i>Theoretical Chemistry Accounts</i> , <b>2008</b> , 119, 329-333	1.9	15
563	A metal-organic framework containing meso-helical chains: Synthesis, characterization and luminescent property. <i>Inorganic Chemistry Communication</i> , <b>2008</b> , 11, 1181-1183	3.1	15
562	Theoretical study on C <sub>32</sub> fullerenes and derivatives. <i>Chemical Physics Letters</i> , <b>2006</b> , 428, 148-151	2.5	15
561	A Mixed-Valence Tin-Oxygen Cluster Containing Six Peripheral Ferrocene Units. <i>Angewandte Chemie</i> , <b>2004</b> , 116, 2463-2465	3.6	15
560	Supramolecular oligourethane gel as a highly selective fluorescent sensor for ions. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 11540-11545	7.1	15

559	A visible-light responsive zirconium metal-organic framework for living photopolymerization of methacrylates. <i>RSC Advances</i> , <b>2016</b> , 6, 66444-66450	3.7	15
558	Connecting effect on the first hyperpolarizability of armchair carbon-boron-nitride heteronanotubes: pattern versus proportion. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 13954-9	3.6	15
557	Reversible tricolour luminescence switching based on a piezochromic iridium(III) complex. <i>Chemical Communications</i> , <b>2019</b> , 55, 14582-14585	5.8	15
556	Synthesis of red-emitting cationic Ir (III) complex and its application in white light-emitting electrochemical cells. <i>Organic Electronics</i> , <b>2017</b> , 42, 303-308	3.5	14
555	Strategic modification of ligands for remarkable piezochromic luminescence (PCL) based on a neutral Ir(III) phosphor. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 10876-10880	7.1	14
554	Guest exchange in a porous cucurbit[6]uril-based metal-organic rotaxane framework probed by NMR and X-ray crystallography. <i>Chemical Communications</i> , <b>2018</b> , 54, 5474-5477	5.8	14
553	Metal-Organic Frameworks with Organogold(III) Complexes for Photocatalytic Amine Oxidation with Enhanced Efficiency and Selectivity. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 15089-15095	4.8	14
552	Polyoxometalates-Based Metal-Organic Frameworks Made by Electrodeposition and Carbonization Methods as Cathodes and Anodes for Asymmetric Supercapacitors. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 16617	4.8	14
551	Green Oxidative Degradation of Methyl Orange with Copper(II) Schiff Base Complexes as Photo-Fenton-Like Catalysts. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2014</b> , 640, 2035-2040	1.3	14
550	A series of coordination compounds containing rigid multi-pyridine based ligands: syntheses, structures and properties. <i>CrystEngComm</i> , <b>2014</b> , 16, 2754	3.3	14
549	Superatoms (Li <sub>3</sub> O and BeF <sub>3</sub> ) induce phenalenyl radical dimer: fascinating interlayer charge-transfer and large NLO responses. <i>Dalton Transactions</i> , <b>2014</b> , 43, 12657-62	4.3	14
548	How does a little difference in structure determine whether molecules have thermally activated delayed fluorescence characteristic or not?. <i>Organic Electronics</i> , <b>2017</b> , 50, 70-76	3.5	14
547	Syntheses, structures, magnetic and luminescence properties of a series of coordination polymers constructed from 1,4-naphthalenedicarboxylate and N-donor ligands. <i>CrystEngComm</i> , <b>2015</b> , 17, 4517-4524	3.3	14
546	The self-assembly mechanism of the Lindqvist anion [W <sub>6</sub> O <sub>19</sub> ] <sup>2-</sup> in aqueous solution: a density functional theory study. <i>Dalton Transactions</i> , <b>2012</b> , 41, 11361-8	4.3	14
545	Ab initio and density functional study on fullerene C <sub>44</sub> and its derivatives. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 978, 166-171	2	14
544	On the origin of the inverted stability order of the reverse-Keggin [(MnO <sub>4</sub> )(CH <sub>3</sub> ) <sub>12</sub> Sb <sub>12</sub> O <sub>24</sub> ] <sup>6-</sup> : a DFT study of alpha, beta, gamma, delta, and epsilon isomers. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 5472-81	5.1	14
543	Theoretical study on the tetranuclear endohedral vanadyl carboxylates with guest-switchable redox properties and large polarizability. <i>Dalton Transactions</i> , <b>2010</b> , 39, 3706-13	4.3	14
542	Organic-inorganic hybrids constructed by Anderson-type polyoxoanions and copper coordination complexes. <i>Journal of Solid State Chemistry</i> , <b>2009</b> , 182, 49-54	3.3	14

541	Broad absorbing low-bandgap polythiophene derivatives incorporating separate and content-tunable benzothiadiazole and carbazole moieties for polymer solar cells. <i>European Polymer Journal</i> , <b>2010</b> , 46, 1770-1777	5.2	14
540	DFT study on second-order nonlinear optical properties of the derivatives of 7-vertex cobaltbarborane metallocenyl. <i>Computational and Theoretical Chemistry</i> , <b>2008</b> , 863, 66-72		14
539	Maximized Schottky Effect: The Ultrafine V O /Ni Heterojunctions Repeatedly Arranging on Monolayer Nanosheets for Efficient and Stable Water-to-Hydrogen Conversion. <i>Small</i> , <b>2021</b> , 17, e2005769	11	14
538	Facile Fabrication of Well-Dispersed Pt Nanoparticles in Mesoporous Silica with Large Open Spaces and Their Catalytic Applications. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 9293-8	4.8	14
537	Large Size Color-tunable Electroluminescence from Cationic Iridium Complexes-based Light-emitting Electrochemical Cells. <i>Scientific Reports</i> , <b>2016</b> , 6, 27613	4.9	14
536	Bottom-Up Construction and Reversible Structural Transformation of Supramolecular Isomers based on Large Truncated Tetrahedra. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 790-794	3.6	14
535	Recent advances in oligomers/polymers with unconventional chromophores. <i>Materials Chemistry Frontiers</i> , <b>2021</b> , 5, 60-75	7.8	14
534	Honeycomb-patterned hybrid films of surfactant-encapsulated polyoxometalates by a breath figure method and its electrocatalysis for BrO. <i>Dalton Transactions</i> , <b>2017</b> , 47, 105-111	4.3	14
533	A multifunctional microporous metal-organic framework: efficient adsorption of iodine and column-chromatographic dye separation.. <i>RSC Advances</i> , <b>2018</b> , 8, 36400-36406	3.7	14
532	Low-cost p-type dye-sensitized solar cells based on Dawson-type transition metal-substituted polyoxometalate inorganic co-sensitizers. <i>Inorganic Chemistry Frontiers</i> , <b>2017</b> , 4, 1187-1191	6.8	13
531	Degradation of azo dyes under visible light with stable MOF based on tetrastylene imidazole ligand. <i>Dalton Transactions</i> , <b>2020</b> , 49, 4352-4357	4.3	13
530	Ultrahigh capacity 2D anode materials for lithium/sodium-ion batteries: an entirely planar B7P2 monolayer with suitable pore size and distribution. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 10301-10309	13	13
529	Theoretical investigation on the 2e/12c bond and second hyperpolarizability of azaphenalenyl radical dimers: strength and effect of dimerization. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 124314	3.9	13
528	Tin Alkylarsonate Clusters: $C_2H_4O_2X$ (X = Cl, O, and $\text{NH}_2$ ) Interaction-Mediated Supramolecular Formation. <i>Crystal Growth and Design</i> , <b>2009</b> , 9, 3881-3888	3.5	13
527	Triphenylamine-based pH chemosensor: Synthesis, crystal structure, photophysical properties and computational studies. <i>Synthetic Metals</i> , <b>2009</b> , 159, 2497-2501	3.6	13
526	A en-templated 3D coordination polymer based on H2pzdc with macrometallo cycles. <i>Inorganic Chemistry Communication</i> , <b>2010</b> , 13, 1227-1230	3.1	13
525	Unprecedented dinuclear tin derivative of deprotonated beta-cyclodextrins. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 2931-3	5.1	13
524	Synthesis and characterization of a new trifunctional magnetic-photoluminescent-oxygen-sensing nanomaterial. <i>Nanotechnology</i> , <b>2008</b> , 19, 495709	3.4	13

- 523 Hierarchical self-assembling of dendritic-linear diblock complex based on hydrogen bonding. *Polymer*, **2007**, 48, 3759-3770 3.9 13
- 522 A novel chiral 3D supramolecular framework based on organooxotin cluster. *Inorganic Chemistry Communication*, **2008**, 11, 220-224 3.1 13
- 521 'One-step' controllable synthesis of Ag and Ag<sub>2</sub>S nanocrystals on a large scale. *Nanotechnology*, **2006**, 17, 5681-5 3.4 13
- 520 Synthesis and self-assembly of silica-coated anisotropic gold nanoparticle films. *Nanotechnology*, **2006**, 17, 1819-1824 3.4 13
- 519 Synthesis, structure and luminescent properties of two three-dimensional d<sup>10</sup> metal complexes constructed from pyridine-3,4-dicarboxylic acid with new network topologies. *Journal of Molecular Structure*, **2006**, 796, 172-178 3.4 13
- 518 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 2.1 13
- 517 Self-assembling structures and thin-film microscopic morphologies of amphiphilic rod-coil block oligomers. *Journal of Colloid and Interface Science*, **2005**, 289, 488-97 9.3 13
- 516 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 3.1 13
- 515 A mechanochromic cyclometalated cationic Ir(III) complex with AIE activity by strategic modification of ligands. *Dalton Transactions*, **2020**, 49, 13066-13071 4.3 13
- 514 Preparation and electrochemical hydrogen storage properties of Ti<sub>49</sub>Zr<sub>26</sub>Ni<sub>25</sub> alloy covered with porous polyaniline. *International Journal of Hydrogen Energy*, **2020**, 45, 11675-11685 6.7 13
- 513 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 3.6 12
- 512 Photosensitizers based on Ir(III) complexes for highly efficient photocatalytic hydrogen generation. *Dyes and Pigments*, **2019**, 170, 107547 4.6 12
- 511 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 3.7 12
- 510 A novel 3D cobalt(II) metal-organic framework to activate peroxymonosulfate for degradation of organic dyes in water. *Journal of Solid State Chemistry*, **2020**, 289, 121443 3.3 12
- 509 Multi-functional TiO<sub>2</sub> nanosheets/carbon nanotubes modified separator enhanced cycling performance for lithium-sulfur batteries. *International Journal of Energy Research*, **2020**, 44, 3231-3240 4.5 12
- 508 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 9.5 12
- 507 Mn-doped CsPb(Br/Cl) mixed-halide perovskites for CO photoreduction. *Nanotechnology*, **2020**, 31, 215605 3.4 12
- 506 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 3.7 12



505	Theoretical studies on organic D-π sensitizers with planar triphenylamine donor and different linkers for dyes-sensitized solar cells. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2309	2	12
504	The structure-property relationship of chiral 1,1'-binaphthyl-based polyoxometalates: TDDFT studies on the static first hyperpolarizabilities and the ECD spectra. <i>Journal of Molecular Graphics and Modelling</i> , <b>2012</b> , 32, 1-8	2.8	12
503	From blue to full color - theoretical design and characterization of a series of Ir(III) complexes containing azoline ligand with potential application in OLEDs. <i>Dalton Transactions</i> , <b>2017</b> , 46, 11491-11502	4.3	12
502	Ag(I)-mediated formation of a 2D cyano-bridged multinuclear silver(I) alkynyl network coupled with the C≡N bond cleavage of acetonitrile. <i>CrystEngComm</i> , <b>2014</b> , 16, 10376-10379	3.3	12
501	TDDFT studies on the determination of the absolute configurations and chiroptical properties of Strandberg-type polyoxometalates. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 2492-8	2.8	12
500	Time-dependent current distributions of a two-terminal carbon nanotube-based electronic device. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 5519-25	3.4	12
499	Building block approach to a series of substituted Keggin-type inorganic-organic hybrids. <i>Solid State Sciences</i> , <b>2011</b> , 13, 1115-1121	3.4	12
498	DFT study on the second-order nonlinear optical property of 12-vertex close-cubane derivatives. <i>International Journal of Quantum Chemistry</i> , <b>2011</b> , 111, 1039-1047	2.1	12
497	Theoretical study on the two-dimensional second-order nonlinear optical properties: a series of charge-transfer covalently bonded organoimido derived hexamolybdate complexes. <i>Theoretical Chemistry Accounts</i> , <b>2009</b> , 122, 217-226	1.9	12
496	Theoretical study on the second-order nonlinear optical properties of nonconjugated D-π chromophores. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 1553-1559	2.1	12
495	Theoretical investigation of structures, electronic spectra and nonlinear optical properties of gold-pentacene (Au <sub>2</sub> C <sub>22</sub> H <sub>14</sub> ) complexes. <i>Journal of Organometallic Chemistry</i> , <b>2009</b> , 694, 1266-1272	2.3	12
494	Interpenetrating metal-organic frameworks formed by self-assembly of tetrahedral and octahedral building blocks. <i>Journal of Solid State Chemistry</i> , <b>2009</b> , 182, 3105-3112	3.3	12
493	A novel luminescent 3D metal-organic framework possessing 4-fold interpenetrating (3,4)-connected net. <i>Inorganic Chemistry Communication</i> , <b>2009</b> , 12, 969-971	3.1	12
492	Theoretical studies on the structure and properties of BN clusters (BN) <sub>n</sub> and endohedral metallo-BN clusters M@BN <sub>n</sub> . <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 964, 56-64	2	12
491	Synthesis and characterizations of novel spindle-like terphenyl-type chromophores for non-linear optical materials. <i>Tetrahedron</i> , <b>2011</b> , 67, 4110-4117	2.4	12
490	A new luminescent 3-D metal-organic framework of diamond-like network possessing 8-fold interpenetration. <i>Journal of Coordination Chemistry</i> , <b>2011</b> , 64, 1578-1585	1.6	12
489	ITO electrode modified by self-assembling multilayer film of polyoxometallate on poly(vinyl alcohol) nanofibers and its electrocatalytic behavior. <i>Electrochimica Acta</i> , <b>2007</b> , 53, 569-574	6.7	12
488	MP2 theory investigation on the halides of D <sub>6h</sub> C <sub>36</sub> :C <sub>36</sub> X <sub>n</sub> (X=F,Cl,Br; n=2,4,6,12). <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 144108	3.9	12

- 487 A Series of New Organotin Cyanometalate Compounds Based on Triorganotin, Diorganotin, and Organooxotin Clusters. *Organometallics*, **2006**, 25, 5996-6006 3.8 12
- 486 Electronic properties of Strandberg anions: A DFT study of  $[X_2Mo_5O_{23}]_n^-$  ( $X = PV, SVI, AsV, SeVI$ ), and  $[(RP)_2Mo_5O_{21}]_4^-$  ( $R = H, CH_3, C_2H_5$ ). *International Journal of Quantum Chemistry*, **2005**, 105, 37-42 2.1 12
- 485 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 3.9 12
- 484 Transition metals doped fullerenes: structures and NLO property relationships. *Molecular Physics*, **2019**, 117, 705-711 1.7 12
- 483 Rational design of iridium-porphyrin conjugates for novel synergistic photodynamic and photothermal therapy anticancer agents.. *Chemical Science*, **2021**, 12, 5918-5925 9.4 12
- 482 Bimetallic Phosphides as High-Efficient Electrocatalysts for Hydrogen Generation. *Inorganic Chemistry*, **2021**, 60, 1624-1630 5.1 12
- 481 Metal-organic framework (MOF) composite materials for photocatalytic CO reduction under visible light. *Dalton Transactions*, **2021**, 50, 3186-3192 4.3 12
- 480 Electrochemical and diffuse reflectance study on tetrahedral Keggin-based metal-organic frameworks. *RSC Advances*, **2017**, 7, 31544-31548 3.7 11
- 479 Ligand-Induced Tunable Dual-Color Emission Based on Lead Halide Perovskites for White Light-Emitting Diodes. *ACS Applied Materials & Interfaces*, **2019**, 11, 15898-15904 9.5 11
- 478 One lithium atom binding with P-nitroaniline: lithium salts or lithium electrides?. *Journal of Molecular Modeling*, **2015**, 21, 23 2 11
- 477 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 9.3 11
- 476 Trimeric hexa-dimethyltin-functionalized selenotungstate  $[\{Sn(CH_3)_2(CH_3COO)\}_3\{Sn(CH_3)_2\}_3\{Se_2W_{18}O_{62}(OH)(H_2O)\}_3]^{18-}$ . *CrystEngComm*, **2016**, 18, 2820-2824 3.3 11
- 475 Evidence of two-state reactivity in water oxidation catalyzed by polyoxometalate-based complex  $[Mn_3(H_2O)_3(SbW_9O_{33})_2]^{12-}$ . *Journal of Catalysis*, **2019**, 376, 146-149 7.3 11
- 474 Bonding interactions between sulfur dioxide (SO<sub>2</sub>) and mono-ruthenium(II)-substituted Keggin-type polyoxometalates: electronic structures of ruthenium-SO<sub>2</sub> adducts. *Physical Chemistry Chemical Physics*, **2014**, 16, 18017-22 3.6 11
- 473 TDDFT studies on the structures and ECD spectra of chiral bisarylimidos bearing different lengths of o-alkoxy chain-substituted polyoxomolybdates. *Journal of Molecular Graphics and Modelling*, **2012**, 35, 49-56 2.8 11
- 472 Density functional studies on photophysical properties and chemical reactivities of the triarylboranes: effect of the constraint of planarity. *Journal of Molecular Modeling*, **2013**, 19, 3437-46 2 11
- 471 Modulating the charge transfer of D-S-A molecules: structures and NLO properties. *Journal of Physical Chemistry A*, **2015**, 119, 767-73 2.8 11
- 470 Assembly of large purely inorganic Ce-stabilized/bridged selenotungstates: from nanoclusters to layers. *Chemistry - an Asian Journal*, **2015**, 10, 1184-91 4.5 11

469	Theoretical study on the charge transport property of Pt(CN(t)Bu) <sub>2</sub> (CN) <sub>2</sub> nanowires induced by Pt⋯Pt interactions. <i>Dalton Transactions</i> , <b>2012</b> , 41, 7272-7	4.3	11
468	TDDFT studies on chiral organophosphonate substituted divacant Keggin-type polyoxotungstate: diplex multistep-redox-triggered chiroptical and NLO switch. <i>Dalton Transactions</i> , <b>2012</b> , 41, 10097-104	4.3	11
467	Theoretical study of isomerism/phase dependent charge transport properties in tris(8-hydroxyquinolino)aluminum(III). <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 9259-64	2.8	11
466	Quantum chemical studies of Lindqvist-type polyoxometalates containing late 3d transition metals ([L(py)M <sub>12</sub> O <sub>18</sub> ] <sub>4</sub> [M = Fe, Co, Ni]): M⋯M bonding and second-order nonlinear optical properties. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 130, 1043-1053	1.9	11
465	Structures and fluorescence properties of two novel metal-organic frameworks based on the bis(2-benzimidazole) and aromatic carboxylate ligands. <i>Inorganic Chemistry Communication</i> , <b>2011</b> , 14, 1077-1081	3.1	11
464	Helical channels, low framework density and structure-directing effect: a novel non-centrosymmetric zinc phosphate NIS-4 prepared by ionothermal reaction. <i>CrystEngComm</i> , <b>2010</b> , 12, 3448	3.3	11
463	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. <i>International Journal of Molecular Sciences</i> , <b>2011</b> , 12, 2242-61	6.3	11
462	Improving the accuracy of low level quantum chemical calculation for absorption energies: the genetic algorithm and neural network approach. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 5124-9	3.6	11
461	Theoretical study on dithieno[3,2-b:2',3'-d]phosphole derivatives: high-efficiency blue-emitting materials with ambipolar semiconductor behavior. <i>Theoretical Chemistry Accounts</i> , <b>2010</b> , 127, 419-427	1.9	11
460	Charge transport and luminescent properties of C <sub>6</sub> F <sub>5</sub> Cu(py) and their relationships with cuprophilic interactions: a density functional theory investigation. <i>Theoretical Chemistry Accounts</i> , <b>2010</b> , 127, 735-742	1.9	11
459	A theoretical study on the efficient reversible redox-based switching of the second-order polarizabilities of two-dimensional nonlinear optical-active donor-acceptor phenanthroline-hexamolybdate. <i>Journal of Molecular Graphics and Modelling</i> , <b>2010</b> , 29, 13-20	2.8	11
458	Electronic structures and spectra of porphyrin with fused benzoheterocycles: DFT and TDDFT-PCM investigations. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 107, 1614-1623	2.1	11
457	A facile method to produce highly monodispersed nanospheres of cystine aggregates. <i>Nanotechnology</i> , <b>2006</b> , 17, 5163-5166	3.4	11
456	Photoelectric properties of material of N,N'-bis(4-aminophenyl)-1,4-quinonediimine doped with heteropolyacid. <i>Synthetic Metals</i> , <b>2002</b> , 129, 15-18	3.6	11
455	Highly Fluorescent Cadmium Based Metal-Organic Frameworks for Rapid Detection of Antibiotic Residues, Fe and CrO Ions. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 9148-9156	5.1	11
454	Sublimable cationic Ir(III) phosphor using chlorine as a counterion for high-performance monochromatic and white OLEDs. <i>Chemical Communications</i> , <b>2018</b> , 54, 11761-11764	5.8	11
453	Phenalenyl Dimer under the External Electric Field: Two-Electron/12-Center Bonding Breaking and Emergence of Electrostatic Interaction. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 3765-3770	3.8	10
452	Copper cyanide polymers with controllable dimensions modulated by rigid and flexible bis-(imidazole) ligands: synthesis, crystal structure and fluorescence properties. <i>CrystEngComm</i> , <b>2019</b> , 21, 1242-1249	3.3	10

- 451 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 3.8 10
- 450 Blue-emitting thermoreversible oligourethane gelators with aggregation-induced emission properties. *Journal of Materials Chemistry C*, **2020**, 8, 5137-5142 7.1 10
- 449 SnO<sub>2</sub>@N-Doped Carbon Hollow Nanoclusters for Advanced Lithium-Ion Battery Anodes. *European Journal of Inorganic Chemistry*, **2016**, 2016, 812-817 2.3 10
- 448 Theoretical Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Polyfluoroarylcyanation of Alkynes: Origin of Selectivity for C≡N Bond Activation. *Organometallics*, **2018**, 37, 2594-2601 3.8 10
- 447 Nonfullerene Acceptors for Organic Photovoltaics: From Conformation Effect to Power Conversion Efficiencies Prediction. *Solar Rrl*, **2019**, 3, 1900258 7.1 10
- 446 Mechanism and kinetic study of 3-fluoropropene with hydroxyl radical reaction. *Journal of Molecular Graphics and Modelling*, **2014**, 48, 18-27 2.8 10
- 445 A novel organic-inorganic hybrid constructed from the Nyman-type dititanoniobate [Ti<sub>2</sub>Nb<sub>8</sub>O<sub>28</sub>](8-) and copper-organic cations. *Dalton Transactions*, **2014**, 43, 9847-50 4.3 10
- 444 The V-shaped polar molecules encapsulated into Cs (10528)-C72: stability and nonlinear optical response. *Dalton Transactions*, **2014**, 43, 9655-60 4.3 10
- 443 Effect of metal ions on the structures of metal-organic frameworks based on mixed ligands. *Inorganic Chemistry Communication*, **2012**, 15, 288-291 3.1 10
- 442 A series of coordination complexes based on unsymmetrical multicarboxylate ligands: syntheses, structures and properties. *CrystEngComm*, **2013**, 15, 6769 3.3 10
- 441 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, 2351-9 3.6 10
- 440 Effect of dehydrogenation/hydrogenation on the linear and nonlinear optical properties of Li@porphyrins. *Journal of Molecular Modeling*, **2012**, 18, 4901-7 2 10
- 439 Mn(III)Salen composite materials based on Keggin heteropolyanions exhibiting photocatalytic and electrocatalytic activities. *Inorganic Chemistry Communication*, **2011**, 14, 1418-1421 3.1 10
- 438 Five supramolecular compounds of water-soluble sulfonylcalix[4]arenetetrasulfonate showing two calixarene conformations. *CrystEngComm*, **2009**, 11, 597-604 3.3 10
- 437 High luminescence, organic-inorganic nanocomposite films with covalently linked 8-hydroxyquinoline anchored to ZnS nanoparticles. *Dyes and Pigments*, **2010**, 85, 66-72 4.6 10
- 436 Time-dependent density functional theory study on electronic and spectroscopic properties for Ph<sub>2</sub>Bq and its complexes. *Theoretical Chemistry Accounts*, **2006**, 117, 1-5 1.9 10
- 435 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, 245106-9 3.9 10
- 434 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 2.6 10

433	A novel cadmium(II) coordination polymer with biphenyl-3,3',4,4'-tetracarboxylic acid and 4,4'-bipyridine. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2005</b> , 61, m469-71		10
432	Theoretical studies on the one- and two-photon absorption of symmetrical stilbene derivatives. <i>Computational and Theoretical Chemistry</i> , <b>2000</b> , 531, 169-174		10
431	A theoretical investigation on promising acceptor groups for POM-based dyes: from electronic structure to photovoltaic conversion efficiency. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 219-227	7.1	10
430	Single Metal-Organic Cage Decorated with an Ir(III) Complex for CO <sub>2</sub> Photoreduction. <i>ACS Catalysis</i> , <b>2021</b> , 11, 7241-7248	13.1	10
429	Mechanistic insight into electroreduction of carbon dioxide on FeN (x = 0-4) embedded graphene. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 23638-23644	3.6	10
428	An unprecedented {CuTe} core incorporated in a 36-tungsto-4-silicate polyoxometalate with visible light-driven catalytic hydrogen evolution activity. <i>Dalton Transactions</i> , <b>2018</b> , 47, 16403-16407	4.3	10
427	The regulation of hydroboration of olefins by oriented external electric field. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 18402-18408	3.6	10
426	A noncovalently connected metal-organic framework assembled from a Ni(III)-supported polyoxometalate-imidazolate hybrid. <i>CrystEngComm</i> , <b>2017</b> , 19, 1721-1724	3.3	9
425	Conductive metal adatoms adsorbed on graphene nanoribbons: a first-principles study of electronic structures, magnetization and transport properties. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 4053-4062	7.1	9
424	A triazine-functionalized nanoporous metal-organic framework for the selective adsorption and chromatographic separation of transition metal ions and cationic dyes and white-light emission by Ln <sup>3+</sup> ion encapsulation. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 8861-8867	7.1	9
423	Terminal Modulation in Search of a Balance between Hole Transport and Electron Transfer at the Interface for BODIPY-Based Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 6407-6415	3.8	9
422	Ammonia borane in an external electric field: structure, charge transfer, and chemical bonding. <i>RSC Advances</i> , <b>2015</b> , 5, 65991-65997	3.7	9
421	Charge transfer and first hyperpolarizability: cage-like radicals C59X and lithium encapsulated Li@C59X (X=B, N). <i>Journal of Molecular Modeling</i> , <b>2015</b> , 21, 258	2	9
420	The research of employing polyoxometalates as pure-inorganic electron-transfer mediators on dye-sensitized solar cells. <i>Inorganic Chemistry Communication</i> , <b>2014</b> , 46, 89-93	3.1	9
419	Theoretical exploration to the substituting effect on second-order nonlinear optical properties for lacunary Keggin polyoxometalates. <i>Chemical Physics Letters</i> , <b>2013</b> , 557, 123-128	2.5	9
418	An unprecedented 3D architecture based on a Nb/W mixed-addendum polyoxometalate and lanthanide-organic complex: synthesis, crystal structure and properties. <i>New Journal of Chemistry</i> , <b>2017</b> , 41, 10532-10536	3.6	9
417	Synergistic Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Cyanoesterification: Effect of Lewis Acid. <i>Organometallics</i> , <b>2017</b> , 36, 4713-4720	3.8	9
416	Tuning the inter-molecular charge transfer, second-order nonlinear optical and absorption spectra properties of a dimer under an external electric field. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 31958-31964	3.6	9

- 415 Theoretical design and study on hexamolybdate-based organic-inorganic hybrids with double D- $\pi$ A chains for high performance p-type dye-sensitized solar cells (DSSCs). *Dyes and Pigments*, **2017**, 137, 372-377 4.6 9
- 414 Enhanced quantum efficiency of cationic iridium(III) complexes with carbazole moiety as a steric hindrance unit. *Journal of Molecular Structure*, **2012**, 1026, 59-64 3.4 9
- 413 Theoretical investigation on two-dimensional molecule-based second-order nonlinear optical materials of the disubstituted o-carborane derivatives. *Computational and Theoretical Chemistry*, **2012**, 992, 142-149 2 9
- 412 Carbonyl amine/Schiff base ligands in manganese complexes: theoretical study on the mechanism, capability of NO release. *Inorganic Chemistry*, **2012**, 51, 3972-80 5.1 9
- 411 Potential of bifluorenylidene derivatives as nonfullerene small-molecule acceptor for heterojunction organic photovoltaics: a density functional theory study. *Theoretical Chemistry Accounts*, **2012**, 131, 1 1.9 9
- 410 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 9
- 409 Synthesis, structure and properties of one 2-D Ag(I) complex based on trinuclear silver(I) cluster and arene-linked bis(pyrazoly)methane ligand. *Inorganic Chemistry Communication*, **2011**, 14, 347-350 3.1 9
- 408 A DFT study on the electronic and redox properties of  $[X_8V_{14}O_{50}]_n$  [X = SiIV, GeIV, PV, and AsV]. *Canadian Journal of Chemistry*, **2010**, 88, 434-442 0.9 9
- 407 Incorporation of Znq2 complexes into mesoporous silica and their transparent polymer luminescent nanocomposites. *Journal of Solid State Chemistry*, **2009**, 182, 1430-1437 3.3 9
- 406 Two novel supramolecular isomers based on 2,2'-biimidazole derivative and zinc ions: Syntheses, structures and luminescent properties. *Inorganic Chemistry Communication*, **2009**, 12, 169-172 3.1 9
- 405 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 0.5 9
- 404 Near-infrared-emitting AIE multinuclear cationic Ir(III) complex-assembled nanoparticles for photodynamic therapy. *Dalton Transactions*, **2020**, 49, 15332-15338 4.3 9
- 403 Copper Dimer Anchored in g-CN Monolayer as an Efficient Electrocatalyst for CO<sub>2</sub> Reduction Reaction: A Computational Study. *Advanced Theory and Simulations*, **2020**, 3, 2000218 3.5 9
- 402 Equi-size nesting of Platonic and Archimedean metal-organic polyhedra into a twin capsid. *Nature Communications*, **2020**, 11, 4103 17.4 9
- 401 Rh@C<sub>8</sub>N<sub>8</sub> monolayer as a promising single-atom-catalyst for overall water splitting. *Applied Surface Science*, **2021**, 549, 149320 6.7 9
- 400 Controllable synthesis of isorecticular pillared-layer MOFs based on N-rich triangular prism building units: gas adsorption and luminescent properties. *New Journal of Chemistry*, **2018**, 42, 20056-20060 3.6 9
- 399 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 3.4 8
- 398 Boron/nitrogen substituted the staggered hetero-dimers: Fascinating intermolecular charge-transfer and large NLO responses. *Dyes and Pigments*, **2017**, 145, 21-28 4.6 8

397	A probe into underlying factors affecting ultrafast charge transfer at Donor/IDIC interface of all-small-molecule nonfullerene organic solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , <b>2019</b> , 375, 1-8	4.7	8
396	Rational synthesis, structural characterization and theoretical exploration on third-order nonlinear optical properties of isolated Ag <sub>n</sub> (n = 5, 8, 12) alkynyl clusters. <i>Dyes and Pigments</i> , <b>2015</b> , 113, 299-306	4.6	8
395	Structural, Optical and Mechanical Properties and Cracking Factors of Large-Sized KBr:Ce <sup>3+</sup> Single Crystal. <i>Journal of Electronic Materials</i> , <b>2020</b> , 49, 4785-4793	1.9	8
394	A ruthenium/polyoxometalate for efficient CO photoreduction under visible light in diluted CO. <i>Nanotechnology</i> , <b>2020</b> , 31, 255402	3.4	8
393	Reduced graphene oxide/TiO <sub>2</sub> (B) nanocomposite-modified separator as an efficient inhibitor of polysulfide shuttling in Li-S batteries.. <i>RSC Advances</i> , <b>2020</b> , 10, 4538-4544	3.7	8
392	Fabrication of a Flowerlike Ag Microsphere Film with Applications in Catalysis and as a SERS Substrate. <i>European Journal of Inorganic Chemistry</i> , <b>2018</b> , 2018, 2835-2840	2.3	8
391	The transport properties of silicon and carbon nanotubes at the atomic scale: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 23643-50	3.6	8
390	Structure and Frontier Molecular Orbital (FMO) energies of Keggin-type polyoxometalate [PW <sub>12</sub> O <sub>40</sub> ] <sup>3-</sup> systematical study with different functionals of density functional theory. <i>Computational and Theoretical Chemistry</i> , <b>2016</b> , 1089, 28-34	2	8
389	Coordination and supramolecular assembly of {Cd <sub>2</sub> Ge <sub>8</sub> V <sub>12</sub> O <sub>48</sub> } building block and cucurbit[6] to form rotaxane-shaped hybrids. <i>Dalton Transactions</i> , <b>2016</b> , 45, 4989-92	4.3	8
388	Orthogonal reactivity of Ni(I)/Pd(0) dual catalysts for Ullmann C-C cross-coupling: theoretical insight. <i>Chemical Communications</i> , <b>2018</b> , 54, 7959-7962	5.8	8
387	Molecular Engineering of Phenylbenzimidazole-Based Orange Ir(III) Phosphors toward High-Performance White OLEDs. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 6029-6037	5.1	8
386	Stimulating intra- and intermolecular charge transfer and nonlinear optical response for biphenalenyl biradicaloid dimer under an external electric field. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 18699-18706	3.6	8
385	Theoretical study on the transport properties of oligothiophene-diketopyrrolopyrrole derivatives: quinoidal versus aromatic. <i>Theoretical Chemistry Accounts</i> , <b>2014</b> , 133, 1	1.9	8
384	Influence of spiral framework on nonlinear optical materials. <i>ChemPhysChem</i> , <b>2014</b> , 15, 929-34	3.2	8
383	Synthesis, structure, and photoluminescent property of a trinuclear CdII complex based on semi-rigid bis(imidazole-4,5-dicarboxylate) ligand. <i>Inorganic Chemistry Communication</i> , <b>2014</b> , 42, 15-19	3.1	8
382	The influence of molecular solid packings on the photoluminescence and carrier transport properties for two bow-shaped thiophene compounds: a theoretical study. <i>Theoretical Chemistry Accounts</i> , <b>2013</b> , 132, 1	1.9	8
381	The symmetric and asymmetric thiophene-fused benzocarborane: structures and first hyperpolarizabilities. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 3741-7	2	8
380	A theoretical exploration of the effect of fluorine and cyano substitutions in diketopyrrolopyrrole-based polymer donor for organic solar cells. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 77, 9-16	2.8	8

- 379 Density Functional Theory Investigation on the Second-Order Nonlinear Optical Properties of Chlorobenzyl-o-Carborane Derivatives. *Chinese Journal of Chemistry*, **2012**, 30, 2349-2355 4.9 8
- 378 Probing the chemical functionalization of single-walled carbon nanotubes with multiple carbon ad-dimer defects. *ChemPhysChem*, **2012**, 13, 1232-9 3.2 8
- 377 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
- 376 Theoretical studies on phosphoraniminato derivatives of Keggin-type polyoxometalates [PW<sub>11</sub>O<sub>39</sub>{MVNPPH<sub>3</sub>}]<sub>3</sub>[M = Fe, Ru]: Electronic structures and bonding features. *Science China Chemistry*, **2012**, 55, 1910-1915 7.9 8
- 375 Theoretical investigation of second-order nonlinear optical response by linking hexamolybdate with graphene in the donor-acceptor (D-A) framework. *Molecular Simulation*, **2013**, 39, 214-219 2 8
- 374 Three-dimensional porous metal-organic replica of natural mineral  $\beta$ -Al<sub>2</sub>O<sub>3</sub> based on hexadentate triazine derivative. *Inorganic Chemistry Communication*, **2011**, 14, 893-896 3.1 8
- 373 A novel 3-connected [3 + 3] topological net showing both rotaxane- and catenane-like motifs. *CrystEngComm*, **2011**, 13, 4945 3.3 8
- 372 Comparative study of the electrostatic potential of perfect and defective single-walled carbon nanotubes. *Computational and Theoretical Chemistry*, **2011**, 966, 1-8 2 8
- 371 Quantum chemistry studies on the Ru-M interactions and the <sup>31</sup>P NMR in [Ru(CO)<sub>3</sub>(Ph<sub>2</sub>Ppy)<sub>2</sub>(MCl<sub>2</sub>)] (M=Zn, Cd, Hg). *Journal of Organometallic Chemistry*, **2006**, 691, 1927-1933 2.3 8
- 370 Synthesis, Crystal Structure and Spectroscopic Studies of a Supramolecular Compound [Cu(IDA)(phen)(H<sub>2</sub>O)]<sub>4</sub>·4H<sub>2</sub>O Built from  $\pi$ -Interactions and Hydrogen Bonds. *Transition Metal Chemistry*, **2004**, 29, 471-476 2.1 8
- 369 Syntheses and Structure of a Novel Layered Lanthanide-Zinc Coordination Polymer: [LaZn(HIDA)(IDA)<sub>2</sub>·0.5H<sub>2</sub>O]<sub>n</sub>. *Chemistry Letters*, **2004**, 33, 446-447 1.7 8
- 368 Electronic property and molecule design for luminescent metal complexes of tris(8-hydroxyquinoline) gallium. *Science in China Series B: Chemistry*, **2000**, 43, 657-669 8
- 367 Effective Hamiltonians of polymethineimine, polyazine and polyazoethene: A density matrix variation approach. *Journal of Chemical Physics*, **1998**, 109, 2565-2571 3.9 8
- 366 Synergetic effect of H adsorption and ethylene functional groups of covalent organic frameworks on the CO photoreduction in aqueous solution. *Chemical Communications*, **2020**, 56, 7261-7264 5.8 8
- 365 Cationic dinuclear Ir(III) complexes based on acylhydrazine ligands: Reversible piezochromic luminescence and AIE behaviours. *Dyes and Pigments*, **2020**, 172, 107855 4.6 8
- 364 Tricopper-polyoxometalate catalysts for water oxidation: Redox-inertness of copper center. *Journal of Catalysis*, **2020**, 381, 402-407 7.3 8
- 363 Preparation and electrochemical hydrogen storage properties of Co<sub>9</sub>S<sub>8</sub> alloy coated with cobalt/graphene composite. *International Journal of Energy Research*, **2020**, 44, 11742-11755 4.5 8
- 362 Optical and mechanical properties of NaCl: Ce<sup>3+</sup> crystal grown by the Czochralski method. *Journal of Materials Science: Materials in Electronics*, **2020**, 31, 13070-13077 2.1 8



361	A photo-activated process cascaded electrocatalysis for the highly efficient CO <sub>2</sub> reduction over a core-shell ZIF-8@Co/C. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 16616-16623	13	8
360	2D luminescent metal-organic framework: efficient and highly selective detection of 2,4,6-trinitrophenol at the ppb level. <i>CrystEngComm</i> , <b>2021</b> , 23, 929-934	3-3	8
359	Be-triple bond in BeXY clusters (X = Li, Na and Y = Li, Na, K) and a perfect classical Be-triple bond presented in BeNaK. <i>Dalton Transactions</i> , <b>2019</b> , 48, 14590-14594	4-3	7
358	A remarkable phosphorescent sensor for acid-base vapours based on an AIPE-active Ir(III) complex. <i>Dalton Transactions</i> , <b>2019</b> , 48, 1955-1959	4-3	7
357	Engineering of Yin Yang-like nanocarriers for varisized guest delivery and synergistic eradication of patient-derived hepatocellular carcinoma. <i>Nanoscale Horizons</i> , <b>2019</b> , 4, 1046-1055	10.8	7
356	Superalkali atoms bonding to the phenalenyl radical: structures, intermolecular interaction and nonlinear optical properties. <i>Journal of Molecular Modeling</i> , <b>2015</b> , 21, 209	2	7
355	Theoretical investigation of armchair silicene nanoribbons with application in stretchable electronics. <i>Journal of Materials Chemistry C</i> , <b>2015</b> , 3, 10085-10090	7.1	7
354	Can we utilize the higher Frenkel exciton state in biazulene diimides-based non-fullerene acceptors to promote charge separation at the donor/acceptor interface?. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 9767-9774	3.6	7
353	Redox-switchable structures and NLO property: Li <sub>2</sub> doped into the cavity of pyridine helix. <i>Organic Electronics</i> , <b>2018</b> , 57, 68-73	3.5	7
352	Theoretical Insight into the Performance of Mn-Monosubstituted Heteropolytungstates as Water Oxidation Catalysts. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 15751-15757	5.1	7
351	Facile assembly of 1D multinuclear Ag <sub>n</sub> (n = 11, 11, 12) alkynyl chains with CF <sub>3</sub> COO <sup>-</sup> /CH <sub>3</sub> COO <sup>-</sup> as the auxiliary ligand. <i>RSC Advances</i> , <b>2014</b> , 4, 60451-60459	3.7	7
350	Red- and white-emitting organic light-emitting diodes based on trimetallic dendritic europium (III) complex: Eu <sub>3</sub> (DBM) <sub>9</sub> (TMMB). <i>Solid-State Electronics</i> , <b>2012</b> , 69, 67-71	1.7	7
349	Synthesis and property investigation of two hexa-cobalt cluster based porous coordination polymers. <i>CrystEngComm</i> , <b>2013</b> , 15, 7402	3-3	7
348	Design and construction of porous metal-organic frameworks based on flexible BPH pillars. <i>Journal of Solid State Chemistry</i> , <b>2013</b> , 198, 143-148	3-3	7
347	Superatoms-Induced Effects of Phenalenyl Dimer on NICS and NLO Properties: Not Always Enhancement. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 20419-20425	3.8	7
346	Two nanoscale Nb containing polyoxometalates based on {PWNbO} clusters and chromium cations. <i>Dalton Transactions</i> , <b>2017</b> , 46, 13345-13348	4-3	7
345	Solvothermal synthesis and structural characterization of a Cd-triazole-benzenedicarboxylate framework. <i>Inorganic Chemistry Communication</i> , <b>2014</b> , 40, 8-10	3.1	7
344	Building blocks and formation thermodynamics of $\beta$ -Keggin-type [PW <sub>12</sub> O <sub>40</sub> ] <sup>3-</sup> anion. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 999, 66-73	2	7

- 343 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 3.3 7
- 342 Quantum chemical investigation on the structure and first hyperpolarizability for N-substituted [n]cyclacene. *Journal of Physical Organic Chemistry*, **2012**, 25, 176-180 2.1 7
- 341 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 2.3 7
- 340 A new (3,4,7)-connected topology framework based on [Cd<sub>2</sub>(CO<sub>2</sub>)<sub>3</sub>O<sub>4</sub>N<sub>2</sub>] second building unit. *Inorganic Chemistry Communication*, **2009**, 12, 1024-1026 3.1 7
- 339 Isophorone-based analogues with A-B-A structure for red organic light emitting devices. *Synthetic Metals*, **2009**, 159, 401-405 3.6 7
- 338 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 3.3 7
- 337 Length-Dependent Direction-Tunable Charge-Transfer Behavior of Second-Order Optical Nonlinearity in Keggin-Type Organosilicone Derivative [PW<sub>11</sub>O<sub>39</sub>(RSi<sub>2</sub>O)<sub>3</sub>]<sup>n-</sup> TDDFT Study. *Journal of Cluster Science*, **2010**, 21, 69-80 3 7
- 336 THEORETICAL STUDY ON ENDOHEDRAL COMPLEXES C<sub>2</sub>H<sub>2</sub>⊂C<sub>60</sub>, C<sub>2</sub>H<sub>4</sub>⊂C<sub>60</sub>, AND C<sub>2</sub>H<sub>6</sub>⊂C<sub>60</sub>. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 1-11 1.8 7
- 335 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 3.9 7
- 334 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 7
- 333 Controlled cutting carbon nanotube with polyoxometalates assisted renewable method. *Materials Letters*, **2006**, 60, 2266-2269 3.3 7
- 332 Theoretical studies on one- and two-photon absorption properties of rubrene and its derivatives. *Synthetic Metals*, **2006**, 156, 1218-1224 3.6 7
- 331 Poly[bis(4,4'-bipyridine)(3,4,4'-dicarboxybiphenyl-3,3'-dicarboxylato)cobalt(II)]. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, m2477-m2479 7
- 330 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 6.8 7
- 329 Two-electron/24-center (2e/24c) bonding in novel diradical dimers. *Physical Chemistry Chemical Physics*, **2016**, 18, 29041-29044 3.6 7
- 328 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 4.7 7
- 327 Phosphorescent iridium(III) complex based photoluminescence sensor for sensitive and selective detection of picric acid. *Dyes and Pigments*, **2020**, 172, 107799 4.6 7
- 326 Hierarchical and Highly Stable Conductive Network Cathode for Ultraflexible LiB Batteries. *ACS Applied Energy Materials*, **2018**, 1, 2689-2697 6.1 7

325	Theoretical studies on tricarbonyl metal derivatives of Lindqvist-type polyoxometalate complexes: electronic structures and nonlinear optical properties. <i>Inorganic Chemistry Frontiers</i> , <b>2015</b> , 2, 544-549	6.8	6
324	A novel [4 + 3] interpenetrated net containing 7-fold interlocking pseudo-helical chains and exceptional catenane-like motifs. <i>Dalton Transactions</i> , <b>2015</b> , 44, 2844-51	4.3	6
323	Ferroelectric Metal-Organic Framework as a Host Material for Sulfur to Alleviate the Shuttle Effect of Lithium-Sulfur Battery. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 13779-13782	4.8	6
322	Theoretical mechanistic study of metallaphotoredox catalysis: C-N cross-coupling via Ni(II)-mediated E-bond metathesis. <i>Organic Chemistry Frontiers</i> , <b>2020</b> , 7, 2168-2178	5.2	6
321	Tuning Second-Order Nonlinear Optical Properties of Cross-Linked Carbon Nanotube via External Electric Field. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 3778-3783	3.8	6
320	Low efficiency roll-off and high performance OLEDs employing alkyl group modified iridium(III) complexes as emitters. <i>RSC Advances</i> , <b>2016</b> , 6, 111556-111563	3.7	6
319	Supramolecular hydrogen-bonded organic networks through acid-base pairs as efficient proton-conducting electrolytes. <i>CrystEngComm</i> , <b>2019</b> , 21, 4996-5001	3.3	6
318	Isomeric thiophene-fused benzocarborane molecules--different lithium doping effect on the nonlinear optical property. <i>Dalton Transactions</i> , <b>2014</b> , 43, 2656-60	4.3	6
317	TD-DFT studies on electronic and spectral properties of platinum(II) complexes with phenol and pyridine groups. <i>Chemical Research in Chinese Universities</i> , <b>2013</b> , 29, 361-365	2.2	6
316	Photosensitive polyoxometalate-induced formation of thermotropic liquid crystal nanomaterial and its photovoltaic effect. <i>RSC Advances</i> , <b>2015</b> , 5, 8194-8198	3.7	6
315	Structure-dependent optical properties of single-walled silicon nanotubes. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 4695-702	3.6	6
314	Influence of the central atom on the electronic properties of Lindqvist polyoxometalates. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 988, 1-5	2	6
313	DFT study of ionic peapod structures from single-walled carbon nanotubes and Lindqvist tungstates. <i>Dalton Transactions</i> , <b>2012</b> , 41, 2798-803	4.3	6
312	One-pot synthesized polyurethane-based nanocomposites filled by original rectorite with enhanced strength and elongation. <i>Journal Wuhan University of Technology, Materials Science Edition</i> , <b>2011</b> , 26, 483-490	1	6
311	The comparative investigation on redox property and second-order nonlinear response of Keggin-type $\beta$ -[PM12O39NPh]3[M = W and Mo) and Mo6NPh. <i>Science Bulletin</i> , <b>2009</b> , 54, 203-211	10.6	6
310	Two new octamolybdate-based metal-organic polymers: Structures, semiconducting and photoluminescent properties. <i>Journal of Molecular Structure</i> , <b>2009</b> , 935, 69-74	3.4	6
309	Syntheses and characterizations of five coordination polymers constructed by 3,5-bis(pyridin-3-ylmethoxy)benzoic acid ligand. <i>Polyhedron</i> , <b>2009</b> , 28, 3155-3161	2.7	6
308	Photophysical and charge-transport properties of hole-blocking material-TAZ: A theoretical study. <i>Synthetic Metals</i> , <b>2009</b> , 159, 1767-1771	3.6	6

- 307 A theoretical study of ambipolar organic transport material: 1,4-Bis(pentafluorobenzyl)[60]-fullerene. *Chemical Physics Letters*, **2011**, 506, 255-259 2.5 6
- 306 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 5.3 6
- 305 A peanut-like Keggin-type POM-incorporated metal-organic framework. *Inorganic Chemistry Communication*, **2010**, 13, 1473-1475 3.1 6
- 304 Density functional study of magnetic exchange of dinuclear manganese complexes with the heteropolymolyanion:  $[Mn^{II} 2(Xn+Mo_9O_{33})_2]_2(n=0)$  (X = PV, AsV, SeVI). *Science in China Series B: Chemistry*, **2008**, 51, 1174-1181 6
- 303 Stabilities, electronic properties of exohedral fluorine and trifluoromethyl derivatives for Td C<sub>28</sub> fullerene C<sub>28</sub>F<sub>4n</sub>(CF<sub>3</sub>)<sub>n</sub> (n = 0,1,2,3,4). *International Journal of Quantum Chemistry*, **2008**, 108, 1391-1399<sup>2.1</sup> 6
- 302 Cooperative enhancement of two-photon absorption cross sections in three-branched oligofluorene with boron center. *Computational and Theoretical Chemistry*, **2008**, 855, 69-76 6
- 301 Soluble dendrimers europium(III) βdiketonate complex for organic memory devices. *Thin Solid Films*, **2008**, 516, 3123-3127 2.2 6
- 300 {1,4-Bis[2-(2-pyridyl)imidazol-1-yl]butane}bis[dichlorocopper(II)]. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, m2586-m2587 6
- 299 cis-Dichlorobis[2-(2-pyridyl)-1H-imidazole-β3]zinc(II) hemihydrate. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, m3479-m3480 6
- 298 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 2.1 6
- 297 Face-Directed Assembly of Molecular Cubes: In Situ Substitution of a Predetermined Concave Cluster. *Angewandte Chemie - International Edition*, **2020**, 59, 22034-22038 16.4 6
- 296 Self-assembly and Li-ion storage performance of three new Nb/W mixed-addendum polyoxometalates based on the {SiNb<sub>3</sub>W<sub>9</sub>O<sub>40</sub>} clusters and transition-metal cations. *CrystEngComm*, **2019**, 21, 1862-1866 3.3 6
- 295 A luminescent metal-organic framework with tetragonal nanochannels as an efficient chemosensor for nitroaromatic explosives detection. *CrystEngComm*, **2021**, 23, 3901-3906 3.3 6
- 294 A tetraphenylethylene-based covalent organic framework for waste gas adsorption and highly selective detection of Fe<sup>3+</sup>. *CrystEngComm*, **2021**, 23, 5569-5574 3.3 6
- 293 Bimetallic Metal-Organic Framework-Derived Graphitic Carbon-Coated Small Co/VN Nanoparticles as Advanced Trifunctional Electrocatalysts. *ACS Applied Materials & Interfaces*, **2021**, 13, 2462-2471 9.5 6
- 292 Dimethyltin-functionalized cyclic selenotungstates based on {SeW} units. *Dalton Transactions*, **2018**, 47, 1393-1397 4.3 6
- 291 Steam-assisted assemblies of {Ni<sub>6</sub>PW<sub>9</sub>}-based inorganic-organic hybrid chains: synthesis, crystal structures and properties. *CrystEngComm*, **2018**, 20, 7507-7512 3.3 6
- 290 Metallic subnanometer porous silicon: A theoretical prediction. *Physical Review B*, **2021**, 103, 3.3 6

289	Syntheses and magnetic properties of high-dimensional cucurbit[6]uril-based metal-organic rotaxane frameworks. <i>Dalton Transactions</i> , <b>2019</b> , 48, 9939-9943	4.3	5
288	Quantum Chemical Insight into the LiF Interlayer Effects in Organic Electronics: Reactions between Al Atom and LiF Clusters. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 2950-8	6.4	5
287	The Structure and Liquid Flow Effect of Melt during NaCl Crystal Growth. <i>Crystal Research and Technology</i> , <b>2020</b> , 55, 1900229	1.3	5
286	Heteroatom-doped C <sub>3</sub> N as a promising metal-free catalyst for a high-efficiency carbon dioxide reduction reaction. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 11824-11828	3.6	5
285	Self-assembly and lithium storage performance of a nanoscale polyoxometalate based on the {MnTa} cluster. <i>Chemical Communications</i> , <b>2020</b> , 56, 2403-2406	5.8	5
284	Promoting visible-light-driven hydrogen production of a zirconium-based metal-organic polyhedron decorated by platinum nanoparticles with different spatial locations. <i>Catalysis Communications</i> , <b>2020</b> , 137, 105930	3.2	5
283	Theoretical insights into the catalytic mechanism for the oxygen reduction reaction on M(hexaiminotriphenylene) (M = Ni, Cu). <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 1821-1828	3.6	5
282	Towards an efficient blue emission cationic Ir(III) complex with azole-type ancillary ligands: a joint theoretical and experimental study. <i>New Journal of Chemistry</i> , <b>2016</b> , 40, 4635-4642	3.6	5
281	An ultra-stable porous coordination polymer for water-mediated proton conduction. <i>Inorganic Chemistry Communication</i> , <b>2018</b> , 96, 153-158	3.1	5
280	Electron transport via phenyl-perfluorophenyl interaction in crystals of fluorine-substituted dibenzalacetones. <i>RSC Advances</i> , <b>2014</b> , 4, 50188-50194	3.7	5
279	Hydrothermal synthesis, crystal structure and properties of a 3D inorganic-organic hybrid based on Keggin-type polyanion and silver-pyrazine circles. <i>Inorganic Chemistry Communication</i> , <b>2014</b> , 47, 48-51	3.1	5
278	Theoretical characterization and design of highly efficient iridium (III) complexes bearing guanidinate ancillary ligand. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 51, 149-57	2.8	5
277	1,4-Azaborine as a controller of triplet energy, exciton distribution, and aromaticity in [6]cycloparaphenylenes. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 9088-9097	7.1	5
276	Redox and acidic properties of chalcogenido-substituted mixed-metal polyoxoanions: a DFT study of [PW <sub>11</sub> O <sub>39</sub> ME] <sub>4</sub> (M = Nb, Ta; E = O, S, Se). <i>Inorganic Chemistry Frontiers</i> , <b>2015</b> , 2, 246-253	6.8	5
275	Theoretical study on the gas phase reaction of allyl chloride with hydroxyl radical. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 084309	3.9	5
274	Hydrothermal synthesis and structural characterization of a new 2D inorganic-organic hybrid compound based on {Ni <sub>6</sub> PW <sub>9</sub> } <sub>2</sub> subunit. <i>Inorganic Chemistry Communication</i> , <b>2012</b> , 23, 21-24	3.1	5
273	First principle investigation of transport properties of Lindqvist derivatives based molecular junction. <i>Journal of Molecular Graphics and Modelling</i> , <b>2012</b> , 38, 220-5	2.8	5
272	The effect of multiple weak interactions on the charge transport ability in polymorphs. <i>Synthetic Metals</i> , <b>2011</b> , 161, 1073-1078	3.6	5

271	DFT study on second-order nonlinear optical properties of Pt(II) complexes with different chromophores. <i>Science in China Series B: Chemistry</i> , <b>2009</b> , 52, 144-152		5
270	DFT STUDIES ON ELECTRONIC STRUCTURES AND THIRD-ORDER NONLINEAR OPTICAL PROPERTIES OF A SERIES OF PtPt BOND-CONTAINING METAL COMPLEXES. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2012</b> , 11, 403-419	1.8	5
269	Two new extended structures built from condensed Keggin-type polyoxotungstates and copper(II)-organic units. <i>Solid State Sciences</i> , <b>2010</b> , 12, 128-133	3.4	5
268	Generalized fabrication of surfactant-stabilized anisotropic metal nanoparticles to amino-functionalized surfaces: application to surface-enhanced Raman spectroscopy. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2008</b> , 8, 5887-95	1.3	5
267	Theoretical study on the structures, isomerization and stability of SiC <sub>3</sub> H isomers. <i>Theoretical Chemistry Accounts</i> , <b>2008</b> , 119, 501-509	1.9	5
266	Theoretical Studies on Electronic Spectra and Second-order Nonlinear Optical Properties of Glucosyl Substituted Barbituric Acid Derivatives. <i>Chinese Journal of Chemistry</i> , <b>2006</b> , 24, 119-123	4.9	5
265	Theoretical studies of ground and excited electronic states of OLED material bis(2-methyl-8-quinolinolato)gallium(iii) chlorine. <i>Computational and Theoretical Chemistry</i> , <b>2005</b> , 722, 161-168		5
264	Two Ni/Co-substituted sandwich-type germanomolybdates based on an unprecedented trivacant polyanion [H-GeMoO]. <i>Dalton Transactions</i> , <b>2020</b> , 49, 977-982	4.3	5
263	A hydrazone-based covalent organic framework/iridium (III) complex for photochemical CO <sub>2</sub> reduction with enhanced efficiency and durability. <i>Journal of Catalysis</i> , <b>2020</b> , 392, 49-55	7.3	5
262	Robust Electrodes for Flexible Energy Storage Devices Based on Bimetallic Encapsulated Core-Multishell Structures. <i>Advanced Science</i> , <b>2021</b> , 8, e2100911	13.6	5
261	From Octahedral to Icosahedral MetalOrganic Polyhedra Assembled from Two Types of Polyoxovanadate Clusters. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 4697-4701	3.6	5
260	Synthesis of novel tetrazol-pyridine based cationic Ir(III) complexes with efficient AIE characteristic and significant mechanochromic luminescence behavior. <i>Dyes and Pigments</i> , <b>2021</b> , 184, 108817	4.6	5
259	Precise Molecular-Level Modification of Nafion with Bismuth Oxide Clusters for High-performance Proton-Exchange Membranes. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 6141-6150	3.6	5
258	Elongated heterometal double-sites promote nitrogen reduction on two-dimensional MM <sub>2</sub> B <sub>7</sub> monolayers. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 10855-10868	13	5
257	A luminescent metalOrganic framework with mixed-linker strategy for white-light-emitting by iridium-complex encapsulation. <i>Inorganic Chemistry Communication</i> , <b>2021</b> , 123, 108359	3.1	5
256	Synthesis, crystal structure and iodine capture of Zr-based metal-organic polyhedron. <i>Inorganica Chimica Acta</i> , <b>2021</b> , 516, 120174	2.7	5
255	A theoretical design of performant chlorinated benzothiadiazole-based polymers as donor for organic photovoltaic devices. <i>Organic Electronics</i> , <b>2018</b> , 61, 46-55	3.5	5
254	Metal-organic frameworks based on multi-carboxylate ligands with threefold symmetries and luminescence properties. <i>Inorganic Chemistry Communication</i> , <b>2017</b> , 79, 69-73	3.1	4

253	Organometallic Ir(III) Phosphors Decorated by Carbazole/Diphenylphosphoryl Units for Efficient Solution-Processable OLEDs with Low Efficiency Roll-Offs. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 13807-13814	5.1	4
252	Self-assembly and photocatalytic properties of three nanosized polyoxometalates based on the {SiNb <sub>3</sub> W <sub>9</sub> O <sub>40</sub> } cluster and transition-metal cations. <i>Journal of Solid State Chemistry</i> , <b>2019</b> , 277, 618-623	3.3	4
251	How do transition-metal-substituted POMs modify the photoanode of dye-sensitized solar cells? A DFT study. <i>Inorganic Chemistry Frontiers</i> , <b>2019</b> , 6, 969-974	6.8	4
250	Exploration of charge transfer and absorption spectra of porphyrin-polyoxometalate hybrids to search for high performance sensitizers. <i>RSC Advances</i> , <b>2015</b> , 5, 93659-93665	3.7	4
249	Luminescent metal-organic frameworks encapsulating polycyclic aromatic hydrocarbons for energy transfer. <i>Dalton Transactions</i> , <b>2020</b> , 49, 5087-5091	4.3	4
248	N-(O-methoxyphenyl)aza-15-crown-5-ether derivatives: Highly efficient and wide range nonlinear optical response based cation recognition. <i>Journal of Molecular Liquids</i> , <b>2020</b> , 301, 112492	6	4
247	Theoretical study on the optical response behavior to hydrogen chloride gas of a series of Schiff-base-based star-shaped structures. <i>Journal of Molecular Modeling</i> , <b>2018</b> , 24, 58	2	4
246	Two polyoxovanadate-based metal-organic polyhedra with undiscovered "near-miss Johnson solid" geometry. <i>Chemical Communications</i> , <b>2019</b> , 55, 10701-10704	5.8	4
245	Spectroscopic behavior, FMO, NLO and substitution effect of 2-(1H-Benzo[d]imidazole-2-ylthio)-N-o-substituted-acetamides: Experimental and theoretical approach. <i>Dyes and Pigments</i> , <b>2019</b> , 171, 107742	4.6	4
244	Metal-oxygen clusters as peroxidase mimics for their multifarious applications in colorimetric sensors. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 13430-13436	3.6	4
243	A comparative DFT study on the mechanism of olefin epoxidation catalyzed by substituted binuclear peroxotungstates ([SeO <sub>4</sub> WO(O <sub>2</sub> ) <sub>2</sub> MO(O <sub>2</sub> ) <sub>2</sub> ] <sup>n-</sup> [M = TiIV, VV, TaV, MoVI, WVI, TcVII, and ReVII]). <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 458-462	2.1	4
242	A DFT study on NLO response of push-pull hybrid porphyrin-polyoxometalate complexes. <i>Russian Journal of Physical Chemistry A</i> , <b>2014</b> , 88, 970-977	0.7	4
241	Structures and electro-optical properties of M-Bis [n]Cyclacenes[13-18]: a theoretical study. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2201	2	4
240	The origin of the unusual broad and intense visible absorption of tetrathiafulvalene-annulated zinc porphyrazine: a density functional theory study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2012</b> , 33, 26-34	2.8	4
239	Structural and Bonding Analyses on a Homologous Metal-Metal Bond Guest-Host Series M <sub>2</sub> @C <sub>50</sub> X <sub>10</sub> (M = Zn, Cd, Hg; X = CH, N, B). <i>European Journal of Inorganic Chemistry</i> , <b>2013</b> , 2013, 2220-2230	2.3	4
238	Unveiling photophysical properties of cyclometalated iridium(III) complexes with azadipyrromethene and dipyrromethene ancillary: a theoretical perspective. <i>RSC Advances</i> , <b>2014</b> , 4, 62197-62208	3.7	4
237	The effect of intermolecular interactions on the charge transport properties of thiazole/thiophene-based oligomers with trifluoromethylphenyl. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 51, 79-85	2.8	4
236	A novel luminescent 3D metal-organic framework possessing 3-fold interpenetrating (3,5)-connected net. <i>Inorganic Chemistry Communication</i> , <b>2012</b> , 26, 42-45	3.1	4

235	Toward design of high-performance optoelectronic materials: comparative theoretical studies on the photophysical and charge transport properties of fluorene-based compounds. <i>Theoretical Chemistry Accounts</i> , <b>2012</b> , 131, 1	1.9	4
234	Theoretical studies on electronic and electron blocking properties of iridium complexes with phenylpyrazolato ligands. <i>Synthetic Metals</i> , <b>2010</b> , 160, 1015-1021	3.6	4
233	Synthesis and characterization of two novel coordination polymers based on the rigid 1H-1,2,3-triazole-4,5-dicarboxylic acid ligand. <i>Science China Chemistry</i> , <b>2010</b> , 53, 2177-2182	7.9	4
232	Computational studies on the mechanism and kinetics of Cl reaction with C <sub>2</sub> H <sub>5</sub> I. <i>Journal of Computational Chemistry</i> , <b>2010</b> , 31, 2263-72	3.5	4
231	Secondary ligand-directed assembly of ZnII and CdII coordination architectures: From 1D to 3D compounds based on pyridine carboxylate ligands. <i>Journal of Molecular Structure</i> , <b>2010</b> , 983, 93-98	3.4	4
230	Hydrothermal syntheses of two novel coordination polymers based on tetranuclear metal cluster constructed by 1,3,5-Tris(2H-tetrazol-5-yl)benzene ligand. <i>Inorganic Chemistry Communication</i> , <b>2010</b> , 13, 1203-1206	3.1	4
229	A novel two-dimensional zinc(II) coordination polymer with 6-mercaptopnicotinic acid. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2008</b> , 64, m70-2		4
228	Bis[2-(2-oxidophenyl)-1H-benzimidazole- $\lambda$ N <sub>3</sub> O]zinc(II) dimethylformamide disolvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2006</b> , 62, m2361-m2362		4
227	Theoretical study on geometrical structure and electronic spectrum properties of two stable conformers of boron hydroxyphenylpyridine excimers. <i>Computational and Theoretical Chemistry</i> , <b>2005</b> , 731, 123-126		4
226	Ground-state reduced density matrices, effective Hamiltonians, and optical properties of Schiff bases of retinal. <i>Chemical Physics</i> , <b>1999</b> , 247, 185-192	2.3	4
225	Single-atom catalysts on supported silicomolybdic acid for CO <sub>2</sub> electroreduction: a DFT prediction. <i>Journal of Materials Chemistry A</i> ,	13	4
224	A BPt <sub>4</sub> S <sub>4</sub> cluster: a planar tetracoordinate boron system with three charges all at their global energy minima. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 767-772	3.6	4
223	All Boron Atoms in a ScB <sub>12</sub> Monolayer Contribute to the Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 23221-23229	3.8	4
222	Octamolybdate-based hybrid constructed by flexible bis-triazole ligands: synthesis, photocatalytic and electrochemical properties. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 13524-13528	3.6	4
221	Understanding Mechanochromic Luminescence on Account of Molecular Level Based on Phosphorescent Iridium(III) Complex Isomers. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 3741-3748	5.1	4
220	The second-order nonlinear optical property of hydrazones-based photochromic complexes: A DFT study. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 327, 114882	6	4
219	The Roles of Polyoxometalates in Photocatalytic Reduction of CO <sub>2</sub> . <i>Materials Today Energy</i> , <b>2021</b> , 21, 100760	7	4
218	Photocatalytic C(sp <sup>3</sup> ) $\pi$ /N Cross-Couplings by NaI $\pi$ Ph <sub>3</sub> /CuBr Cooperative Catalysis: Computational Design and Experimental Verification. <i>ACS Catalysis</i> , <b>2021</b> , 11, 6633-6642	13.1	4



217	PL sensor for sensitive and selective detection of 2,4,6-trinitrophenol based on carbazole and tetraphenylsilane polymer. <i>Dyes and Pigments</i> , <b>2021</b> , 191, 109379	4.6	4
216	A substrate-free Mo <sub>2</sub> C-based electrocatalyst by facile glucose-blowing for efficient hydrogen production. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 18970-18974	3.6	4
215	Computational Study of sp <sup>x</sup> (x=1-3)-Hybridized Be-Be Bonds Stabilized by Amidinate Ligands. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 10891-10895	4.8	4
214	Achieving highly electrochemically active maricite NaFePO <sub>4</sub> with ultrafine NaFePO <sub>4</sub> @C subunits for high rate and low temperature sodium-ion batteries. <i>Chemical Engineering Journal</i> , <b>2021</b> , 405, 126689	14.7	4
213	Synthesis, characterization of mechanochromic luminescent-active mono-/dinuclear iridium(III) complexes with near-infrared emission. <i>Journal of Organometallic Chemistry</i> , <b>2021</b> , 931, 121628	2.3	4
212	An EPR-independent therapeutic strategy: Cancer cell-mediated dual-drug delivery depot for diagnostics and prevention of hepatocellular carcinoma metastasis. <i>Biomaterials</i> , <b>2021</b> , 268, 120541	15.6	4
211	Stepwise Construction of Multivariate Metal-Organic Frameworks from a Predesigned Zr <sub>16</sub> Cluster. <i>CCS Chemistry</i> , 287-293	7.2	4
210	Constructing Stable $\pi$ -Dimers: Two Parallel Pancake $\pi$ -Bonds. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 16919-16924	4.8	4
209	Fine-tuning emission color of aggregation-induced emission-active Ir(III) phosphors through simple ligand modification. <i>Dyes and Pigments</i> , <b>2021</b> , 192, 109439	4.6	4
208	Effective CO Migration among Multiadsorbed Sites Achieves the Low-Barrier and High-Selective Conversion to C <sub>2</sub> Products on the NiB Monolayer. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 3845-3855	9.5	4
207	Theoretical studies on lindqvist polyoxometalates [M <sub>6</sub> O <sub>19</sub> ] <sup>n-</sup> (M = Mo, W, n=2; M = V, Nb, Ta, n=8) and derivatives: Electronic structures, stability and bonding. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2017</b> , 16, 1750054	1.8	3
206	Polyoxovanadate-Based Metal-Organic Octahedron Based on 1,4-Naphthalenedicarboxylic Acid. <i>Israel Journal of Chemistry</i> , <b>2019</b> , 59, 306-310	3.4	3
205	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). <i>Small</i> , <b>2015</b> , 11, 3082-3082	11	3
204	A simple synthesis of highly ordered microporous carbon nanospheres for high performance potassium-ion batteries. <i>Journal of Power Sources</i> , <b>2020</b> , 479, 229113	8.9	3
203	Synthesis, characterization, photo-and-electrochemical properties of cationic iridium(III) complexes by using 1,3,4-oxadiazole cyclometallating ligand. <i>Inorganic Chemistry Communication</i> , <b>2020</b> , 118, 107980	3.1	3
202	Structural Extension from 0D to 3D Pillared Heterometallic 3d-4f Polyoxometalate Hybrids. <i>Crystal Growth and Design</i> , <b>2020</b> , 20, 2706-2712	3.5	3
201	Syntheses of cucurbit[6]uril-based metal-organic rotaxane networks by the anion regulation strategy and their proton conduction properties. <i>Dalton Transactions</i> , <b>2020</b> , 49, 1747-1751	4.3	3
200	The interaction between Boron-carbon-nitride heteronanotubes and lithium atoms: Role of composition proportion. <i>Chemical Physics Letters</i> , <b>2016</b> , 658, 230-233	2.5	3

199	Metal ions doped into merocyanine form of coumarin derivatives: nonlinear optical molecular switches. <i>Journal of Molecular Modeling</i> , <b>2019</b> , 25, 212	2	3
198	Probe the accumulation modes of the Au <sub>2</sub> H <sub>14</sub> dimer on the structure and NLO properties. <i>Molecular Physics</i> , <b>2014</b> , 112, 1918-1923	1.7	3
197	Suitable helical cavity, suitable alkali metal, larger first hyperpolarizability. <i>Chemical Physics Letters</i> , <b>2014</b> , 600, 123-127	2.5	3
196	Simple Copper(II) Schiff Base Complex as Efficient Heterogeneous Photo-Fenton-like Catalyst. <i>Chemistry Letters</i> , <b>2014</b> , 43, 1158-1160	1.7	3
195	Two metal-organic frameworks based on a flexible dithioether spacer with luminescence and sensing properties. <i>Inorganic Chemistry Communication</i> , <b>2017</b> , 86, 271-275	3.1	3
194	The effect of boron nitride nanotubes size on the HArF interaction by NBO and AIM analysis. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 1692-1696	2.1	3
193	Density functional theory studies on structures and absorption spectra of [Au(tpy)Cl] <sub>2</sub> <sup>+</sup> and its derivatives: Role of basis set, functional, solvent effect, and spin orbit effect. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 1642-1653	2.1	3
192	Determination of the charge transport abilities of polymorphs [C <sub>6</sub> F <sub>5</sub> Cu] <sub>2</sub> (4,4'-bipy) with different interactions: a density functional theoretical investigation. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 129, 45-51	1.9	3
191	Synthesis, Characterization, and Luminescence of Two New Zinc(II) Coordination Polymers Constructed by 5-(4-Carboxybenzyloxy)isophthalic Acid Ligand. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2011</b> , 637, 1414-1418	1.3	3
190	DFT STUDY ON SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF THE DERIVATIVES OF DISUBSTITUTED SEVEN-VERTEX COBALTACARBORANE METALLOCENYL. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2010</b> , 09, 219-231	1.8	3
189	Theoretical investigation of electronic properties and redox properties for purely inorganic and aryloxy substituted Ti-containing POM derivatives. <i>Molecular Physics</i> , <b>2010</b> , 108, 1553-1560	1.7	3
188	The modulation of electronic and optical properties of OXD-X through introduction of the electron-withdrawing groups: a DFT study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2010</b> , 28, 427-34 <sup>2.8</sup>		3
187	Theoretical studies on electronic spectra and second-order nonlinear optical properties of barbituric acid derivatives substituted with schiff base. <i>Chinese Journal of Chemistry</i> , <b>2010</b> , 22, 425-429	4.9	3
186	A new 2D 5-connected coordination polymer based on 3,4-bis(pyridin-4-ylmethoxy)benzoic acid ligand. <i>Inorganic Chemistry Communication</i> , <b>2010</b> , 13, 932-934	3.1	3
185	A novel large heteropolytungstate constructed from two types of lacunary Keggin anions: K <sub>7</sub> Na <sub>13</sub> [(PW <sub>11</sub> O <sub>39</sub> ) <sub>2</sub> (PW <sub>9</sub> O <sub>34</sub> ) <sub>2</sub> (W <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> ] · 25H <sub>2</sub> O. <i>Inorganica Chimica Acta</i> , <b>2007</b> , 360, 3376-3379	2.7	3
184	Synthesis and characterization of three Cu(II), Zn(II), Cd(II) supramolecular complexes bridged by biphenyl 2,2'-dicarboxylate. <i>Solid State Sciences</i> , <b>2007</b> , 9, 1006-1011	3.4	3
183	Self-assembly of bimetallic polyoxometalates and dicyandiamide to form Co/WC@NC for efficient electrochemical hydrogen generation. <i>New Journal of Chemistry</i> , <b>2021</b> , 46, 178-184	3.6	3
182	Manipulating charge carrier transporting of disubstituted phenylbenzimidazole-based host materials for efficient full-color PhOLEDs. <i>Organic Electronics</i> , <b>2020</b> , 77, 105513	3.5	3

181	Syntheses, structure and properties of an especially stable Cd metal-organic framework driven by benzotriazole-5-carboxylic acid. <i>Inorganic Chemistry Communication</i> , <b>2020</b> , 112, 107726	3.1	3
180	A theoretical mechanistic study of Ir/Cu-metallaphotoredox catalyzed asymmetric radical decarboxylative cyanation. <i>Dalton Transactions</i> , <b>2020</b> , 49, 15276-15286	4.3	3
179	The AlAl triple bond in Al <sub>2</sub> X <sub>5</sub> <sup>+</sup> and Al <sub>2</sub> X <sub>6</sub> <sup>2+</sup> (X = Li, Na) clusters with multiple alkali metal coordination. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 21119-21124	3.6	3
178	Exploring Charge Dissociation in a Statistical Sample of Active-Layer Models of an Organic Solar Cell. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 18840-18846	3.8	3
177	High-Performance and Stable Warm White OLEDs Based on Orange Iridium(III) Phosphors Modified with Simple Alkyl Groups. <i>Organometallics</i> , <b>2020</b> , 39, 3384-3393	3.8	3
176	Second-order nonlinear optical property of carbonBoronNitride heterostructure: Vertical carbon-segment into the BN nanosheet. <i>Computational and Theoretical Chemistry</i> , <b>2021</b> , 1198, 113177	2	3
175	Transition-Metal-Modified Vanadoborate Clusters as Stable and Efficient Photocatalysts for CO Reduction. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 7364-7371	5.1	3
174	Co/WC@NC electrocatalysts derived from polyoxometalates (POM) for efficient hydrogen evolution. <i>Nanotechnology</i> , <b>2021</b> , 32,	3.4	3
173	Dinuclear Ir(III) complexes with asymmetrical bridging ligands as highly efficient phosphors for single-layer electroluminescent devices. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 13461-13467	7.1	3
172	Near-infrared (NIR-II) luminescence for the detection of cyclotetramethylene tetranitramine based on stable Nd-MOF. <i>Journal of Solid State Chemistry</i> , <b>2021</b> , 294, 121789	3.3	3
171	Mechanistic insight into photocatalytic CO <sub>2</sub> reduction by a Z-scheme g-C <sub>3</sub> N <sub>4</sub> /TiO <sub>2</sub> heterostructure. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 11474-11480	3.6	3
170	PMO <sub>12</sub> @ZIF-8/ZnO-derived hierarchical porous molybdenum carbide as efficient electrocatalysts for hydrogen evolution. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 9456-9461	3.6	3
169	Structure-property relationships of coronene in external electric field. <i>Organic Electronics</i> , <b>2018</b> , 59, 196-201	3.9	3
168	Switching of second-order nonlinear response effected by different acceptors: The impacts of environment and frequency dispersion. <i>Dyes and Pigments</i> , <b>2021</b> , 193, 109502	4.6	3
167	Self-Assembled Polyoxometalate-Based Metal-Organic Polyhedra as an Effective Heterogeneous Catalyst for Oxidation of Sulfide. <i>Crystal Growth and Design</i> , <b>2021</b> , 21, 1028-1034	3.5	3
166	Activating room-temperature phosphorescence of 1,8-naphthalimide by doping into aromatic dicarboxylic acids.. <i>Chemical Communications</i> , <b>2022</b> ,	5.8	3
165	Encapsulation of AlEgens within MetalOrganic Framework toward High-Performance White Light-Emitting Diodes. <i>Advanced Optical Materials</i> , <b>2020</b> , 174	8.1	3
164	Insight into spin-orbital interaction using MCSCF method: A special analysis of the electronic state in C and the linear polyacetylenic C and C. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 1338-1343	3.5	2

163	Exploring the electronic properties and cation complexation of polyoxoaurates [Au(III)4X4Om](n-) (X = Si(IV), P(V), Ge(IV), As(V), and Se(IV)) using quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 11521-6	3.6	2
162	"Dancing inside the ball": the structures and nonlinear optical properties of three Sc2S@C3v(8)-C82 isomers. <i>Journal of Molecular Modeling</i> , <b>2015</b> , 21, 259	2	2
161	Configuration effect in polyoxometalate-based dyes on the performance of DSSCs: an insight from a theoretical perspective. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 16032-16039	3.6	2
160	Hollow Porous MnFe O Sphere Grown on Elm-Money-Derived Biochar towards Energy-Saving Full Water Electrolysis. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 14397-14404	4.8	2
159	Hydrogen Migration-Triggered Diradicaloid Singlet-Fission Switch. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 11791-11803	16.4	2
158	Two anthracene chromophore based metal-organic frameworks for gas adsorption and promising nitro aromatic sensing. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 12496-12502	3.6	2
157	Sulfur-doping polyoxometallate-metal-organic intercalation compound with PPy coating as highly efficient photocatalyst for visible light degradation. <i>Polyhedron</i> , <b>2020</b> , 179, 114350	2.7	2
156	NICS values scan in three-dimensional space of the hoop-shaped $\pi$ -conjugated molecules [6]8cyclacene and [16]trannulene. <i>New Journal of Chemistry</i> , <b>2018</b> , 42, 1987-1994	3.6	2
155	Theoretical investigation on the effect of fluorine and carboxylate substitutions on the performance of benzodithiophene-diketopyrrolopyrrole-based polymer solar cells. <i>Theoretical Chemistry Accounts</i> , <b>2018</b> , 137, 1	1.9	2
154	Theoretical studies on oxidation-switchable second-order nonlinear optical responses of Metallosalen-Keggin polyoxometalate derivatives. <i>RSC Advances</i> , <b>2016</b> , 6, 53438-53443	3.7	2
153	TDDFT studies on the chiroptical properties of a chiral inorganic polythioanion Mbius strip. <i>Inorganic Chemistry Frontiers</i> , <b>2016</b> , 3, 86-91	6.8	2
152	Two Novel Lanthanide Metal-Organic Frameworks Constructed by Tetracarboxylate Ligands: Synthesis, Structures; and Luminescent Properties. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2019</b> , 645, 940-943	1.3	2
151	Electronic properties and stabilities of methoxy-substituted Lindqvist polyoxometalates [Nb2W4O19CH3]3 by DFT. <i>Science Bulletin</i> , <b>2012</b> , 57, 976-982		2
150	Rational modifications on ruthenium terpyridine sensitizers with large Jsc for dye-sensitized solar cells: combined DFT and relativistic TDDFT studies. <i>RSC Advances</i> , <b>2015</b> , 5, 100169-100175	3.7	2
149	A TiO2@{Mo368} composite: synthesis, characterization, and application in dye-sensitized solar cells. <i>Journal of Coordination Chemistry</i> , <b>2014</b> , 67, 3873-3883	1.6	2
148	A DFT study on the second-order nonlinear optical properties of the plenary mixed-metal polyoxometalate. <i>Molecular Simulation</i> , <b>2012</b> , 38, 518-524	2	2
147	DFT studies on the electronic properties of organometallic-polyoxomolybdate anions [Cpn*Mo6O19B](2B)(n = 1 or 2): Revealing bonding features of Cp*Mo. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 976, 1-7	2	2
146	A novel route for designing C60 derivatives with large first hyperpolarizability: Cage-opened cases. <i>Synthetic Metals</i> , <b>2011</b> , 161, 2185-2191	3.6	2

145	Theoretical study on stability and nonlinear optical properties of tetrahydropyrrole diradical and its isoelectronic systems in different electronic states. <i>Science China Chemistry</i> , <b>2011</b> , 54, 1086-1093	7.9	2
144	Synthesis and Luminescent Properties of Two Zinc(II) Coordination Polymers Constructed by 4-(Pyridin-4-ylmethoxy)benzoic Acid Ligand. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2011</b> , 637, 1419-1422	1.3	2
143	Synthesis, Crystal Structure, and Fluorescent Property of A Chiral 2D Polymer Based on Bis(2-benzimidazoles) and Aromatic Carboxylate Ligands. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2011</b> , 637, 2211-2214	1.3	2
142	TDDFT study on the second-order nonlinear optical properties of a series of mono- and di-nuclear [60]fullerene complexes. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 963, 98-103	2	2
141	A facile method for preparation of dye-doped silica-based raspberry-like microspheres and fluorescent films. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2009</b> , 9, 6594-9	1.3	2
140	Theoretical study on the structures, isomerization and stability of SiC <sub>4</sub> isomers. <i>Theoretical Chemistry Accounts</i> , <b>2010</b> , 126, 15-25	1.9	2
139	Theoretical investigation on structures, electronic spectra and nonlinear optical properties of gold compounds [X-Au(PMe <sub>3</sub> ) <sub>2</sub> ]. <i>Science China Chemistry</i> , <b>2010</b> , 53, 1149-1154	7.9	2
138	Molecular simulation study of the binding mechanism of [H-PTiWO] for its promising broad-spectrum inhibitory activity to FluV-A neuraminidase. <i>Science Bulletin</i> , <b>2010</b> , 55, 2497-2504		2
137	Quantum chemical study on the reaction mechanism of OBrO radical with OH radical. <i>Chinese Journal of Chemistry</i> , <b>2010</b> , 22, 611-615	4.9	2
136	Theoretical study of the impact factor on redox property and second-order nonlinear response for organoimido derivatives of [Mo <sub>6</sub> O <sub>19</sub> ] <sup>2-</sup> Electron donors with magnitude of conjugated groups or length of conjugated chain. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 947, 9-15		2
135	Theoretical Study on One- and Two-Photon Absorption Properties of PPV Derivative with Electron-Donor Phenylanthracene as Pendent Group. <i>Chinese Journal of Chemistry</i> , <b>2007</b> , 25, 465-471	4.9	2
134	Bis[2,2'-(butane-1,4-diyl)bis(1H-benzimidazolium)] H <sup>-</sup> octamolybdate(VI). <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2007</b> , 63, m584-m586		2
133	Theoretical Studies on Proton Transfer Reactions of 8-Hydroxyquinoline Monomers and Dimers. <i>Chinese Journal of Chemistry</i> , <b>2006</b> , 24, 724-730	4.9	2
132	Density functional theory study on isomerization reactions of pyridazine derivatives bearing N,N-dialkylaminoethyl group. <i>International Journal of Quantum Chemistry</i> , <b>2004</b> , 98, 515-521	2.1	2
131	Tetraaqua(2,2'-bipyridine)zinc(II) terephthalate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2004</b> , 60, m142-m144		2
130	Non-metal boron atoms on a CuB monolayer as efficient catalytic sites for urea production.. <i>Chemical Science</i> , <b>2022</b> , 13, 1342-1354	9.4	2
129	Establishing the Principal Descriptor for Electrochemical Urea Production via the Dispersed Dual-Metals Anchored on the N-Decorated Graphene.. <i>Advanced Science</i> , <b>2022</b> , e2105697	13.6	2
128	Polymers and polyoxometalate induced Co/WC@NC for electrocatalytic hydrogen production. <i>Journal of Solid State Chemistry</i> , <b>2022</b> , 308, 122879	3.3	2

- 127 A metal-free covalent organic framework as a photocatalyst for CO<sub>2</sub> reduction at low CO<sub>2</sub> concentration in a gas-solid system. *Journal of Materials Chemistry A*, **2021**, 9, 24895-24902 13 2
- 126 A thiol-functionalized zirconium metal-organic cage for the effective removal of Hg from aqueous solution. *Nanotechnology*, **2021**, 32, 075602 3-4 2
- 125 All-Metallic Zn=Zn Double-Bonded Octahedral Zn M (M=Li, Na) Clusters with Negative Oxidation State of Zinc. *ChemPhysChem*, **2020**, 21, 459-463 3-2 2
- 124 External Electric Field-Phenyl interaction boosts hydrosilylation of substituted alkynes to  $\beta$ -vinylsilane. *International Journal of Quantum Chemistry*, **2020**, 120, e26134 2-1 2
- 123 Self-assembly of zirconocene-based metal-organic capsules: the structure, luminescence sensing of Fe<sup>3+</sup> and iodine capture. *New Journal of Chemistry*, **2020**, 44, 21255-21260 3-6 2
- 122 Ultrafast Absorption of Polysulfides through Electrostatic Confinement by Protonated Molecules for Highly Efficient Li-S Batteries. *ACS Applied Materials & Interfaces*, **2020**, 12, 36220-36227 9-5 2
- 121 Cu/Cu S-Embedded N,S-Doped Porous Carbon Derived in Situ from a MOF Designed for Efficient Catalysis. *Chemistry - A European Journal*, **2021**, 27, 11468-11476 4-8 2
- 120 Co<sub>2</sub>P@C derived from metal-organic coordinate interactions using polyaniline as soft template for electrocatalytic hydrogen production. *Journal of Solid State Chemistry*, **2021**, 299, 122184 3-3 2
- 119 The inner-induced effects of YCN in C76 on the structures and nonlinear optical properties. *Journal of Molecular Modeling*, **2016**, 22, 174 2 2
- 118 The directions of an external electric field control the catalysis of the hydroboration of C-O unsaturated compounds.. *RSC Advances*, **2019**, 9, 29331-29336 3-7 2
- 117 Superiority of Iridium Photocatalyst and Role of Quinuclidine in Selective  $\beta$ -C(sp)-H Alkylation: Theoretical Insights. *Journal of Organic Chemistry*, **2021**, 86, 484-492 4-2 2
- 116 Integration of zirconium-based metal-organic framework with CdS for enhanced photocatalytic conversion of CO to CO. *Nanoscale*, **2021**, 13, 16977-16985 7-7 2
- 115 Er, Yb:CeF<sub>3</sub> red emission nanoparticles with controllable size and enhanced luminescence properties. *Journal of Materials Science: Materials in Electronics*, **2021**, 32, 8213-8225 2-1 2
- 114 A stable Cd metal-organic framework as efficient fluorescent probe for sensing Fe<sup>3+</sup> in water. *Inorganica Chimica Acta*, **2021**, 528, 120635 2-7 2
- 113 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 3-6 2
- 112 Rational Design of Ir(III) Phosphors to Strategically Manage Charge Recombination for High-Performance White Organic Light-Emitting Diodes.. *Inorganic Chemistry*, **2022**, 61, 1211-1218 5-1 2
- 111 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**, 129234 5-1 2
- 110 Demulsification-induced Fast Solidification: a Novel Strategy for Preparation of Polymer Encapsulations. *Chemical Research in Chinese Universities*, **2019**, 35, 1082-1088 2-2 1

109	Strong Pancake 2e/12c Bond in $\pi$ -Stacking Phenalenyl Derivatives Avoiding Bond Conversion. <i>ChemPhysChem</i> , <b>2019</b> , 20, 1879-1884	3.2	1
108	Multifunctional Dicyandiamide Blowing-Induced Formation of Electrocatalysts for the Hydrogen Evolution Reaction. <i>ACS Omega</i> , <b>2019</b> , 4, 10347-10353	3.9	1
107	A theoretical exploration on why the replacement of hexyl group by alkoxy carbonyl in P3HT could greatly improve the performance of non-fullerene organic solar cell. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , <b>2019</b> , 100, 160-167	5.3	1
106	Theoretical exploration to the cation effect on the second-order nonlinear optical properties of Strandberg-type polyoxometalates. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2015</b> , 14, 1550007	1.8	1
105	A comparative computational analysis on the photophysical and charge transport properties of three 5,5-bis(2,2-diphenylvinyl)-bicyclic compounds. <i>Chemical Physics Letters</i> , <b>2020</b> , 748, 137348	2.5	1
104	Synthesis and proton-conducting performance of crystalline hydrogen-bonded organic networks. <i>Journal of Solid State Chemistry</i> , <b>2020</b> , 290, 121550	3.3	1
103	Retraction: Sublimable cationic Ir(III) phosphor using chlorine as a counterion for high-performance monochromatic and white OLEDs. <i>Chemical Communications</i> , <b>2020</b> , 56, 1609-1610	5.8	1
102	Theoretical design of organic-inorganic hybrids based on hexamolybdate toward high performance dye-sensitized solar cells. <i>Molecular Simulation</i> , <b>2016</b> , 42, 688-692	2	1
101	Single step synthesized three dimensional spindle-like nanoclusters as lithium-ion battery anodes. <i>CrystEngComm</i> , <b>2018</b> , 20, 3043-3048	3.3	1
100	Hydrothermal synthesis and structure characterization of two six-connected metal-organic frameworks based on the mixed ligands. <i>Solid State Sciences</i> , <b>2014</b> , 34, 8-11	3.4	1
99	A novel nitrogen-containing compound with D <sub>3h</sub> structure: theoretical and experimental study. <i>Canadian Journal of Chemistry</i> , <b>2014</b> , 92, 411-416	0.9	1
98	Probing the relationship between spin contamination and first hyperpolarizability: Open-shell M <sub>3</sub> Bi <sub>3</sub> anion. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 720-724	2.1	1
97	Reply to Comment on How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 725-728	3.8	1
96	Recent Theoretical Advances in Understanding the Mechanism of Aggregation-Induced Emission for Small Organic Molecules <b>2013</b> , 399-418		1
95	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. <i>Journal of Molecular Modeling</i> , <b>2017</b> , 23, 231	2	1
94	Molecular dynamic and quantum mechanics study of drug recognition for the extremity of DNA G-quadruplex groove. <i>Medicinal Chemistry Research</i> , <b>2012</b> , 21, 4010-4016	2.2	1
93	TDDFT studies on electronic structures, chiroptical properties and solvent effect on the CD spectra of diphosphonate-functionalized polyoxomolybdates. <i>Journal of Molecular Graphics and Modelling</i> , <b>2013</b> , 44, 26-32	2.8	1
92	Structure and mechanical properties of waterborne polyurethane-based composites filled with self-assembled supramolecular nanoplatelets. <i>Journal Wuhan University of Technology, Materials Science Edition</i> , <b>2013</b> , 28, 773-780	1	1

91	Theoretical investigation of second-order nonlinear optical response of Hexamolybdate as a superior donor over metal carbonyl complexes in the D <sub>3h</sub> model. <i>Canadian Journal of Chemistry</i> , <b>2011</b> , 89, 61-67	0.9	1
90	Theoretical Investigation on Electronic Transition of Tris(8-quinolinolate) Aluminum Grafted on Poly(p-phenylenevinylene) Units with the Localized-density-matrix Method. <i>Chinese Journal of Chemistry</i> , <b>2009</b> , 27, 1891-1896	4.9	1
89	Investigation on fluorescence properties of ultrafine PVA fiber mats-contained polyoxometalate with different molecular structure. <i>Journal of Applied Polymer Science</i> , <b>2009</b> , 113, 1369-1374	2.9	1
88	The influence of M <sup>n</sup> M <sup>m</sup> attraction on nonlinear optical properties of (XMPH <sub>3</sub> ) <sub>2</sub> (X = F, Cl; and M = Au, Ag and Cu): A theoretical study. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 110, NA-NA	2.1	1
87	Theoretical study on the second-order nonlinear optical properties of gold (III) alkyl complexes. <i>Synthetic Metals</i> , <b>2009</b> , 159, 2406-2409	3.6	1
86	QUANTUM CHEMISTRY STUDIES ON THE Fe-Hg INTERACTIONS AND <sup>31</sup> P NMR IN [Fe(CO) <sub>3</sub> (RPhPpy) <sub>2</sub> (HgCl <sub>2</sub> )] (R = Me, Et, Ph). <i>Journal of Theoretical and Computational Chemistry</i> , <b>2011</b> , 10, 53-63	1.8	1
85	Theoretical studies on the structures and absorption spectra of $R_2n+1$ (R = H, F; n = 1, 2) substituted 5-(2-pyridyl) pyrazolate boron complexes. <i>Molecular Physics</i> , <b>2009</b> , 107, 2511-2520	1.7	1
84	A theoretical study of ground and excited state proton transfer and rotamerism in salicylanilide and its 1:1 complex with methanol. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 945, 110-115		1
83	Two inorganic-organic hybrid compounds based on [Ni <sub>2</sub> (V <sub>3</sub> O <sub>9</sub> ) <sub>2</sub> ] <sub>2</sub> cluster and {Co <sub>2</sub> V <sub>2</sub> } cage subunits. <i>Inorganic Chemistry Communication</i> , <b>2010</b> , 13, 981-984	3.1	1
82	THEORETICAL STUDIES ON THE FORMATION MECHANISM AND STRUCTURE OF PENTAFULVENONE AND AZAFULVENONE. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2008</b> , 07, 233-246	1.8	1
81	Bis{4,4'-[(2,2'-bi-1H-imidazole-1,1'-diyl)dimethylene]dipyridinium} hexamolybdate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2007</b> , 63, m2817-m2817		1
80	Electronic Properties and Stability of Ditungsten Substituted Keggin Polyoxotungstate with Heteroatom Phosphorus by DFT. <i>ChemInform</i> , <b>2005</b> , 36, no		1
79	Anisotropic conductivity of undoped and [FeCl <sub>4</sub> ] <sup>-</sup> doped trans-polyacetylene. <i>Computational and Theoretical Chemistry</i> , <b>2001</b> , 540, 1-4		1
78	Ammonium polyphosphate induced bimetallic phosphides nanoparticles coated with porous N-doped carbon for efficiently electrochemical hydrogen evolution. <i>Chemical Engineering Journal</i> , <b>2021</b> , 431, 133696	14.7	1
77	Two-dimensional graphdiyne analogue containing Mo-coordinated porphyrin covalent organic framework as a high-performance electrocatalyst for nitrogen fixation. <i>Applied Surface Science</i> , <b>2022</b> , 580, 152359	6.7	1
76	CO <sub>2</sub> electroreduction performance of transition metals supported on g-C <sub>3</sub> (CN) <sub>3</sub> monolayer with specific TMN <sub>3</sub> active sites. <i>Applied Surface Science</i> , <b>2022</b> , 573, 151544	6.7	1
75	A theoretical exploration of charge transfer dynamics in PTB7Ir/PC71BM triplet-material-based organic photovoltaics. <i>Organic Electronics</i> , <b>2020</b> , 87, 105956	3.5	1
74	Face-Directed Assembly of Molecular Cubes: In Situ Substitution of a Predetermined Concave Cluster. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 22218-22222	3.6	1



73	Investigation of the Structural and Luminescent Properties and the Chromium Ion Valence of Li <sub>2</sub> CaGeO <sub>4</sub> Crystals Doped with Cr <sup>4+</sup> Ions. <i>Crystals</i> , <b>2020</b> , 10, 1019	2.3	1
72	Tunable Dual-Color Emission Perovskites via Post-Synthetic Modification Strategy for Near-Unity Photoluminescence Quantum Yield. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 21645-21652	9.5	1
71	Enhanced Fluorescence of La <sup>3+</sup> , Gd <sup>3+</sup> doped EuW <sub>10</sub> for Temperature sensing performance. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2021</b> , 647, 1221-1226	1.3	1
70	Close-packed storage of potassium metallic clusters achieved through nanostructure engineering of ultrafine hollow nanoparticles-based carbon nanoclusters. <i>EcoMat</i> , <b>2021</b> , 3, e12105	9.4	1
69	Radical Mechanism of Ir III /Ni II -Metallaphotoredox-Catalyzed C(sp <sup>3</sup> ) Functionalization Triggered by Proton-Coupled Electron Transfer: Theoretical Insight. <i>CCS Chemistry</i> , 1456-1467	7.2	1
68	Temperature sensitive properties and preparation of europium complexes with double ligands. <i>Luminescence</i> , <b>2021</b> , 36, 1476-1482	2.5	1
67	Near-infrared luminescence investigation of Cr <sup>4+</sup> ions doped Li <sub>2</sub> TiGeO <sub>5</sub> . <i>Journal of Materials Science: Materials in Electronics</i> , <b>2021</b> , 32, 18544-18550	2.1	1
66	Metal-free catalysis for the Markovnikov hydrosilylation of styrene. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 18339-18344	3.6	1
65	Theoretical investigation of the influence of different electric field directions and strengths on a POM-based dye for dye-sensitized solar cells. <i>Materials Chemistry Frontiers</i> , <b>2021</b> , 5, 929-936	7.8	1
64	An octahedral polyoxomolybdate-organic molecular cage. <i>Chemical Communications</i> , <b>2021</b> , 57, 1042-1045	5.8	1
63	Efficient catalytic reduction of 4-nitrophenol by Cu <sub>1.96</sub> S/NSC hybrid material derived from metal-organic framework. <i>E3S Web of Conferences</i> , <b>2021</b> , 252, 02065	0.5	1
62	Assembly of tetra-nuclear Yb-containing selenotungstate clusters: synthesis, structures, and magnetic properties. <i>Dalton Transactions</i> , <b>2021</b> , 50, 11535-11541	4.3	1
61	Carbon nitride derivatives as photocatalysts for the CO reduction reaction: computational study. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 3401-3406	3.6	1
60	Periodic B- and N-doped phenalenyl aggregates: unexpected nonlinear optical properties by tuning pancake bonding. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 23998-24003	3.6	1
59	High performance doping-free WOLEDs based on rationally designed asymmetric orange-red Ir(III) emitter with balanced charge mobility. <i>Organic Electronics</i> , <b>2021</b> , 89, 106022	3.5	1
58	Doping alkali metal ions and introducing electron donor groups to fulleropyrrolidine derivatives: Large second-order nonlinear optical responses. <i>Computational and Theoretical Chemistry</i> , <b>2021</b> , 1201, 113254	2	1
57	Activation of Peroxymonosulfate by Co-Metal-Organic Frameworks as Catalysts for Degradation of Organic Pollutants. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2021</b> , 60, 13223-13232	3.9	1
56	N-Donor flexible ligands for constructing polyoxometalate-based metal-organic frameworks as multifunctional electrocatalysts. <i>CrystEngComm</i> , <b>2022</b> , 24, 2705-2708	3.3	1

55	Aspects of the Nonlinear Optical Properties as a Guide to Protonation Sites: A Theoretical Study upon $\beta$ -Keggin [SiW <sub>12</sub> O <sub>40</sub> ] <sup>4-</sup> and [SiV <sub>3</sub> W <sub>9</sub> O <sub>40</sub> ] <sup>7-</sup> <i>Chemistry Letters</i> , <b>2010</b> , 39, 580-581	1.7	○
54	The effect of conformational dependent properties of radical cations on poly(N,N-dimethylaniline). <i>Macromolecular Chemistry and Physics</i> , <b>2000</b> , 201, 1774-1779	2.6	○
53	Metal-free C <sub>2</sub> N doped with sp <sup>2</sup> hybridized B atom as high efficiency photocatalyst for nitrobenzene reduction reaction: A density functional theory study. <i>Molecular Catalysis</i> , <b>2022</b> , 518, 112080	3.3	○
52	Theoretical mechanistic study of 4CzIPN/Ni-metallaphotoredox catalyzed enantioselective desymmetrization of cyclic -anhydrides. <i>Dalton Transactions</i> , <b>2021</b> , 50, 17675-17687	4.3	○
51	Computational evaluation of FeMo heteroatom coeffect induced high electroreduction activity of N <sub>2</sub> -to-NH <sub>3</sub> . <i>Applied Surface Science</i> , <b>2022</b> , 579, 152214	6.7	○
50	Metal-Free Z-Scheme aza-CMP/C <sub>2</sub> N Heterostructure to Facilitate Photocatalytic CO <sub>2</sub> Reduction: A Computational Study. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 23133-23141	3.8	○
49	Study on the photoluminescence properties and magnetization performance of Lu <sup>3+</sup> , Tb <sup>3+</sup> : CeF <sub>3</sub> nanoparticles. <i>Journal of Materials Science: Materials in Electronics</i> , <b>2021</b> , 32, 28098	2.1	○
48	Synthesis, Crystal Structure, and Luminescent Properties of a New Holmium(III) Coordination Polymer Involving 2,5-Dihydroxy-1,4-terephthalic Acid Dianion as Ligand. <i>Crystals</i> , <b>2021</b> , 11, 1294	2.3	○
47	ZIF-8 and polyaniline modified coconut gel to fabricate composite aerogel for efficient removal of tetracycline. <i>E3S Web of Conferences</i> , <b>2020</b> , 185, 04055	0.5	○
46	Theoretical Simulations of Thermo-chromic and Aggregation-Induced Emission Behaviors of a Series of Red-Light Anthracene-o-carborane Derivatives. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 9571-9579	4.8	○
45	A typical 2D covalent organic polymer as multifunctional sensor and assemble a WLED. <i>Journal of Solid State Chemistry</i> , <b>2021</b> , 297, 122101	3.3	○
44	The nonlinear optics property of heterodinuclear (Li and Na) sexipyridine helix: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26478	2.1	○
43	Regioisomeric BODIPY derivatives: second-order nonlinear optical properties under an external electric field. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 4335-4339	3.6	○
42	A fluorescent porous covalent-organic polymer (COP-3) for highly selective and sensitive detection of Fe <sup>3+</sup> in aqueous solution. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 2370-2373	3.6	○
41	Tuning the NLO response of bis-cyclometalated iridium(III) complexes by modifying ligands: experimental and structural DFT analysis. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 5491-5496	3.6	○
40	Two functional hybrids based on polyoxometalate coordination polymers: Synthesis, electrochemical and photocatalytic properties. <i>Inorganic Chemistry Communication</i> , <b>2021</b> , 130, 108673	3.1	○
39	Novel acetylene-terminated thermosetting polyisoimides with excellent solubility and performed as efficient heat shields composites. <i>Journal of Applied Polymer Science</i> , 51559	2.9	○
38	Cubic Ba <sub>2</sub> LaF <sub>7</sub> :Yb <sup>3+</sup> /Ln (Ln = Er <sup>3+</sup> , Ho <sup>3+</sup> ) up-conversion submicron particles controllable synthesis and luminescence properties. <i>Journal of Materials Science: Materials in Electronics</i> , <b>2021</b> , 32, 24856	2.1	○

37	Theoretical design and characterization of new terpolymer donors based on PTB7Ir for high-efficiency triplet-material-based organic photovoltaics.. <i>RSC Advances</i> , <b>2022</b> , 12, 8578-8587	3.7	○
36	Theoretical search of a simple characteristic for long-lived organic room-temperature phosphorescence materials with H aggregation. <i>Journal of Materials Chemistry C</i> , <b>2022</b> , 10, 5425-5432	7.1	○
35	Coordination Environment Regulation of Cucurbit[6]uril-Based Metal-Organic Rotaxane Networks for Proton Conduction. <i>Crystal Growth and Design</i> ,	3.5	○
34	Lanthanide metal-organic frameworks based on planar $\pi$ -conjugated ligands for white light emission, temperature and chemical sensing. <i>Dyes and Pigments</i> , <b>2022</b> , 202, 110256	4.6	○
33	Stable zinc metal-organic framework as efficient bifunctional fluorescent probe for selective detection of nitrobenzene and Fe(III). <i>Journal of Solid State Chemistry</i> , <b>2022</b> , 310, 123093	3.3	○
32	Improved ablation resistance and thermal insulation performances of polyimide composites by introducing albite/glass powder composition. <i>Polymers and Polymer Composites</i> , <b>2022</b> , 30, 096739112210878	0.8	○
31	Three Cd-MOFs with water stability act as novel fluorescent probes for detecting nitrofurantoin and Fe <sup>3+</sup> . <i>Journal of Solid State Chemistry</i> , <b>2022</b> , 123170	3.3	○
30	Syntheses, Structures, and Photophysical Properties of Two Coordination Polymers Based on 2,3-Dioxo-1,2,3,4-tetrahydroquinoxaline-6-carboxylic Acid. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2017</b> , 643, 531-535	1.3	
29	A new covalent organic polymer used to highly selective detection of Fe <sup>3+</sup> ions. <i>E3S Web of Conferences</i> , <b>2020</b> , 213, 01008	0.5	
28	Theoretical studies on the chiral polyoxoanions [P <sub>2</sub> Mo <sub>18</sub> O <sub>62</sub> ] <sup>6-</sup> and [PMo <sub>9</sub> O <sub>31</sub> (OH) <sub>2</sub> ] <sub>3</sub> <sup>3-</sup> with histidine: chiral inversion and chiral induction. <i>Inorganic Chemistry Frontiers</i> , <b>2018</b> , 5, 1992-1997	6.8	
27	The Effect of the different spin multiplicity on nonlinear optical properties of lithium decahydroborate dimers. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2415	2	
26	Theoretical study on photophysical properties of Pt(II) triarylborons with a 2,2-bpy core derivatives. <i>Journal of Molecular Graphics and Modelling</i> , <b>2013</b> , 44, 311-7	2.8	
25	Inside Cover: Spiral Intramolecular Charge Transfer and Large First Hyperpolarizability in M <sup>B</sup> ius Cyclacenes: New Insight into the Localized $\pi$ Electrons (ChemPhysChem 9/2012). <i>ChemPhysChem</i> , <b>2012</b> , 13, 2222-2222	3.2	
24	NOVEL ANODE Li-ION SECONDARY BATTERIES DERIVED FROM NANOCRYSTALLINE Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> /POLYACENE MATERIALS. <i>International Journal of Nanoscience</i> , <b>2009</b> , 08, 333-336	0.6	
23	Mechanism and Kinetics for the Reaction of NCS and OH Radicals. <i>Chinese Journal of Chemistry</i> , <b>2010</b> , 22, 590-593	4.9	
22	Density functional study on the mechanism of collision reaction among protons, N <sub>2</sub> and water vapor. <i>Chinese Journal of Chemistry</i> , <b>2010</b> , 22, 594-598	4.9	
21	Theoretical study on the mechanism for the reaction of pentafulvenone with HNC in singlet and triplet states, interconversions and solvation effect. <i>Molecular Physics</i> , <b>2008</b> , 106, 1767-1776	1.7	
20	catena-Poly[[diaquabis(2-methoxymethyl-1H-benzimidazole- $\kappa$ 3)cadmium(II)]- $\mu$ -terephthalato- $\kappa$ O:O?]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2007</b> , 63, m292-m293		

- 19 A tetranuclear copper(II) complex constructed from the salen ligand with alkoxo groups. *Acta Crystallographica Section E: Structure Reports Online*, **2007**, 63, m2932-m2932
- 18 A one-dimensional nickel(II) coordination polymer with pyridine and isophthalate. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, m322-m324
- 17 Ab initio and DFT study on  $[\text{Si}(\text{O}2\text{Ph})_n\text{m}]^{\pm}$  ( $n=1,2$ ,  $m=0,1,2$ ). *Computational and Theoretical Chemistry*, **2002**, 578, 159-167
- 16 Quantum chemical study on ferromagnetic property on the N,N-dimethylaniline dimer radical cation. *International Journal of Quantum Chemistry*, **2002**, 89, 484-488 2.1
- 15 Electrical anisotropy of oriented trans-polyacetylene undoped and doped with  $\text{SO}_3$ . *Science Bulletin*, **2000**, 45, 893-896
- 14 Electronic Properties Of The Model Organometallic Polymer  $[\text{M}-\text{C}=\text{C}(\text{N})]_n$  ( $\text{M} = \text{Cu}(\text{I}), \text{Ag}(\text{I}), \text{Au}(\text{I})$ ). *Materials Research Society Symposia Proceedings*, **1999**, 576, 389
- 13 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 7.1
- 12 Green Catalytic Method for Hydrothiolation of Allylamines: An External Electric Field.. *ACS Omega*, **2022**, 7, 5782-5790 3.9
- 11 The interesting luminescence behavior and rare nonlinear optical properties of the  $\{\text{AgMo}\}$  nanocluster.. *RSC Advances*, **2021**, 11, 38814-38819 3.7
- 10 Hexanuclear nickel-based  $[\text{P}_4\text{Mo}_{11}\text{O}_{50}]$  with photocatalytic reduction of  $\text{CO}_2$  activity. *Inorganic Chemistry Communication*, **2021**, 109009 3.1
- 9 Tetra-aqua-bis(2-oxo-1,2-dihydro-quinoline-4-carboxyl-ato- $\text{O}$ )nickel(II). *Acta Crystallographica Section E: Structure Reports Online*, **2008**, 64, m389-90
- 8 A new polyniobotungstate based on  $\{\text{GeW}_9\text{Nb}_3\text{O}_{40}\}$  clusters and nickel cation with photocatalytic properties. *Inorganic Chemistry Communication*, **2020**, 120, 108151 3.1
- 7 An efficient strategy for improving the water stability of a nearinfrared- emissive lanthanide MOF. *E3S Web of Conferences*, **2020**, 185, 04070 0.5
- 6 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 6.7
- 5 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 1.6
- 4 Synthesis and characterization of two isostructural 3d-4f coordination compounds based on pyridine-2,6-dicarboxylic acid and 4,4'-bipyridine. *Acta Crystallographica Section C, Structural Chemistry*, **2019**, 75, 723-727 0.8
- 3 Machine Learning Corrections for DFT Noncovalent Interactions. *Springer Series in Materials Science*, **2021**, 183-212 0.9
- 2 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*, **2021**, 1 2.2

- 1 Post-decorated synthesis of metal-organic frameworks derived Ni/Ni<sub>3</sub>S<sub>2</sub>@CN electrocatalyst for efficient hydrogen evolution. *Journal of Solid State Chemistry*, **2022**, 123287 33