Wei Guan

List of Publications by Year
in descending order

137 papers	4,611 citations	117625 34 h-index	118850 62 g-index
145 all docs	145 docs citations	145 times ranked	4919 citing authors

#	Article	IF	Citations
1	Ultrastable Polymolybdate-Based Metalâ€“Organic Frameworks as Highly Active Electrocatalysts for Hydrogen Generation from Water. Journal of the American Chemical Society, 2015, 137, 7169-7177.	13.7	584
2	Effect of Imidazole Arrangements on Proton-Conductivity in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2017, 139, 6183-6189.	13.7	436
3	Creating Well-Defined Hexabenzocoronene in Zirconium Metalâ€“Organic Framework by Postsynthetic Annulation. Journal of the American Chemical Society, 2019, 141, 2054-2060.	13.7	148
4	A highly efficient Z-scheme B-doped g-C₃N₄/SnS₂photocatalyst for CO₂reduction reaction: a computational study. Journal of Materials Chemistry A, 2018, 6, 21056-21063.	10.3	134
5	Multielectron transportation of polyoxometalate-grafted metalloporphyrin coordination frameworks for selective CO2-to-CH4 photoconversion. National Science Review, 2020, 7, 53-63.	9.5	127
6	Photoinduced Copper-Catalyzed Asymmetric Câ€“O Cross-Coupling. Journal of the American Chemical Society, 2021, 143, 13382-13392.	13.7	118
7	A DFT Study on The Twoâ€Dimensional Secondâ€Order Nonlinear Optical (NLO) Response of Terpyridineâ€Substituted Hexamolybdates: Physical Insight on 2D Inorganicâ€“Organic Hybrid Functional Materials. European Journal of Inorganic Chemistry, 2012, 2012, 705-711.	2.0	109
8	Redox-Switchable Second-Order Nonlinear Optical Responses of Pushâˆ’Pull Monotetrathiafulvalene-Metalloporphyrins. Inorganic Chemistry, 2009, 48, 6548-6554.	4.0	103
9	Prediction of Remarkably Large Second-Order Nonlinear Optical Properties of Organoimido-Substituted Hexamolybdates. Journal of Physical Chemistry A, 2009, 113, 3576-3587.	2.5	102
10	Theoretical Study on the Electronic Spectrum and the Origin of Remarkably Large Third-Order Nonlinear Optical Properties of Organoimide Derivatives of Hexamolybdates. Journal of Physical Chemistry B, 2006, 110, 23092-23098.	2.6	84
11	Directed Copper-Catalyzed Intermolecular Aminative Difunctionalization of Unactivated Alkenes. Journal of the American Chemical Society, 2019, 141, 18475-18485.	13.7	81
12	Gold with +4 and +6 Oxidation States in AuF₄ and AuF₆. Journal of the American Chemical Society, 2018, 140, 9545-9550.	13.7	80
13	Multicolor Carbon Dots Prepared by Singleâ€Factor Control of Graphitization and Surface Oxidation for Highâ€Quality White Lightâ€Emitting Diodes. Advanced Optical Materials, 2021, 9, 2100688.	7.3	79
14	Directed Copper-Catalyzed Intermolecular Heck-Type Reaction of Unactivated Olefins and Alkyl Halides. Journal of the American Chemical Society, 2018, 140, 16929-16935.	13.7	72
15	Second-Order Nonlinear Optical Properties of Transition-Metal-Trisubstituted Polyoxometalateâˆ’Diphosphate Complexes: A Donorâˆ’Conjugated Bridgeâˆ’Acceptor Paradigm for Totally Inorganic Nonlinear Optical Materials. Journal of Physical Chemistry C, 2009, 113, 19672-19676.	3.1	61
16	Ïƒ-Bond Activation of Small Molecules and Reactions Catalyzed by Transition-Metal Complexes: Theoretical Understanding of Electronic Processes. Inorganic Chemistry, 2014, 53, 6444-6457.	4.0	60
17	Density Functional Theory Study on the First Hyperpolarizabilities of Organoimido Derivatives of Hexamolybdates. Journal of Physical Chemistry B, 2005, 109, 22332-22336.	2.6	59
18	Reasons Two Nonstrained Câ€“C Ïƒ-Bonds Can Be Easily Cleaved in Decyanative [4 + 2] Cycloaddition Catalyzed by Nickel(0)/Lewis Acid Systems. Theoretical Insight. ACS Catalysis, 2015, 5, 1-10.	11.2	55

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19	Electronic Properties and Stability of DititaniumIV Substituted Î±-Keggin Polyoxotungstate with Heteroatom Phosphorus by DFT. Inorganic Chemistry, 2005, 44, 100-107.	4.0	53
20	Two-State Reactivity Mechanism of Benzene Câ€“C Activation by Trinuclear Titanium Hydride. Journal of the American Chemical Society, 2016, 138, 11069-11072.	13.7	50
21	Ambient-Light-Promoted Three-Component Annulation: Synthesis of Perfluoroalkylated Pyrimidines. Organic Letters, 2017, 19, 2358-2361.	4.6	49
22	Theoretical investigation of structural and electronic propertyies of [PW12O40]3â^' on graphene layer. Dalton Transactions, 2012, 41, 4602.	3.3	48
23	Reversible Redox-Switchable Second-Order Optical Nonlinearity in Polyoxometalate: A Quantum Chemical Study of [PW₁₁O₃₉(ReN)]^{nâ^'} (n = 3â^'7). Inorganic Chemistry, 2008, 47, 5245-5252.	4.0	47
24	Second-Order Nonlinear Optical Properties of Trisubstituted Keggin and Wellsâ^'Dawson Polyoxometalates: Density Functional Theory Investigation of the Inorganic Donor-Conjugated Bridgeâ^'Acceptor Structure. Inorganic Chemistry, 2009, 48, 8115-8119.	4.0	46
25	Prediction of second-order optical nonlinearity of porphyrinâ€“metalâ€“polyoxometalate sandwich compounds. Dalton Transactions, 2010, 39, 7645.	3.3	46
26	How Does Iridium(III) Photocatalyst Regulate Nickel(II) Catalyst in Metallaphotoredox-Catalyzed Câ€“S Cross-Coupling? Theoretical and Experimental Insights. ACS Catalysis, 2019, 9, 3858-3865.	11.2	45
27	Prediction of Second-Order Optical Nonlinearity of Trisorganotin-Substituted Î²-Keggin Polyoxotungstate. Inorganic Chemistry, 2006, 45, 7864-7868.	4.0	44
28	DFT/TD-DFT Study on the Electronic Structures and Optoelectronic Properties of Several Blue-Emitting Iridium(III) Complexes. Journal of Physical Chemistry A, 2010, 114, 6559-6564.	2.5	44
29	Anion-specific aggregation induced phosphorescence emission (AIPE) in an ionic iridium complex in aqueous media. Chemical Communications, 2015, 51, 16924-16927.	4.1	43
30	Cooperative Catalysis of Combined Systems of Transitionâ€Metal Complexes with Lewis Acids: Theoretical Understanding. Chemical Record, 2016, 16, 2405-2425.	5.8	42
31	Quantum Chemical Studies on High-Valent Metal Nitrido Derivatives of Keggin-Type Polyoxometalates ([PW11O39{MVIN}]4â^' (M = Ru, Os, Re)): MVIâ^'N Bonding and Electronic Structures. Inorganic Chemistry, 2009, 48, 541-548.	4.0	40
32	Why Does Disubstituted Hexamolybdate with Arylimido Prefer to Form an Orthogonal Derivative? Analysis of Stability, Bonding Character, and Electronic Properties on Molybdate Derivatives by Density Functional Theory (DFT) Study. Journal of Physical Chemistry B, 2004, 108, 17337-17343.	2.6	38
33	Inorganicâ€“organic hybrid compounds based on the co-existence of different isomers or forms of polymolybdate. CrystEngComm, 2010, 12, 3684.	2.6	38
34	Atomic Nb Anchoring on Graphdiyne as a New Potential Electrocatalyst for Nitrogen Fixation: A Computational View. Advanced Theory and Simulations, 2019, 2, 1900132.	2.8	38
35	Ir^{III}/Ni^{II}-Metallaphotoredox catalysis: the oxidation state modulation mechanism versus the radical mechanism. Chemical Communications, 2018, 54, 5968-5971.	4.1	36
36	Tuning Second-Order Non-linear (NLO) Optical Response of Organoimido-Substituted Hexamolybdates through Halogens: Quantum Design of Novel Organic-Inorganic Hybrid NLO Materials. Australian Journal of Chemistry, 2010, 63, 836.	0.9	35

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37	Crystalline Ni3C as both carbon source and catalyst for graphene nucleation: a QM/MD study. Scientific Reports, 2015, 5, 12091.	3.3	35
38	On the Origin of the Relative Stability of Wellsâ€“Dawson Isomers: A DFT Study of Î±-, Î²-, Î³-, Î±*-, Î²*-, and Î³*-[(PO₄)₂W₁₈O₅₄]^{6â€“}Anions. Inorganic Chemistry, 2011, 50, 4967-4977.	4.0	34
39	How Do the Different Defect Structures and Element Substitutions Affect the Nonlinear Optical Properties of Lacunary Keggin Polyoxometalates? A DFT Study. European Journal of Inorganic Chemistry, 2006, 2006, 4179-4183.	2.0	33
40	A Wellâ€Established POMâ€based Singleâ€Crystal Protonâ€Conducting Model Incorporating Multiple Weak Interactions. Chemistry - A European Journal, 2018, 24, 2365-2369.	3.3	32
41	Theoretical studies on POM-based organicâ€“inorganic hybrids containing double Dâ€“A1â€“Ïâ€“A2 chains for high-performance p-type, dye-sensitized solar cells (DSSCs). Physical Chemistry Chemical Physics, 2015, 17, 5459-5465.	2.8	31
42	Studies on the interactions of Ti-containing polyoxometalates (POMs) with SARS-CoV 3CLpro by molecular modeling. Journal of Inorganic Biochemistry, 2007, 101, 89-94.	3.5	30
43	Prediction of robustly large molecular second-order nonlinear optical properties of terpyridine-substituted hexamolybdates: Structural modelling towards a rational entry to NLO materials. Journal of Molecular Graphics and Modelling, 2010, 28, 735-745.	2.4	30
44	DFT characterization on the mechanism of water splitting catalyzed by single-Ru-substituted polyoxometalates. Dalton Transactions, 2013, 42, 10617.	3.3	30
45	Photocatalytic Cross-Couplings of Aryl Halides Enabled by o-Phosphinophenolate and o-Phosphinothiophenolate. ACS Catalysis, 2022, 12, 2788-2795.	11.2	29
46	Copper-Catalyzed Asymmetric Hydroamination: A Unified Strategy for the Synthesis of Chiral Î²-Amino Acid and Its Derivatives. CCS Chemistry, 2021, 3, 1737-1745.	7.8	28
47	Theoretical investigation on electronic structure and second-order nonlinear optical properties of novel hexamolybdate-organoimido-(car)borane hybrid. Physical Chemistry Chemical Physics, 2012, 14, 5605.	2.8	27
48	Theoretical insights into [PMo12O40]3â^' grafted on single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 9177.	2.8	27
49	A theoretical design and investigation on Zn-porphyrin-polyoxometalate hybrids with different Ïâ€linkers for searching high performance sensitizers of p-type dye-sensitized solar cells. Dyes and Pigments, 2016, 130, 168-175.	3.7	27
50	Quantum Chemical Design for Enhanced Secondâ€Order NLO Response of Terpyridineâ€Substituted Hexamolybdates. European Journal of Inorganic Chemistry, 2010, 2010, 3466-3472.	2.0	26
51	Prediction of second-order nonlinear optical properties of Wellsâ€“Dawson polyoxometalate derivatives [Xâ€“C(CH₂O)₃P₂Mâ€²₃M₁₅O₅₉]^{6â^'}(X Chemistry Frontiers, 2014, 1, 65-70.	6.1	26
52	An unusual three-dimensional self-penetrating network derived from cross-linking of two-fold interpenetrating nets via ligand-unsupported Agâ€“Ag bonds: synthesis, structure, luminescence, and theoretical study. New Journal of Chemistry, 2012, 36, 877.	2.8	25
53	Density functional study of protonation sites of Î±-Keggin isopolyanions. International Journal of Quantum Chemistry, 2006, 106, 1860-1864.	2.0	24
54	Theoretical Mechanistic Study of Novel Ni(0)-Catalyzed [6 â€“ 2 + 2] Cycloaddition Reactions of Isatoic Anhydrides with Alkynes: Origin of Facile Decarboxylation. Organometallics, 2013, 32, 7564-7574.	2.3	24

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55	Photocatalytic C(sp³)â€“O/N Cross-Couplings by Naâ€“PPh₃/CuBr Cooperative Catalysis: Computational Design and Experimental Verification. ACS Catalysis, 2021, 11, 6633-6642.	11.2	24
56	Theoretical Studies on Metalloporphyrinâ€“Polyoxometalates Hybrid Complexes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2014, 118, 29623-29628.	3.1	23
57	Monodisperse and Tiny Co₂N_{0.67} Nanocrystals Uniformly Embedded over Two Curving Surfaces of Hollow Carbon Microfibers as Efficient Electrocatalyst for Oxygen Evolution Reaction. ACS Applied Nano Materials, 2018, 1, 4461-4473.	5.0	23
58	An Nâ€Trifluoromethylation/Cyclization Strategy for Accessing Diverse Nâ€Trifluoromethyl Azoles from Nitriles and 1,3â€Dipoles. Angewandte Chemie - International Edition, 2022, 61, .	13.8	23
59	A DFT Study on the Electronic and Redox Properties of [PW11O39(ReN)]nâ€“(n = 3, 4, 5) and [PW11O39(OsN)]2â€“. European Journal of Inorganic Chemistry, 2006, 2006, 5126-5129.	2.0	22
60	Theoretical Study on a Novel Series of Fullerene-Containing Organometallics Fe(Î·5-C55X5)2 (X = CH, N,) Tj ETQq0 0 0 rgBT /Overlock 10 8086-8092.	2.5	22
61	Three Competitive Transition States at the Glycosidic Bond of Sucrose in Its Acid-Catalyzed Hydrolysis. Journal of Organic Chemistry, 2013, 78, 2527-2533.	3.2	20
62	A Quantum Mechanical Study of the Second-Order Nonlinear Optical Properties of Aryldiazenido-Substituted Hexamolybdates: A Surprising Charge Transfer. European Journal of Inorganic Chemistry, 2009, 2009, 5181-5188.	2.0	19
63	Quantum chemical study of redox-switchable second-order optical nonlinearity in Keggin-type organoimido derivative [PW11O39(ReNC6H5)] nâ^' (nÂ=Â2â€“4). Theoretical Chemistry Accounts, 2009, 122, 265-273.	1.4	19
64	Theoretical studies on nitrido ruthenium (VI) porphyrin and high valent ruthenium nitrido derivatives of Keggin typical polyoxometalate ([PW11O39{RuVIN}]4â^'): electronic structures and bonding features. Dalton Transactions, 2009, , 6208.	3.3	19
65	A DFT study on the electronic and redox properties of [X₈V₁₄O₅₀]^{nâ€“} (X = Si^{IV},) Tj ETQq1 1 0.784314 rgBT /Overlock 434-442.	1.1	18
66	Quantum chemical characterization of the generation of high-valent oxoruthenium species of Keggin type polyoxometalates: electronic structure and bonding features. Dalton Transactions, 2011, 40, 2967.	3.3	17
67	Bonding Interactions between Nitrous Oxide (N₂O) and Monoâ€Ruthenium Substituted Kegginâ€Type Polyoxometalates: Electronic Structures of Ruthenium/N₂O Adducts. European Journal of Inorganic Chemistry, 2011, 2011, 489-494.	2.0	17
68	Insight into a class of cobalt nitrides for oxygen evolution catalysis: Nitrogen-rich matters. Electrochimica Acta, 2019, 323, 134684.	5.2	17
69	Theoretical mechanistic study of metallaphotoredox catalysis: Câ€“N cross-coupling via Ni(<scp>ii</scp>)-mediated if-bond metathesis. Organic Chemistry Frontiers, 2020, 7, 2168-2178.	4.5	17
70	DFT/TDDFT Study on the electronic structures and optoelectronic properties of several red-emitting osmium(ii) complexes with different Pâ^§P ancillary ligands. Dalton Transactions, 2011, 40, 11131.	3.3	15
71	The self-assembly mechanism of the Lindqvist anion [W6O19]2â^' in aqueous solution: a density functional theory study. Dalton Transactions, 2012, 41, 11361.	3.3	15
72	Theoretical studies on the photoisomerization-switchable second-order nonlinear optical responses of DTE-linked polyoxometalate derivatives. Journal of Molecular Graphics and Modelling, 2013, 40, 110-115.	2.4	15

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73	Orthogonal reactivity of Ni(<scp>i</scp>)/Pd(0) dual catalysts for Ullmann Câ€“C cross-coupling: theoretical insight. Chemical Communications, 2018, 54, 7959-7962.	4.1	15
74	On the Origin of the Inverted Stability Order of the Reverse-Keggin [(MnO₄)(CH₃)₁₂Sb₁₂O₂₄]^{6â^'}: A DFT Study of Î±, Î², Î³, Î´, and Îµ Isomers. Inorganic Chemistry, 2010, 49, 5472-5481.	4.0	14
75	Theoretical study on the tetranuclear endohedral vanadyl carboxylates with guest-switchable redox properties and large polarizability. Dalton Transactions, 2010, 39, 3706.	3.3	14
76	S_N1â€“S_N2 and S_N2â€“S_N3 mechanistic changes revealed by transition states of the hydrolyses of benzyl chlorides and benzenesulfonyl chlorides. Journal of Computational Chemistry, 2014, 35, 1140-1148.	3.3	14
77	Theoretical screening of promising donor and Ï€-linker groups for POM-based Znâ€“porphyrin dyes in dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2019, 21, 3822-3831.	2.8	14
78	Evidence of two-state reactivity in water oxidation catalyzed by polyoxometalate-based complex [Mn3(H2O)3(SbW9O33)2]12â^'. Journal of Catalysis, 2019, 376, 146-149.	6.2	13
79	A theoretical study on the efficient reversible redox-based switching of the second-order polarizabilities of two-dimensional nonlinear optical-active donorâ€“acceptor phenanthroline-hexamolybdate. Journal of Molecular Graphics and Modelling, 2010, 29, 13-20.	2.4	12
80	Quantum chemical studies of Lindqvist-type polyoxometalates containing late 3d transition metals ([(py)MIIW5O18]4â^' (MÂ=ÂFe, Co, Ni)): MIIâ€“N bonding and second-order nonlinear optical properties. Theoretical Chemistry Accounts, 2011, 130, 1043-1053.	1.4	12
81	The structureâ€“property relationship of chiral 1,1â€²-binaphthyl-based polyoxometalates: TDDFT studies on the static first hyperpolarizabilities and the ECD spectra. Journal of Molecular Graphics and Modelling, 2012, 32, 1-8.	2.4	12
82	TDDFT studies on the structures and ECD spectra of chiral bisarylimidos bearing different lengths of o-alkoxy chain-substituted polyoxomolybdates. Journal of Molecular Graphics and Modelling, 2012, 35, 49-56.	2.4	12
83	Interest in new heterodinuclear transition-metal/main-group-metal complexes: DFT study of electronic structure and mechanism of fluoride sensing function. Dalton Transactions, 2013, 42, 8717.	3.3	12
84	Theoretical Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Polyfluoroarylcyanation of Alkynes: Origin of Selectivity for Câ€“CN Bond Activation. Organometallics, 2018, 37, 2594-2601.	2.3	12
85	Tricopper-polyoxometalate catalysts for water oxidation: Redox-inertness of copper center. Journal of Catalysis, 2020, 381, 402-407.	6.2	12
86	Organoborohydride-catalyzed Chichibabin-type C4-position alkylation of pyridines with alkenes assisted by organoboranes. Chemical Science, 2020, 11, 11554-11561.	7.4	12
87	TDDFT studies on chiral organophosphonate substituted divacant Keggin-type polyoxotungstate: diplex multistep-redox-triggered chiroptical and NLO switch. Dalton Transactions, 2012, 41, 10097.	3.3	11
88	DFT study of ionic peapod structures from single-walled carbon nanotubes and Lindqvist tungstates. Dalton Transactions, 2012, 41, 2798.	3.3	11
89	An aniline dication-like transition state in the Bamberger rearrangement. Beilstein Journal of Organic Chemistry, 2013, 9, 1073-1082.	2.2	11
90	Substrate dependent reaction channels of the Wolffâ€“Kishner reduction reaction: A theoretical study. Beilstein Journal of Organic Chemistry, 2014, 10, 259-270.	2.2	11

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91	Synergistic Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Cyanoesterification: Effect of Lewis Acid. Organometallics, 2017, 36, 4713-4720.	2.3	11
92	The Effect of Dyes with Different Ï€-Linkers on the Overall Performance of P-DSSCs: Lessons from Theory. Journal of Physical Chemistry A, 2018, 122, 7491-7496.	2.5	11
93	A theoretical investigation on promising acceptor groups for POM-based dyes: from electronic structure to photovoltaic conversion efficiency. Journal of Materials Chemistry C, 2020, 8, 219-227.	5.5	11
94	Radical Mechanism of Ir III /Ni II -Metallaphotoredox-Catalyzed C(sp 3)â€“H Functionalization Triggered by Proton-Coupled Electron Transfer: Theoretical Insight. CCS Chemistry, 0, , 1456-1467.	7.8	11
95	Ruthenium-based catalysts for water oxidation: the key role of carboxyl groups as proton acceptors. Physical Chemistry Chemical Physics, 2020, 22, 5249-5254.	2.8	11
96	Aza-tricycles containing a perfluoroalkyl group: synthesis, structure and fluorescence. Organic and Biomolecular Chemistry, 2018, 16, 8950-8954.	2.8	10
97	A theoretical mechanistic study of Ir^{III}/Cu^I-metallaphotoredox catalyzed asymmetric radical decarboxylative cyanation. Dalton Transactions, 2020, 49, 15276-15286.	3.3	10
98	Role of Terminal Positions of Aryl Ring Towards Second-Order Nonlinearity in Arylimido-Substituted Molybdates: An Interesting Quantum Study of Organic-Inorganic Hybrid Composites. Current Physical Chemistry, 2011, 1, 99-105.	0.2	10
99	Origin and Regioselectivity of Direct Hydrogen Atom Transfer Mechanism of C(sp3)â€“H Arylation by [W10O32]4â€“/Ni Metallaphotoredox Catalysis. Inorganic Chemistry, 2021, , .	4.0	10
100	The comparative investigation on redox property and second-order nonlinear response of Keggin-type Î±-[PM12O39NPh]3â^' (M = W and Mo) and Mo6NPh. Science Bulletin, 2009, 54, 203-211.	9.0	8
101	Length-Dependent Direction-Tunable Charge-Transfer Behavior of Second-Order Optical Nonlinearity in Keggin-Type Organosilicone Derivative [PW11O39(RSi)2O]3â^': A TDDFT Study. Journal of Cluster Science, 2010, 21, 69-80.	3.3	8
102	First principle investigation of transport properties of Lindqvist derivatives based molecular junction. Journal of Molecular Graphics and Modelling, 2012, 38, 220-225.	2.4	8
103	A water cluster (H2O)12 guested coordination polymer as proton conducting solid electrolytes. Solid State Ionics, 2018, 321, 43-47.	2.7	8
104	Building blocks and formation thermodynamics of Î±-Keggin-type [PW12O40]3â^' anion. Computational and Theoretical Chemistry, 2012, 999, 66-73.	2.5	7
105	Theoretical studies on tricarbonyl metal derivatives of Lindqvist-type polyoxometalate complexes: electronic structures and nonlinear optical properties. Inorganic Chemistry Frontiers, 2015, 2, 544-549.	6.0	7
106	Photo- and dioxygen-enabled radical C(sp³)â€“N(sp²) cross-coupling between guanidines and perfluoroalkyl iodides. Organic and Biomolecular Chemistry, 2019, 17, 8695-8700.	2.8	7
107	How do transition-metal-substituted POMs modify the photoanode of dye-sensitized solar cells? A DFT study. Inorganic Chemistry Frontiers, 2019, 6, 969-974.	6.0	7
108	Springboard Role for Iridium Photocatalyst: Theoretical Insight of C(sp³)â^'N Crossâ€Coupling by Photoredoxâ€Mediated Iridium/Copper Dual Catalysis versus Singleâ€Copper Catalysis. ChemCatChem, 2022, 14, .	3.7	7

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109	Density functional study of magnetic exchange of dinuclear manganese complexes with the heteropolymolyanion: [MnII 2(X n+Mo9O33)2]2(nâˆ'10)âˆ' (X = PV, AsV, SeVI). Science in China Series B: Chemistry, 2008, 51, 1174-1181.	0.8	6
110	An Nâ€Trifluoromethylation/Cyclization Strategy for Accessing Diverse Nâ€Trifluoromethyl Azoles from Nitriles and 1,3â€Dipoles. Angewandte Chemie, 0, , .	2.0	6
111	Presence or absence of a novel charge-transfer complex in the base-catalyzed hydrolysis of N-ethylbenzamide or ethyl benzoate. Beilstein Journal of Organic Chemistry, 2013, 9, 185-196.	2.2	5
112	Proton transfers in the Strecker reaction revealed by DFT calculations. Beilstein Journal of Organic Chemistry, 2014, 10, 1765-1774.	2.2	5
113	A DFT study on proton transfers in hydrolysis reactions of phosphate dianion and sulfate monoanion. Journal of Computational Chemistry, 2014, 35, 2195-2204.	3.3	5
114	Theoretical mechanistic study of 4CzIPN/Ni0-metallaphotoredox catalyzed enantioselective desymmetrization of cyclic meso-anhydrides. Dalton Transactions, 2021, 50, 17675-17687.	3.3	5
115	DFT characterization on the mechanism of sulfoxidation with H2O2catalyzed by tetranuclear peroxotungstates [XO4{WO(O2)2}4]nâˆ'(X = SiIV, PV, SVI, AsV, and SeVI). Dalton Transactions, 2015, 44, 9063-9070.	3.3	4
116	Nanographeneâˆ'rhenium complex as efficient catalyst for electrochemical reduction: A computational study. Molecular Catalysis, 2020, 484, 110736.	2.0	4
117	Ultrafast Absorption of Polysulfides through Electrostatic Confinement by Protonated Molecules for Highly Efficient Liâ€"S Batteries. ACS Applied Materials & Interfaces, 2020, 12, 36220-36227.	8.0	4
118	Electronic Properties and Stability of DititaniumIV Substituted ?-Keggin Polyoxotungstate with Heteroatom Phosphorus by DFT. ChemInform, 2005, 36, no.	0.0	3
119	Theoretical investigation of electronic properties and redox properties for purely inorganic and aryloxide substituted Ti-containing POM derivatives. Molecular Physics, 2010, 108, 1553-1560.	1.7	3
120	DFT studies on the electronic properties of organometallic-polyoxomolybdate anions [<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>Cp</mml:mtext></mml:mrow><mml:mrow><mml:mi>n</mml:mi></mr (n= 1 or 2): Revealing bonding features of Cpâˆ—â€"Mo. Computational and Theoretical Chemistry, 2011, 976, 1-7.	2.0	3
121	Unveiling the relative stability and proton binding of non-classical Wellsâ€"Dawson isomers of [(NaF6)W18O54(OH)2]7âˆ' and [(SbO6)W18O54(OH)2]9âˆ': a DFT study. Dalton Transactions, 2017, 46, 16145-16158.	3.3	3
122	Configuration effect in polyoxometalate-based dyes on the performance of DSSCs: an insight from a theoretical perspective. Physical Chemistry Chemical Physics, 2020, 22, 16032-16039.	2.8	3
123	Superiority of Iridium Photocatalyst and Role of Quinuclidine in Selective Î±-C(sp³)â€"H Alkylation: Theoretical Insights. Journal of Organic Chemistry, 2021, 86, 484-492.	3.2	3
124	Theoretical insight into decatungstate photocatalyzed alkylation of N-tosylimine via hydrogen atom transfer and proton-coupled electron transfer. Dalton Transactions, 2022, , .	3.3	3
125	Ir^{III}/Ni^{II}-Metallaphotoredox-Catalyzed Enantioselective Decarboxylative Arylation of Î±-Amino Acids: Theoretical Insight of Enantio-Determining Outer-Sphere Reductive Elimination. Inorganic Chemistry, 0, , .	4.0	3
126	Reassembly and functionalization ofN-CF₃pyridinium salts: synthesis of nicotinaldehydes. Organic Chemistry Frontiers, 2022, 9, 4549-4553.	4.5	3

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127	Theoretical study of the impact factor on redox property and second-order nonlinear response for organoimido derivatives of [Mo6O19]2â^': Electron donors with magnitude of conjugated groups or length of conjugated chain. Computational and Theoretical Chemistry, 2010, 947, 9-15.	1.5	2
128	Theoretical investigation of second-order nonlinear optical responseâ€‰â€”â€‰Hexamolybdate as a superior donor over metal carbonyl complexes in the Dâ€“Ï€â€“A model. Canadian Journal of Chemistry, 2011, 89, 61-67.	1.1	2
129	Electronic properties and stabilities of methoxy-substituted Lindqvist polyoxometalates [Nb2W4O19CH3]3â^' by DFT. Science Bulletin, 2012, 57, 976-982.	1.7	2
130	Theoretical exploration to the cation effect on the second-order nonlinear optical properties of Strandberg-type polyoxometalates. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550007.	1.8	2
131	Theoretical investigation of the influence of different electric field directions and strengths on a POM-based dye for dye-sensitized solar cells. Materials Chemistry Frontiers, 2021, 5, 929-936.	5.9	2
132	Theoretical mechanistic study of nickelâ€catalyzed antiâ€Markovnikov hydroarylation of alkenes. International Journal of Quantum Chemistry, 2021, 121, e26621.	2.0	2
133	Theoretical study of Ni^Iâ€“Ni^{III} cycle mediated by heterogeneous zinc in Câ€“N cross-coupling reaction. Physical Chemistry Chemical Physics, 2022, 24, 7617-7623.	2.8	2
134	Aspects of the Nonlinear Optical Properties as a Guide to Protonation Sites: A Theoretical Study upon Î±-Keggin [SiW12O40]4â^' and [SiV3W9O40]7â^'. Chemistry Letters, 2010, 39, 580-581.	1.3	1
135	How is the anionic tetrahedral intermediate involved in the isomerization of aspartyl peptides to iso-aspartyl ones? A DFT study on the tetra-peptide. Organic and Biomolecular Chemistry, 2012, 10, 8007.	2.8	1
136	Theoretical design of organic-inorganic hybrids based on hexamolybdate toward high performance dye-sensitized solar cells. Molecular Simulation, 2016, 42, 688-692.	2.0	1
137	POM-based dyes featuring rigidified bithiophene Ï€ linkers: potential high-efficiency dyes for dye-sensitized solar cells. New Journal of Chemistry, 2020, 44, 8996-9003.	2.8	0