

Li-Li Zhao

List of Publications by Year in descending order

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108
papers

3,694
citations

126708

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h-index

149479

56
g-index

117
all docs

117
docs citations

117
times ranked

2275
citing authors

#	ARTICLE	IF	CITATIONS
1	Energy decomposition analysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1345.	6.2	369
2	Chemical Bonding and Bonding Models of Main-Group Compounds. Chemical Reviews, 2019, 119, 8781-8845.	23.0	232
3	Observation of alkaline earth complexes $M(\text{CO})_8$ ($M = \text{Ca}, \text{Sr}, \text{or Ba}$) that mimic transition metals. Science, 2018, 361, 912-916.	6.0	207
4	The Lewis electron-pair bonding model: modern energy decomposition analysis. Nature Reviews Chemistry, 2019, 3, 48-63.	13.8	197
5	Dative bonding in main group compounds. Coordination Chemistry Reviews, 2017, 344, 163-204.	9.5	174
6	Dinitrogen complexation and reduction at low-valent calcium. Science, 2021, 371, 1125-1128.	6.0	131
7	Transition-Metal Chemistry of Alkaline-Earth Elements: The Trisbenzene Complexes $M(\text{Bz})_3$ ($M = \text{Sr}, \text{Ba}$). Angewandte Chemie - International Edition, 2019, 58, 17365-17374.	7.2	82
8	Octa-coordinated alkaline earth metal dinitrogen complexes $M(\text{N}_2)_8$ ($M = \text{Ca}, \text{Sr}, \text{Ba}$). Nature Communications, 2019, 10, 3375.	5.8	79
9	Aromaticity, the Hückel 4n+2 Rule and Magnetic Current. ChemistrySelect, 2017, 2, 863-870.	0.7	66
10	NHC-Stabilised Acetylene: How Far Can the Analogy Be Pushed?. Chemistry - A European Journal, 2017, 23, 2926-2934.	1.7	65
11	Direct C(sp ²) Arylsulfonylation of Enamides via Iridium(III)-Catalyzed Insertion of Sulfur Dioxide with Aryldiazonium Tetrafluoroborates. Advanced Synthesis and Catalysis, 2019, 361, 3593-3598.	2.1	64
12	Double dative bond between divalent carbon(0) and uranium. Nature Communications, 2018, 9, 4997.	5.8	63
13	Alkali Metal Covalent Bonding in Nickel Carbonyl Complexes $\text{ENi}(\text{CO})_3^+$. Angewandte Chemie - International Edition, 2019, 58, 1732-1738.	7.2	62
14	Unusually Short Be-Be Distances with and without a Bond in Be_2F_2 and in the Molecular Discs Be_2B_8 and Be_2B_7^+ . Angewandte Chemie - International Edition, 2016, 55, 7841-7846.	7.2	60
15	Barium as Honorary Transition Metal in Action: Experimental and Theoretical Study of $\text{Ba}(\text{CO})^+$ and $\text{Ba}(\text{CO})^+$. Angewandte Chemie - International Edition, 2018, 57, 3974-3980.	7.2	60
16	Carbodicarbenes: Unexpected π -Accepting Ability during Reactivity with Small Molecules. Journal of the American Chemical Society, 2017, 139, 12830-12836.	6.6	57
17	Response to Comment on "Observation of alkaline earth complexes $M(\text{CO})_8$ ($M = \text{Ca}, \text{Sr}$)". Tj ETQq1.1 0.784314 rgBT / 6.0 54	6.0	54
18	Alkali Metal Covalent Bonding in Nickel Carbonyl Complexes $\text{ENi}(\text{CO})_3^+$. Angewandte Chemie, 2019, 131, 1746-1752.	1.6	53

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19	The Lewis electron-pair bonding model: the physical background, one century later. <i>Nature Reviews Chemistry</i> , 2019, 3, 35-47.	13.8	52
20	Side-On Bonded Beryllium Dinitrogen Complexes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 10603-10609.	7.2	51
21	Bonding in Binuclear Carbonyl Complexes $M_2(CO)_9$ (M = Fe, Ru, Os). <i>Inorganic Chemistry</i> , 2018, 57, 7780-7791.	1.9	50
22	A Very Short Be-Be Distance but No Bond: Synthesis and Bonding Analysis of $Ng_2Be_2O_2Ng_2$ (Ng, $Ng_2 = Ne, Ar, Kr, Xe$). <i>Chemistry - A European Journal</i> , 2017, 23, 2035-2039.	7.23	46
23	Computational design of metal-free catalysts for catalytic hydrogenation of imines. <i>Dalton Transactions</i> , 2010, 39, 4038.	1.6	45
24	Reaction Mechanism of Phosphane-Catalyzed [4+2] Annulations between \pm -Alkylallenoates and Activated Alkenes: A Computational Study. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 3587-3597.	1.2	45
25	Carbones and Carbon Atom as Ligands in Transition Metal Complexes. <i>Molecules</i> , 2020, 25, 4943.	1.7	43
26	Coinage metal aluminyl complexes: probing regiochemistry and mechanism in the insertion and reduction of carbon dioxide. <i>Chemical Science</i> , 2021, 12, 13458-13468.	3.7	42
27	Donor-Stabilized Antimony(I) and Bismuth(I) Ions: Heavier Valence Isoelectronic Analogues of Carbones. <i>Journal of the American Chemical Society</i> , 2021, 143, 1301-1306.	6.6	40
28	Parent Thioketene Sulfide H_2CCSO : Gas-Phase Generation, Structure, and Bonding Analysis. <i>Chemistry - A European Journal</i> , 2017, 23, 16566-16573.	1.7	39
29	Encumbering the intramolecular π donation by using a bridge: A strategy for designing metal-free compounds to hydrogen activation. <i>Science Bulletin</i> , 2010, 55, 239-245.	1.7	38
30	Octacarbonyl Ion Complexes of Actinides $[An(CO)_8]^{+}$ (An=Th, U) and the Role of f Orbitals in Metal-Ligand Bonding. <i>Chemistry - A European Journal</i> , 2019, 25, 11772-11784.	1.7	38
31	Octacarbonyl Anion Complexes of the Late Lanthanides $Ln(CO)_8^{-}$ (Ln=Tm, Yb). <i>TJ ETQq</i> 1.1 0.784314 rgBT 1.7 38	1.7	38
32	Nickel-Catalyzed Heteroarenes Cross Coupling via Tandem C-H/C-O Activation. <i>ACS Catalysis</i> , 2018, 8, 11368-11376.	5.5	37
33	Reversible Heterolytic Methane Activation of Metal-Free Closed-Shell Molecules: A Computational Proof-of-Principle Study. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 2254-2260.	1.0	35
34	Computational Mechanistic Study of PMe_3 and <i>N</i> -Heterocyclic Carbene Catalyzed Intramolecular Morita-Baylis-Hillman-Like Cycloalkylations: The Origins of the Different Reactivity. <i>Journal of Organic Chemistry</i> , 2011, 76, 2733-2743.	1.7	34
35	Electronic Structure and Bonding Situation in M_2O_2 (M = Be, Mg, Ca) Rhombic Clusters. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2816-2822.	1.1	34
36	Visible-Light-Induced Regio- and Stereoselective $C(sp^2)$ -H Trifluoroethylation of Enamides with 2,2,2-Trifluoroethyl Iodide. <i>Organic Letters</i> , 2020, 22, 9029-9035.	2.4	34

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37	Cyanide \leftrightarrow isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides (metal =) Tj ETQq1 1.0.784314 rgBT / Overloc	1.3	32
38	Beryllium Atom Mediated Dinitrogen Activation via Coupling with Carbon Monoxide. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 18201-18207.	7.2	29
39	The strength of a chemical bond. <i>International Journal of Quantum Chemistry</i> , 2022, 122, e26773.	1.0	29
40	A C(sp ²) δ^{\sim} H Dehydrogenation of Heteroarenes and Arenes by a Functionalized Aluminum Hydride. <i>Chemistry - A European Journal</i> , 2017, 23, 13633-13637.	1.7	28
41	Transition \rightarrow Metal Chemistry of Alkaline \rightarrow Earth Elements: The Trisbenzene Complexes M(Bz) ₃ (M= Sr, Ba). <i>Angewandte Chemie</i> , 2019, 131, 17526-17535.	1.6	28
42	Palladium-Catalyzed Hydroxycarbonylation of Pentenoic Acids. Computational and Experimental Studies on the Catalytic Selectivity. <i>ACS Catalysis</i> , 2017, 7, 7070-7080.	5.5	27
43	Isolation of Transient Acyclic Germanium(I) Radicals Stabilized by Cyclic Alkyl(amino) Carbenes. <i>Journal of the American Chemical Society</i> , 2019, 141, 1908-1912.	6.6	27
44	Highly responsive ethylenediamine vapor sensor based on a perylenediimide \leftrightarrow camphorsulfonic acid complex via ionic self-assembly. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7644-7651.	2.7	26
45	Computational Insights into the Catalytic Mechanism of Bacterial Carboxylic Acid Reductase. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 832-841.	2.5	26
46	Metal-free catalysts for hydrogenation of both small and large imines: a computational experiment. <i>Dalton Transactions</i> , 2011, 40, 1929.	1.6	25
47	A diradical based on odd-electron σ -bonds. <i>Nature Communications</i> , 2020, 11, 3441.	5.8	22
48	A Strained Ion Pair Permits Carbon Dioxide Fixation at Atmospheric Pressure by C \leftrightarrow H H-Bonding Organocatalysis. <i>Journal of Organic Chemistry</i> , 2021, 86, 3422-3432.	1.7	22
49	Invisible Chelating Effect Exhibited between Carbodicarbene and Phosphine through σ - π Interaction and Implication in the Cross-Coupling Reaction. <i>Organometallics</i> , 2017, 36, 4287-4297.	1.1	21
50	Filling a Gap: The Coordinatively Saturated Group \rightarrow 4 Carbonyl Complexes TM(CO) ₈ (TM=Zr,) Tj ETQq0 0 0 rgBT / Overloc	1.7	21
51	Isolable cyclic radical cations of heavy main-group elements. <i>Chemical Communications</i> , 2020, 56, 2167-2170.	2.2	21
52	Cerium \leftrightarrow carbon dative interactions supported by carbodiphosphorane. <i>Dalton Transactions</i> , 2019, 48, 16108-16114.	1.6	20
53	Double donation in trigonal planar iron \leftrightarrow carbodiphosphorane complexes \leftrightarrow a concise study on their spectroscopic and electronic properties. <i>Dalton Transactions</i> , 2020, 49, 2537-2546.	1.6	20
54	CO \leftrightarrow Induced Dinitrogen Fixation and Cleavage Mediated by Boron. <i>Chemistry - A European Journal</i> , 2021, 27, 2131-2137.	1.7	20

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55	A computational experiment to study hydrogenations of various unsaturated compounds catalyzed by a rationally designed metal-free catalyst. <i>Dalton Transactions</i> , 2012, 41, 4674.	1.6	19
56	Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound $M@B_{10}^+$ Clusters (M=Nb, Ta). <i>Chemistry - A European Journal</i> , 2018, 24, 3590-3598.	1.7	19
57	$CaCl_2$ molten salt hydrate-promoted conversion of carbohydrates to 5-hydroxymethylfurfural: an experimental and theoretical study. <i>Green Chemistry</i> , 2021, 23, 2058-2068.	4.6	19
58	Heterobimetallic Complexes Featuring $Fe(CO)_5$ as a Ligand on Gold. <i>Chemistry - A European Journal</i> , 2017, 23, 17222-17226.	1.7	18
59	Highly Coordinated Heteronuclear Calcium-Iron Carbonyl Cation Complexes $[CaFe(CO)_n]^+$ ($n=5-12$) with d Bonding. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13865-13870.	7.2	18
60	Synergistic Catalysis by Brønsted Acid/Carbodicarbene Mimicking Frustrated Lewis Pair-Like Reactivity. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 19949-19956.	7.2	18
61	Barium as Honorary Transition Metal in Action: Experimental and Theoretical Study of $Ba(CO)_+$ and $Ba(CO)^+$. <i>Angewandte Chemie</i> , 2018, 130, 4038-4044.	1.6	16
62	Metal-free [3+3] benzannulation of 1-indanylidene-malononitrile with Morita-Baylis-Hillman carbonates: direct access to functionalized fluorene and fluorenone derivatives. <i>Chemical Communications</i> , 2020, 56, 1948-1951.	2.2	15
63	Isolable dicarbon stabilized by a single phosphine ligand. <i>Nature Chemistry</i> , 2021, 13, 89-93.	6.6	15
64	The nature of the polar covalent bond. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	15
65	An Experimental and Theoretical Study of the Structures and Properties of $[CDP^+Me^-Ni(CO)_3]$ and $[Ni_2(CO)_4](\mu_2^2-CO)(\mu_2^2-CDP^+Me^-)$. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4546-4554.	1.0	13
66	Synthesis and characterization of heterometallic complexes involving coinage metals and isoelectronic $Fe(CO)_5$, $[Mn(CO)_5]^+$ and $[Fe(CO)_4CN]^+$ ligands. <i>Dalton Transactions</i> , 2020, 49, 8566-8581.	1.6	13
67	Side-On Bonded Beryllium Dinitrogen Complexes. <i>Angewandte Chemie</i> , 2020, 132, 10690-10696.	1.6	13
68	Photomediated core modification of organic photoredox catalysts in radical addition: mechanism and applications. <i>Chemical Science</i> , 2021, 12, 9432-9441.	3.7	13
69	Aluminum alkoxy-catalyzed biomass conversion of glucose to 5-hydroxymethylfurfural: Mechanistic study of the cooperative bifunctional catalysis. <i>Journal of Computational Chemistry</i> , 2019, 40, 1599-1608.	1.5	12
70	Bonding Analysis of the Shortest Bond between Two Atoms Heavier than Hydrogen and Helium: O_2^+ . <i>Journal of Physical Chemistry A</i> , 2020, 124, 1087-1092.	1.1	12
71	Copper-catalyzed regioselective [3+2] annulation of malonate-tethered acyl oximes with isatins. <i>Chemical Communications</i> , 2021, 57, 3379-3382.	2.2	12
72	Dinitrogen Functionalization Affording Structurally Well-Defined Cobalt Diazenido Complexes. <i>CCS Chemistry</i> , 2022, 4, 532-539.	4.6	12

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73	Isolation of a Uranium(III)â€Carbon Multiple Bond Complex. <i>Chemistry - A European Journal</i> , 2021, 27, 10006-10011.	1.7	12
74	An Isolable Mononuclear Palladium(I) Amido Complex. <i>Journal of the American Chemical Society</i> , 2021, 143, 10751-10759.	6.6	11
75	Intriguing structural, bonding and reactivity features in some beryllium containing complexes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27476-27495.	1.3	10
76	Directing Groupâ€Promoted Inert CâˆO Bond Activation Using Versatile Boronic Acid as a Coupling Agent. <i>Chemistry - A European Journal</i> , 2020, 26, 17021-17026.	1.7	10
77	Carbodicarbene: geminal â€Bimetallic Coordination in Selective Manner. <i>Chemistry - A European Journal</i> , 2020, 26, 17350-17355.	1.7	10
78	Covalent Bonding Between Be⁺ and CO₂ in BeOCO⁺ with a Surprisingly High Antisymmetric OCO Stretching Vibration. <i>Journal of the American Chemical Society</i> , 2021, 143, 14300-14305.	6.6	10
79	Synthesis of cAAC stabilized biradical of â€œMe₂Siâ€ and â€œMe₂SiClâ€ monoradical from Me₂SiCl₂ â€“ an important feedstock material. <i>Chemical Communications</i> , 2019, 55, 4534-4537.	2.2	9
80	Complex Featuring Two Double Dative Bonds Between Carbon(0) and Uranium. <i>CCS Chemistry</i> , 2022, 4, 1921-1929.	4.6	9
81	A <i>i>Bis</i>â€(carbene) Pincer Ligand and Its Coordinative Behavior toward Multiâ€Metallic Configurations. <i>Angewandte Chemie - International Edition</i>, 2022, 61, .</i>	7.2	9
82	Generation and Identification of the Linear OCBNO and OBNCO Molecules with 24 Valence Electrons. <i>Chemistry - A European Journal</i> , 2021, 27, 412-418.	1.7	8
83	Carbodiphosphorane-Stabilized Parent Dioxophosphorane: A Valuable Synthetic HO₂P Source. <i>Journal of the American Chemical Society</i> , 2022, 144, 7357-7365.	6.6	7
84	Inverse sandwich complexes of B₇M₂^{âˆ}, B₈M₂, and B₉M₂⁺ (M = Zr, Hf): the nonclassical Mâ€M bonds embedded in monocyclic boron rings. <i>New Journal of Chemistry</i> , 2020, 44, 17705-17713.	1.4	6
85	Synergistic Catalysis by BrÃnsted Acid/Carbodicarbene Mimicking Frustrated Lewis Pairâ€Like Reactivity. <i>Angewandte Chemie</i> , 2021, 133, 20102-20109.	1.6	6
86	Mechanistic insight into the highly regioselective Ni(0)-catalyzed [2 + 2] self-cycloaddition of electron-deficient allenoates. <i>Catalysis Science and Technology</i> , 2019, 9, 1273-1278.	2.1	5
87	Mechanistic insight into the organocalcium-mediated nucleophilic alkylation of benzene and further rational design. <i>Catalysis Science and Technology</i> , 2020, 10, 950-958.	2.1	4
88	Mechanistic Study of Unprecedented Highly Regioselective Hydrocyanation of Terminal Alkynes: Insight into the Origins of the Regioselectivity and Ligand Effects. <i>Journal of Computational Chemistry</i> , 2020, 41, 279-289.	1.5	4
89	Bonding in M(NHBMMe) ₂ and M[Mn(CO) ₅] ₂ complexes (M=Zn, Cd, Hg; NHBMMe=(HCNMe) ₂ B): divalent group 12 metals with zero oxidation state. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	4
90	Divergent Metal-Free [4 + 2] Cascade Reaction of 1-Indanylidene malononitrile with 3-Benzylidenebenzofuran-2(3 <i>H</i>)-one: Access to Spiro-dihydrofluorene-benzofuranone and Axially Chiral Fluorenylamine-phenol Derivatives. <i>Organic Letters</i> , 2021, 23, 5611-5615.	2.4	4

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91	Beryllium Atom Mediated Dinitrogen Activation via Coupling with Carbon Monoxide. <i>Angewandte Chemie</i> , 2020, 132, 18358-18364.	1.6	3
92	Mechanistic Study of the <i>N</i> -Quaternized Pyridoxal-Catalyzed Biomimetic Asymmetric Mannich Reaction: Insights into the Origins of Enantioselectivity and Diastereoselectivity. <i>Journal of Organic Chemistry</i> , 2021, 86, 6592-6599.	1.7	3
93	Improvement in hydrogen binding ability of closo-dicboranes via functionalization and designing of extended frameworks. <i>Journal of Molecular Modeling</i> , 2018, 24, 307.	0.8	2
94	Bent Phosphaallenes With "Hidden" Lone Pairs as Ligands. <i>Chemistry - A European Journal</i> , 2019, 25, 7912-7920.	1.7	2
95	Linear group 13 E-E triple bonds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11611-11615.	1.3	2
96	Computational Mechanistic Study of Brønsted Acid-Catalyzed Unsymmetrical 1,2,4,5-Tetrazines Synthesis. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4715-4726.	1.1	2
97	Application of sugar-containing biomass: one-step synthesis of 2-furyl glyoxylic acid and its derivatives from a vitamin C precursor. <i>Green Chemistry</i> , 2022, 24, 2000-2009.	4.6	2
98	A <i>Bis</i> (carbone) Pincer Ligand and Its Coordinative Behavior toward Multi-Metallic Configurations. <i>Angewandte Chemie</i> , , , .	1.6	1
99	A multi-input/multi-output molecular system based on lanthanide(ⁱⁱⁱ) complexes. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2668-2675.	3.0	1
100	Berichtigung: Barium as Honorary Transition Metal in Action: Experimental and Theoretical Study of Ba(CO) ⁺ and Ba(CO) ⁺ . <i>Angewandte Chemie</i> , 2018, 130, 15856-15857.	1.6	0
101	Monitoring the Hierarchical Evolution from a Double-Stranded Helix to a Well-Defined Microscopic Morphology Based on a Turbine-like Aromatic Molecule. <i>ACS Omega</i> , 2020, 5, 16612-16618.	1.6	0
102	E-E triple bonds (E = Group 13) promoted by charge transfer from alkali metals. <i>New Journal of Chemistry</i> , , , .	1.4	0
103	Mechanistic study of the cooperative palladium/Lewis acid-catalyzed transfer hydrocyanation reaction: the origin of the regioselectivity. <i>Dalton Transactions</i> , 2021, 50, 1233-1238.	1.6	0
104	Highly Coordinated Heteronuclear Calcium-Iron Carbonyl Cation Complexes [CaFe(CO) _n] ⁺ (n = 5-12) with d ^π -d Bonding. <i>Angewandte Chemie</i> , 2021, 133, 13984-13989.	1.6	0
105	Mechanistic study of cobalt(I)-catalyzed asymmetric coupling of ethylene and enynes to functionalized cyclobutanes. <i>Journal of Computational Chemistry</i> , 2022, 43, 440-447.	1.5	0
106	Frontispiz: A <i>Bis</i> (carbone) Pincer Ligand and Its Coordinative Behavior toward Multi-Metallic Configurations. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	0
107	Frontispiece: A <i>Bis</i> (carbone) Pincer Ligand and Its Coordinative Behavior toward Multi-Metallic Configurations. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	0
108	How to capture C ₂ O ₂ : Structures and bonding of neutral and charged complexes [(NHC)-C ₂ O ₂ -(NHC)] _q (NHC = N-heterocyclic carbene; q = 0, 1+, 2+). <i>Physical Chemistry Chemical Physics</i> , , , .	1.3	0