Lingpeng Meng

List of Publications by Year
in descending order

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93 papers	1,141 citations	361413 20 h-index	501196 28 g-index
93 all docs	93 docs citations	93 times ranked	726 citing authors

#	Article	IF	Citations
1	Electronic and Photovoltaic Properties of Superlattices Constructed by Organicâ€“Inorganic Perovskites: a Theoretical Perspective. ACS Applied Energy Materials, 2022, 5, 2430-2441.	5.1	3
2	Halogen Bond Catalysis on Carbonylâ€“Olefin<scp>Ringâ€Closing</scp>Metathesis Reaction: Comparison with Lewis Acid Catalysis. Chinese Journal of Chemistry, 2022, 40, 1275-1284.	4.9	4
3	Mechanism and origin of the stereoselectivity of manganese-catalyzed hydrosilylation of alkynes: a DFT study. Catalysis Science and Technology, 2022, 12, 2649-2658.	4.1	6
4	Photocatalytic Reduction of CO₂ with H₂O Mediated by Ce-Tailored Bismuth Oxybromide Surface Frustrated Lewis Pairs. ACS Catalysis, 2022, 12, 4016-4025.	11.2	95
5	Mechanism, Stereoselectivity, and Role of O₂ in Aza-Dielsâ€“Alder Reactions Catalyzed by Dinuclear Molybdenum Complexes: A Theoretical Study. Inorganic Chemistry, 2022, 61, 4714-4724.	4.0	3
6	<scp> BF ₃ â€Catalyzed </scp> Mukaiyama aldol reaction of acetaldehyde with 2â€siloxyâ€1â€propene. Journal of Computational Chemistry, 2022, 43, 402-412.	3.3	1
7	Charge-regulated regioselective mechanism of bicobalt-catalyzed hydrogermylation of alkynes: DFT investigation. Molecular Catalysis, 2022, 526, 112379.	2.0	4
8	Mechanistic insights into the reaction Cp2Nb(CO)H (Cpâ€²=â€²Î·5-C5H5) with acetylenedicarboxylic acid (ADCA): DFT studies. Inorganica Chimica Acta, 2021, 514, 119990.	2.4	0
9	Competition and conversion between pnicogen bonds and hydrogen bonds involving prototype organophosphorus compounds. Physical Chemistry Chemical Physics, 2021, 23, 18794-18805.	2.8	2
10	Improving the stability of perovskite by covering graphene on <scp> FAPbI ₃ </scp> surface. International Journal of Energy Research, 2021, 45, 10808-10820.	4.5	7
11	Comparison of Anionâ€Anion Halogen Bonds with Neutralâ€Anion Halogen Bonds in the Gas Phase and Polar Solvents. ChemPlusChem, 2021, 86, 232-240.	2.8	15
12	Control of the Regioselectivity of Alkyne Hydrostannylation by Tuning the Metal Pair of Heterobimetallic Catalysts: A Theoretical Study. Organometallics, 2021, 40, 654-662.	2.3	6
13	Mechanism and regioselectivity of [Cu-Fe] heterobimetallic-catalyzed hydroboration of pyridines: DFT investigation. Molecular Catalysis, 2021, 511, 111722.	2.0	4
14	Mechanism and Stereoselectivity of the Elementometalation Process of Activated Alkyne RCï£½CR(Rï£¾CO 2) Tj ETQq0 0 0 rgBT /Over	3.3	7
15	Electronic structure of triangular M₃ (M = B, Al, Ga): nonclassical three-center two electron ï€ bond and ïƒ delocalization. Physical Chemistry Chemical Physics, 2020, 22, 18071-18077.	2.8	5
16	Nb(i PrNPMe 2) 3 Feâ€“PMe 3 : A potential high reactivity heterobimetallic catalyst for acetylene cycloadditions. Applied Organometallic Chemistry, 2020, 34, e5966.	3.5	4
17	Substituent-regulated mechanism on reaction Cp2NbH3 (Cp = Î·5-C5H5) with RCî€CR (R = COOMe and Me). Dalton Transactions, 2020, 49, 15376-15384.	3.3	0
18	Stereoselectivity and nonmigratory insertion mechanism of dimethylacetylene dicarboxylate into metalloceneâ€hydride of Cp 2 M(L)H [Cp = Î· 5 â€C 5 H 5 ; M = Nb, V; L = CO, P (OMe) 3]: A DFT study. Applied Organometallic Chemistry, 2020, 34, e5601.	3.5	2

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19	Reaction Mechanism and Kinetics study on Addition of CCl 4 to 1â€hexene Catalyzed by Moâ€Mo Quintuplyâ€bond. Applied Organometallic Chemistry, 2020, 34, e5726.	3.5	2
20	The roles of native defects and transition metal additives in the dehydrogenation mechanism of Mg(AlH4)2. International Journal of Hydrogen Energy, 2020, 45, 17625-17636.	7.1	1
21	Effect of Sr substitution on the property and stability of CH₃NH₃SnI₃perovskite: A firstâ€principles investigation. International Journal of Energy Research, 2020, 44, 5765-5778.	4.5	19
22	Enhancing the stability of perovskites by constructing heterojunctions of graphene/MASnI₃. Physical Chemistry Chemical Physics, 2020, 22, 3724-3733.	2.8	6
23	Effects of halogen substitutions on the properties of CH3NH3Sn0.5Pb0.5I3 perovskites. Computational Materials Science, 2020, 177, 109576.	3.0	5
24	Organocatalysis by Halogen, Chalcogen, and Pnictogen Bond Donors in Halide Abstraction Reactions: An Alternative to Hydrogen Bond-Based Catalysis. Journal of Physical Chemistry A, 2020, 124, 3815-3824.	2.5	23
25	Investigation on the intramolecular proton transfer mechanism of [Cp2MHn](Cpâ€¯=â€¯C5H5, Mâ€¯=â€¯Mo, W, Re;) Tj ETQq1 1 0.784	2.4	2
26	Aromaticity analysis of fused heterometallacycles containing M M(Mâ€¯=â€¯Cr, Mo and W) quintuple bond. Chemical Physics Letters, 2019, 731, 136600.	2.6	7
27	The mechanism of ringâ€opening polymerization of Lâ€lactide by ICl₃ catalysts: Halogen bond catalysis or participating in reactions?. Journal of Computational Chemistry, 2019, 40, 2827-2833.	3.3	7
28	Coinage metal dimers as the noncovalent interaction acceptors: study of the Ï*f*-lump interactions. Physical Chemistry Chemical Physics, 2019, 21, 21152-21161.	2.8	11
29	Comparison of pnicogen and tetrel bonds in complexes containing CX2 carbenes (X = F, Cl, Br, OH,) Tj ETQq1 1 0.784314 rgBT /Overl	2.8	9
30	Predicting the halogenâ€n (n = 3â€“6) synthons to form the â€œwindmillâ€•pattern bonding based on the halogenâ€bonded interactions. Journal of Computational Chemistry, 2019, 40, 1219-1226.	3.3	13
31	Insight into the Effects of Electrostatic Potentials on the Conversion Mechanism of the Hydrogen-Bonded Complexes and Carbon-Bonded Complexes: An Ab Initio and Quantum Theory of â€œAtoms in Moleculesâ€•Investigation. ACS Omega, 2019, 4, 231-241.	3.5	3
32	Nature of MoHÂ·Â·Â·I bonds in Cp₂Mo(L)HÂ·Â·Â·Iâ€Câ‰¡Câ€R Complexes (L=H, CN, PPh₂,) Tj ETQq0 0 0 rgBT Applied Organometallic Chemistry, 2018, 32, e4258.	3.5	4
33	ClË‰ as the halogen bond acceptor: studies on strong halogen bonds. Structural Chemistry, 2018, 29, 503-511.	2.0	1
34	Insight into the Ï€â€holeÂ·Â·Â·Ï€â€electrons tetrel bonds between F₂ZO (Zâ€‰=â€‰C, Si, Ge) and unsaturated hydrocarbons. International Journal of Quantum Chemistry, 2018, 118, e25521.	2.0	13
35	Nature of non-nuclear (3, â^’3) Ï€-attractor and Ï€-bonding: Theoretical analysis on Ï€-electron density. Chemical Physics Letters, 2018, 691, 347-350.	2.6	2
36	Stability and donor-acceptor bond in dinuclear organometallics CpM1â€“M2Cl3 (M1, M2â€‰=â€‰B, Al, Ga, In; Cpâ€‰=â€‰Î·) Tj ETQ	1.8	3

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37	The enhancing effects of molecule X (Xâ€‰=â€‰PH₂Cl, SHCl, ClCl) on chalcogenâ€“chalcogen interactions in cyclic trimers YÂ·Â·Â·YÂ·Â·Â·X (Yâ€‰=â€‰SHCl, SeHCl). International Journal of Quantum Chemistry, 2017, 117, e25354.	2.0	4
38	The ground and excited-state electronic structures of sandwich compounds Cp2(ME)2 contain an (ME)2 four-membered ring (Cp = C5H5; M = Ni, Pd, Pt; E = O, S, Se, Te). New Journal of Chemistry, 2017, 41, 12028-12034.	2.8	3
39	Insight into Ï€-hole interactions containing the inorganic heterocyclic compounds S2N2/SN2P2. Journal of Molecular Modeling, 2017, 23, 233.	1.8	2
40	Mechanism and kinetics for the reactions of methacrolein and methyl vinyl ketone with HO₂ radical. New Journal of Chemistry, 2017, 41, 7714-7722.	2.8	5
41	Inorganic benzenes as the noncovalent interaction donor: a study of the Ï€-hole interactions. Journal of Molecular Modeling, 2017, 23, 335.	1.8	2
42	Chalcogen- and halogen-bonds involving SX2 (X = F, Cl, and Br) with formaldehyde. Journal of Molecular Modeling, 2016, 22, 167.	1.8	4
43	The mutual influence between Ï€-hole pnicogen bonds and Ïƒ-hole halogen bonds in complexes of PO2Cl and XCN/C6H6 (XÂ=ÂF, Cl, Br). Structural Chemistry, 2016, 27, 1427-1437.	2.0	18
44	Insight into the pseudo Ï€-hole interactions in the M₃H₆â‹¯(NCF)_n(M) Tj ETQq0 0 0 rgBT /Overlo	2.8	36
45	Comparative studies on group III Ïƒ-hole and Ï€-hole interactions. Journal of Computational Chemistry, 2016, 37, 1321-1327.	3.3	49
46	Intriguing Eâ€¦E' bonding in [Nap(EPh)(E'Ph)]^{â€¢+}(E, E'=O, S, Se, Te). International Journal of Quantum Chemistry, 2016, 116, 1090-1096.	2.0	3
47	Dinuclear first-row transition metalâ€“(C8Me6)2complexes: metalâ€“metal and metalâ€“ligand bonds determined by the d electron configuration of the metal atom. New Journal of Chemistry, 2016, 40, 1988-1996.	2.8	9
48	Comparison of the directionality of the halogen, hydrogen, and lithium bonds between HOOOH and XF (XÂ=ÂCl, Br, H, Li). Journal of Molecular Modeling, 2016, 22, 52.	1.8	4
49	Mutual enhancing effects of the Ïƒ-hole interactions and halogen/hydrogen-bonded interactions in the iodine-ylide containing complexes. Structural Chemistry, 2016, 27, 927-937.	2.0	4
50	Improvement in dehydrogenation performance ofÂMg(BH4)2Â·2NH3 doped with transition metal: First-principles investigation. International Journal of Hydrogen Energy, 2015, 40, 8721-8731.	7.1	15
51	A comprehensive analysis of PÂ·Â·Â·Ï€ pnicogen bonds: substitution effects and comparison with BrÂ·Â·Â·Ï€ halogen bonds. Journal of Molecular Modeling, 2015, 21, 143.	1.8	24
52	Understanding the Properties of Inorganic Benzenes Based on Ï€-Electron Densities. Journal of Physical Chemistry A, 2015, 119, 2091-2097.	2.5	15
53	Influences of the substituents on the Mâ€“M bonding in Cp₄Al₄ and Cp₂M₂X₂ (M = B, Al, Ga; Cp = C₅H₅, X =) Tj ETQq1 1 0.784314 rgB	3.1	13
54	The competition of Yâ‹¯o and Xâ‹¯n halogen bonds to enhance the group V Ïƒ-hole interaction in the NCYâ‹¯oï£¾PH₃â‹¯NCX and Oï£¾PH₃â‹¯NCXâ‹¯NCY (X, Yï£¾F, Cl, and Br) complexes. Journal of Computational Chemistry, 2015, 36, 1349-1358.	3.3	27

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55	Influences of Al, Ti and Nb doping on the structure and hydrogen storage property of Mg(BH 4) 2 (001) surface â€“ A theoretical study. International Journal of Hydrogen Energy, 2015, 40, 10516-10526.	7.1	12
56	Enhancing Ïƒ/Ï€-type copper(<scp>i</scp>)â‹¯thiophene interactions by metal doping (metal = Li, Na, K, Ca, Sc). Dalton Transactions, 2015, 44, 1283-1291.	3.3	12
57	The cooperativity between the Ïƒ-hole and Ï€-hole interactions in the ClOÂ·Â·Â·XONO2/XONOÂ·Â·Â·NH3 (XÂ=ÂCl, Br, I) complexes. Structural Chemistry, 2015, 26, 213-221.	2.0	29
58	Influence of titanium and nickel dopants on the dehydrogenation properties of Mg(AlH4)2: Electronic structure mechanisms. International Journal of Hydrogen Energy, 2014, 39, 9276-9287.	7.1	8
59	A comparative study of some lithium and hydrogen-bonded complexes: Ab initio and QTAIM studies. International Journal of Quantum Chemistry, 2014, 114, 400-408.	2.0	4
60	Regulatory factors and the nature of Cuâ‹¯Cu interaction in copper(i) complexes with NHC and NHCP ligands: a theoretical assessment. New Journal of Chemistry, 2014, 38, 5786-5792.	2.8	5
61	Effects of Mg and Al doping on the electronic structure and dehydrogenation of LiBH4Â·NH3. International Journal of Hydrogen Energy, 2014, 39, 17144-17152.	7.1	8
62	The enhancing effects of group V Ïƒ-hole interactions on the Fâ‹¯O halogen bond. Physical Chemistry Chemical Physics, 2014, 16, 19282-19289.	2.8	29
63	NÂ·Â·Â·I Halogen Bonding Interactions: Influence of Lewis Bases on Their Strength and Characters. Journal of Physical Chemistry A, 2014, 118, 7058-7065.	2.5	27
64	Nature of the Mâ€“M bonding (MÂ=ÂCr, Mo, and W) in [CpM(CO)3]2: Covalent single bond or noncovalent interaction?. Journal of Organometallic Chemistry, 2014, 769, 106-111.	1.8	7
65	Enhancing effects of hydrogen/halogen bonds on Ïƒ-hole interactions involving ylide. Journal of Molecular Modeling, 2014, 20, 2282.	1.8	4
66	Influence of Cr/Zr doping on the electronic structure and hydrogen storage properties of the Mg2Ni (010) surface: A first principles study. Journal of Alloys and Compounds, 2014, 601, 280-288.	5.5	7
67	Interplay between halogen bonds and hydrogen bonds in OH/SHÂ·Â·Â·HOXÂ·Â·Â·HY (X = Cl, Br; Y = F, Cl, Br) complexes. Journal of Molecular Modeling, 2013, 19, 1069-1077.	1.8	21
68	First-principles study of hydrogen vacancies in lithium amide doped with titanium and niobium. International Journal of Hydrogen Energy, 2013, 38, 11303-11312.	7.1	9
69	Discovery of Ïƒ-hole interactions involving ylides. Journal of Molecular Modeling, 2013, 19, 4887-4895.	1.8	8
70	Metalâ€“Metal and Metalâ€“Ligand Bonds in (Î·⁵-C₅H₅)₂M₂ (M = Be, Mg, Ca, Ni, Cu, Zn). Organometallics, 2013, 32, 1060-1066.	2.3	43
71	Influence of the Liâ‹¯â‹¯Â·Â·Â·Ïƒ Interaction on the H/Xâ‹¯â‹¯Â·Â·Â·Ïƒ Interactions in HOLiâ‹¯â‹¯Â·Â·Â·C₆H₆â‹¯â‹¯Â·Â·Â·HOX/XOH (X=F, Cl, Br, I) Complexes. ChemPhysChem, 2013, 14, 1591-1600.	3.2	18
72	Electron Structure of Arxâ€²ZnZnArxâ€² (Arxâ€² = C₆H₃-2,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (6-(C Hydrogen/Sodium Atoms on Znâ€“Zn Interactions. Organometallics, 2012, 31, 6582-6588.	2.3	9

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73	Assessment of intermolecular interactions at three sites of the arylalkyne in phenylacetyleneâ€containing lithiumâ€bonded complexes: Ab initio and QTAIM studies. Journal of Computational Chemistry, 2012, 33, 1321-1327.	3.3	15
74	Substituent effects on the intramolecular hydrogen bond in 1-hydroxyanthraquinone: AIM and NBO analyses. Structural Chemistry, 2012, 23, 1233-1240.	2.0	13
75	Computational studies of Ïƒ-type weak interactions between NCO/NCS radicals and XY(X = H, Cl; Y = F, Cl,) Tj ETQq1 1 0.784314 rgBT	8.2	2
76	Cooperativity between SÂ·Â·Â·Ï€ and RgÂ·Â·Â·Ï€ in the OCSÂ·Â·Â·C₆H₆Â·Â·Â·Rg (Rg = He, Ne, Ar, and) Tj ETQq0	2.5	10
77	A computational study on the nature of the halogen bond between sulfides and dihalogen molecules. Structural Chemistry, 2011, 22, 567-576.	2.0	40
78	Insight into the lithium/hydrogen bonding in (CH2)2X...LiY/HY (X: C=CH2, O, S; Y=F, Cl, Br) complexes. Journal of Molecular Modeling, 2011, 17, 757-767.	1.8	26
79	Insight into the nature of the interactions of furan and thiophene with hydrogen halides and lithium halides: ab initio and QTAIM studies. Journal of Molecular Modeling, 2011, 17, 2907-2918.	1.8	24
80	Ab initio and AIM studies on typical Ï€â€type and pseudoâ€Ï€â€type halogen bonds: Comparison with hydrogen bonds. International Journal of Quantum Chemistry, 2011, 111, 3725-3740.	2.0	20
81	AIM and ELF Analyses of Halogen Bonding in NCS:BrCl Complexes. Chinese Journal of Chemistry, 2011, 29, 2416-2420.	4.9	0
82	The Role of Molecular Electrostatic Potentials in the Formation of a Halogen Bond in Furanâ‹…â‹…â‹…XY and Thiopheneâ‹…â‹…â‹…XY Complexes. ChemPhysChem, 2011, 12, 1080-1087.	2.1	24
83	The Role of Ï€ Electrons in the Formation of Benzeneâ€Containing Lithiumâ€Bonded Complexes. ChemPhysChem, 2011, 12, 3584-3590.	2.1	19
84	First-principles studies of the structures and properties of Al- and Ag-substituted Mg2Ni alloys and their hydrides. International Journal of Hydrogen Energy, 2010, 35, 10349-10358.	7.1	23
85	Theoretical Studies on the Isomerizations of CH₃NO₂. Chinese Journal of Chemistry, 2009, 27, 1025-1030.	4.9	0
86	Topological Characteristics of Electron Density Distribution in SSXY â†' XSSY (X or Y = F, Cl, Br, I) Isomerization Reactions. Journal of Physical Chemistry A, 2007, 111, 9093-9101.	2.5	27
87	Theoretical Investigation on Stability and Isomerizations of CH3SO Isomers. Journal of Physical Chemistry A, 2007, 111, 2343-2350.	2.5	23
88	Topological Characterization of HXO2 (X = Cl, Br, I) Isomerization. Journal of Physical Chemistry A, 2007, 111, 1530-1535.	2.5	17
89	A DFT study of the generation of interstellar species XN (X=Cl, and Br) activated by molecular sieve clusters. Chemical Physics Letters, 2004, 400, 394-400.	2.6	5
90	AIM Studies on Reactions FNCX â†' FXCN (X = O, S, and Se). Journal of Physical Chemistry A, 2004, 108, 10527-10534.	2.5	14

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91	Studies on Reactions INCX â†' IXCN (X = O, S, and Se). Inorganic Chemistry, 2004, 43, 5311-5320.	4.0	26
92	Topological studies on IRC paths of X+H2?XH+H reactions. Journal of Computational Chemistry, 1997, 18, 1167-1174.	3.3	13
93	Theoretical investigation on the nature of substituted benzeneâ‹¯AuX interactions: covalent or noncovalent?. New Journal of Chemistry, 0, , .	2.8	2