Hai-Gang Lu

List of Publications by Year
in descending order

75 papers	2,853 citations	218662 26 h-index	175241 52 g-index
78 all docs	78 docs citations	78 times ranked	1812 citing authors

#	Article	IF	Citations
1	La@[La5&B30]0/â^'/2â^': endohedral trihedral metallo-borospherenes with spherical aromaticity. Physical Chemistry Chemical Physics, 2022, 24, 3918-3923.	2.8	4
2	The unified quantum mechanical structure of tubular molecular rotors with multiple equivalent global minimum structures: the 18*C2h â† D9d case of La-[B2@B18]-La. Physical Chemistry Chemical Physics, 2021, 23, 19146-19149.	2.8	1
3	B111, B112, B113, and B114: The most stable core-shell borospherenes with an icosahedral B12 core at the center exhibiting superatomic behaviors. Nano Research, 2021, 14, 4719-4724.	10.4	16
4	Cage-like La4B24 and Core-Shell La4B290/+/â^'â€‰: perfect spherically aromatic tetrahedral metallo-borospherenes. Journal of Molecular Modeling, 2021, 27, 130.	1.8	7
5	Perfect Spherical Tetrahedral Metallo-Borospherene Ta₄B₁₈ as a Superatom Following the 18-Electron Rule. ACS Omega, 2021, 6, 10991-10996.	3.5	13
6	Metal-centered monocyclic carbon wheel clusters with record coordination numbers in planar species. RSC Advances, 2021, 11, 27193-27198.	3.6	10
7	(C6H6Cr)n&B40 (nâ€‰=â€‰1â€“6): Exohedral Borospherene Complexes with Cage-like B40 as an Effective Ligand with Multiple Coordination Sites. Journal of Cluster Science, 2020, 31, 1363-1369.	3.3	2
8	Sea-shell-like B31+ and B32: two new axially chiral members of the borospherene family. RSC Advances, 2020, 10, 10129-10133.	3.6	10
9	Perfect cubic La-doped boron clusters La₆&[La@B₂₄]^{+/0}as the embryos of low-dimensional lanthanide boride nanomaterials. RSC Advances, 2020, 10, 12469-12474.	3.6	9
10	Predicting two-dimensional semiconducting boron carbides. Nanoscale, 2019, 11, 11099-11106.	5.6	29
11	K(CO) 8 â^' and Rb(CO) 8 â^' : Cube-Like Alkali Octacarbonyls Satisfying the 18-Electron Rule. Journal of Cluster Science, 2019, 30, 621-626.	3.3	4
12	Fluxional bonds in quasiâ€planar and halfâ€sandwich (M = K, Rb, and Cs). Journal of Computational Chemistry, 2019, 40, 1227-1232.	3.3	8
13	Low-dimensional functional networks of cage-like B₄₀ with effective transition-metal intercalations. Physical Chemistry Chemical Physics, 2019, 21, 22611-22617.	2.8	5
14	Probing the Fluxional Bonding Nature of Rapid Cope rearrangements in Bullvalene C10H10 and Its Analogs C8H8, C9H10, and C8BH9. Scientific Reports, 2019, 9, 17074.	3.3	12
15	Predicting lanthanide boride inverse sandwich tubular molecular rotors with the smallest coreâ€“shell structure. Nanoscale, 2019, 11, 21311-21316.	5.6	19
16	Azugraphene: a new graphene-like hexagonal carbon allotrope with Dirac cones. RSC Advances, 2019, 9, 34481-34485.	3.6	17
17	NiB10, NiB11â^', NiB12, and NiB13+: Half-Sandwich Complexes with the Universal Coordination Bonding Pattern of Ïƒ Plus Ï€ Double Delocalization. Journal of Cluster Science, 2019, 30, 115-121.	3.3	14
18	Fluxional Bonds in Planar B₁₉^{â^'}, Tubular Ta@B₂₀^{â^'}, and Cageâ€Like B₃₉^{â^'}. Journal of Computational Chemistry, 2019, 40, 966-970.	3.3	23

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19	Aromatic cage-like B₃₄ and B₃₅⁺: new axially chiral members of the borospherene family. Physical Chemistry Chemical Physics, 2018, 20, 15344-15349.	2.8	13
20	Cage-like Ta@Bqn complexes (n = 23â€“28, q = â˜'1â€“+ 3) in 18-electron configurations with the highest coordination number of twenty-eight. Nanoscale, 2018, 10, 7451-7456.	5.6	23
21	A DFT based method for calculating the surface energies of asymmetric MoP facets. Applied Surface Science, 2018, 427, 357-362.	6.1	81
22	High-symmetry tubular Ta@B₁₈^{3â˜'}, Ta₂@B₁₈, and Ta₂@B₂₇⁺ as embryos of Î±-boronanotubes with a transition-metal wire coordinated inside. Physical Chemistry Chemical Physics, 2018, 20, 25009-25015.	2.8	9
23	Charge-induced structural transition between seashell-like B₂₉^{â˜'} and B₂₉⁺ in 18 Ï€-electron configurations. Physical Chemistry Chemical Physics, 2018, 20, 15330-15334.	2.8	12
24	Planar B₃₈^{â˜'}and B₃₇^{â˜'}clusters with a double-hexagonal vacancy: molecular motifs for borophenes. Nanoscale, 2017, 9, 4550-4557.	5.6	76
25	A novel borophene featuring heptagonal holes: a common precursor of borospherenes. Physical Chemistry Chemical Physics, 2017, 19, 19890-19895.	2.8	12
26	Cage-like B₃₉⁺clusters with the bonding pattern of Ïƒ + Ï€ double delocalization: new members of the borospherene family. Physical Chemistry Chemical Physics, 2017, 19, 10998-11003.	2.8	23
27	Which Density Functional Should Be Used to Describe Protonated Water Clusters?. Journal of Physical Chemistry A, 2017, 121, 3117-3127.	2.5	27
28	Structural transition in metal-centered boron clusters: from tubular molecular rotors Ta@B₂₁and Ta@B₂₂⁺to cage-like endohedral metalloborospherene Ta@B₂₂^{â˜'}. Physical Chemistry Chemical Physics, 2017, 19, 27025-27030.	2.8	38
29	Heteroborospherene clusters Niâ€‰â˜†â€‰B40 (nâ€‰=â€‰1â€“4) and heteroborophene monolayers Ni2â€‰â˜†â€‰B14 with pla heptacoordinate transition-metal centers in Î·7-B7 heptagons. Scientific Reports, 2017, 7, 5701.	3.3	16
30	Double-ring tubular (B2O2)nclusters (n = 6â€“42) rolled up from the most stable BO double-chain ribbon in boron monoxides. Physical Chemistry Chemical Physics, 2017, 19, 23213-23217.	2.8	3
31	â€œW-X-Mâ€•transformations in isomerization of B39â˜' borospherenes. AIP Advances, 2016, 6, .	1.3	11
32	Cage-like B40 +: a perfect borospherene monocation. Journal of Molecular Modeling, 2016, 22, 124.	1.8	16
33	Endohedral charge-transfer complex Ca@B₃₇^{â˜'}: stabilization of a B₃₇^{3â˜'}borospherene trianion by metal-encapsulation. Physical Chemistry Chemical Physics, 2016, 18, 14186-14190.	2.8	45
34	From Quasi-Planar B56 to Penta-Ring Tubular CaÂ©B56: Prediction of Metal-Stabilized CaÂ©B56 as the Embryo of Metal-Doped Boron Î±-Nanotubes. Scientific Reports, 2016, 6, 37893.	3.3	7
35	Saturn-like charge-transfer complexes Li₄&B₃₆, Li₅&B₃₆⁺, and Li₆&B₃₆²⁺: exohedral metalloborospherenes with a perfect cage-like B₃₆^{4â˜'}core. Physical Chemistry Chemical Physics, 2016, 18, 9922-9926.	2.8	58
36	Endohedral Ca@B₃₈: stabilization of a B₃₈^{2â˜'}borospherene dianion by metal encapsulation. Physical Chemistry Chemical Physics, 2016, 18, 11610-11615.	2.8	50

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37	Cageâ€Like B₄₁⁺ and B₄₂²⁺: New Chiral Members of the Borospherene Family. Angewandte Chemie, 2015, 127, 8278-8282.	2.0	11
38	IhSymmetrical (4,6)-Fullerenes and Their Local Ring Aromaticity: A First Principle Study. Journal of Nanomaterials, 2015, 2015, 1-5.	2.7	0
39	Experimental and Theoretical Evidence of an Axially Chiral Borospherene. ACS Nano, 2015, 9, 754-760.	14.6	228
40	Strain-induced metal-semimetal transition of BeB₂ monolayer. RSC Advances, 2015, 5, 11392-11396.	3.6	19
41	Ribbon Aromaticity of Double-Chain B2n C2H2 Clusters (nÂ=Â2â€“9): A First Principle Study. Journal of Cluster Science, 2015, 26, 2043-2050.	3.3	4
42	Endohedral C₃Ca@B₃₉⁺and C₂Ca@B₃₉⁺: axially chiral metalloborospherenes based on B₃₉^{â^'}. Physical Chemistry Chemical Physics, 2015, 17, 19690-19694.	2.8	31
43	Cageâ€Like B₄₁⁺ and B₄₂²⁺: New Chiral Members of the Borospherene Family. Angewandte Chemie - International Edition, 2015, 54, 8160-8164.	13.8	105
44	D3h [A-CE3-A]â^' (E = Al and Ga, A = Si, Ge, Sn, and Pb): A new class of hexatomic mono-anionic species with trigonal bipyramidal carbon. Journal of Chemical Physics, 2014, 140, 104302.	3.0	5
45	Chemical bonding in electron-deficient boron oxide clusters: core boronyl groups, dual 3câ€“4e hypervalent bonds, and rhombic 4câ€“4e bonds. Physical Chemistry Chemical Physics, 2014, 16, 7274.	2.8	29
46	Thermodynamic Stability versus Kinetic Stability: Is the Planar Hexacoordinate Carbon Species D_{3h} CN₃Mg₃⁺ Viable?. Journal of Physical Chemistry A, 2014, 118, 3319-3325.	2.5	23
47	Observation of an all-boron fullerene. Nature Chemistry, 2014, 6, 727-731.	13.6	724
48	Planar D 2h B26H8, D 2h B26H8 2+, and C 2h B26H6: Building Blocks of Stable Boron Sheets with Twin-Hexagonal Holes. Journal of Cluster Science, 2013, 24, 1127-1137.	3.3	6
49	Covalent Bonding in Au(BO) 2 â^' and Au(BS) 2 â^'. Journal of Cluster Science, 2013, 24, 233-241.	3.3	9
50	Two-dimensional carbon allotropes from graphene to graphyne. Journal of Materials Chemistry C, 2013, 1, 3677.	5.5	116
51	Perfectly planar boronyl boroxine D3h B6O6: A boron oxide analog of boroxine and benzene. Journal of Chemical Physics, 2013, 138, 244304.	3.0	43
52	B30H8, B39H9 2â^', B42H10, B48H10, and B72H12: polycyclic aromatic snub hydroboron clusters analogous to polycyclic aromatic hydrocarbons. Journal of Molecular Modeling, 2013, 19, 1195-1204.	1.8	15
53	Face-Capping Î¼3-BO in B6(BO)7â€“: Boron Oxide Analogue of B6H7â€“ with Rhombic 4câ€“2e Bonds. Journal of Physical Chemistry A, 2013, 117, 11587-11591.	2.5	12
54	Binary nature of monolayer boron sheets from ab initio global searches. Journal of Chemical Physics, 2013, 138, 024701.	3.0	44

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55	Ribbon aromaticity in double-chain planar BnH22â˜ and Li2BnH2 nanoribbon clusters up to n = 22: lithiated boron dihydride analogues of polyenes. Physical Chemistry Chemical Physics, 2013, 15, 18872.	2.8	31
56	M(C6X6Li6)2 (M=Cr, Mo, W; X=O, S): Transition-metal sandwich complexes with Ï€-aromatic C6X6Li6 ligands. Computational and Theoretical Chemistry, 2013, 1018, 95-101.	2.5	6
57	First-principles investigations on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>5</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML". Computational and Theoretical Chemistry, 2013, 1007, 9-14.	2.5	35
58	Comment on â€œTwo-Dimensional Boron Monolayer Sheetsâ€. ACS Nano, 2013, 7, 879-879.	14.6	6
59	Pi and sigma double conjugations in boronyl polyboroene nanoribbons: B_n(BO)₂^{â˜} and B_n(BO)₂ (n = 5â˜12). Journal of Chemical Physics, 2013, 139, 174301.	3.0	40
60	Three-chain B6n+14 cages as possible precursors for the syntheses of boron fullerenes. Journal of Chemical Physics, 2013, 139, 224307.	3.0	16
61	D3h CN3Be3+ and CO3Li3+: viable planar hexacoordinate carbon prototypes. Physical Chemistry Chemical Physics, 2012, 14, 14760.	2.8	59
62	Double-chain planar D2h B4H2, C2h B8H2, and C2h B12H2: conjugated aromatic borenes. Physical Chemistry Chemical Physics, 2012, 14, 14769.	2.8	51
63	CAl₂Be₃^{2â€“} and Its Salt Complex LiCAl₂Be₃^{â€“}: Anionic Global Minima with Planar Pentacoordinate Carbon. Journal of Physical Chemistry A, 2012, 116, 3290-3294.	2.5	54
64	Planar Ï€-aromatic C3h B6H 3 + and Ï€-antiaromatic C2h B8H2: boron hydride analogues of D3h C3H 3 + and D2h C4H4. Journal of Molecular Modeling, 2012, 18, 3161-3167.	1.8	18
65	Deciphering the mystery of hexagon holes in an all-boron graphene Î±-sheet. Physical Chemistry Chemical Physics, 2011, 13, 11575.	2.8	136
66	Starlike Aluminumâ€“Carbon Aromatic Species. Chemistry - A European Journal, 2011, 17, 714-719.	3.3	45
67	Dâžh B2 (BS)2 â˜/2â˜ and Td B(BS)4 â˜ : Boron sulfide clusters containing BB multiple bonds and Bâ˜ tetrahedral centers. International Journal of Quantum Chemistry, 2010, 110, 2689-2696.	2.0	6
68	Hydration and coordination of K+ solvation in water from ab initio molecular-dynamics simulation. Journal of Chemical Physics, 2010, 132, 124503.	3.0	42
69	T_d B(BO)₄^{â˜}: A Tetrahedral Boron Oxide Cluster Analogous to Boron Hydride T_d BH₄^{â˜}. Journal of Physical Chemistry A, 2009, 113, 2561-2564.	2.5	39
70	Simplest Neutral Singlet C₂E₄(E = Al, Ga, In, and Tl) Global Minima with Double Planar Tetracoordinate Carbons: Equivalence of C₂Moieties in C₂E₄to Carbon Centers in CAl₄^{2â˜}and CAl₅⁺. Journal of Physical Chemistry A, 2009, 113, 3395-3402.	2.5	73
71	Hydrogen-bond network and local structure of liquid water: An atoms-in-molecules perspective. Journal of Chemical Physics, 2008, 129, 124512.	3.0	22
72	Hydrometal Complexes with More than One Planar and Quasi-Planar Tetracoordinate Carbon Atom:â€‰ From Hydrogen-Surrounded Pieces to the Rudiment of Hydrogen-Sealed Nanotubes. Organometallics, 2007, 26, 4395-4401.	2.3	21

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73	Atomic orbitals in molecules: general electronegativity and improvement of Mulliken population analysis. Physical Chemistry Chemical Physics, 2006, 8, 340-346.	2.8	17
74	Density functional study on zerovalent lanthanide bis(arene)-sandwich complexes. Theoretical Chemistry Accounts, 1999, 102, 121-126.	1.4	18
75	Half-Sandwich LaBnâˆ’/0 (nâ€‰=â€‰14â€“17): Ï€ Dually Aromatic Lanthanide Boride Complexes with Multicenter Fluxional Bonds. Journal of Cluster Science, 0, , 1.	3.3	3