Si-Dian Li

List of Publications by Year in Descending Order

164 papers	5,417 citations	39 h-index	67 g-index
176 ext. papers	6,370 ext. citations	6.6 avg, IF	5.95 L-index

#	Paper	IF	Citations
164	AuB: an Au-borozene complex.. *Chemical Communications*, **2022**,	5.8	1
163	SrCo0.4Fe0.4Zr0.1Y0.1O3-□A new CO2 tolerant cathode for proton-conducting solid oxide fuel cells. *Renewable Energy*, **2022**, 185, 8-16	8.1	1
162	Monovalent lanthanide(I) in borozene complexes. *Nature Communications*, **2021**, 12, 6467	17.4	3
161	Predicting bilayer B, B, B, and B: structural evolution in bilayer B-B clusters. *Journal of Molecular Modeling*, **2021**, 27, 364	2	1
160	Scalable Production of Freestanding Few-Layer ⊞-Borophene Single Crystalline Sheets as Efficient Electrocatalysts for Lithium-Sulfur Batteries. *ACS Nano*, **2021**,	16.7	5
159	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	10	2
158	Expanded Inverse-Sandwich Complexes of Lanthanum Borides: LaB and LaB. *Journal of Physical Chemistry A*, **2021**, 125, 2622-2630	2.8	10
157	Cage-like LaB and Core-Shell LaB : perfect spherically aromatic tetrahedral metallo-borospherenes. *Journal of Molecular Modeling*, **2021**, 27, 130	2	3
156	Perfect Spherical Tetrahedral Metallo-Borospherene TaB as a Superatom Following the 18-Electron Rule. *ACS Omega*, **2021**, 6, 10991-10996	3.9	2
155	Predicting the Structural Transition in Medium-Sized Boron Nanoclusters: From Bilayer B64, B66, B68, B70, and B72 to Core-Shell B74. *European Journal of Inorganic Chemistry*, **2021**, 2021, 2618-2624	2.3	3
154	An oxygen-passivated vanadium cluster [V@VO] with metal-metal coordination produced by reacting V with O. *Physical Chemistry Chemical Physics*, **2021**, 23, 921-927	3.6	4
153	Interactions between water and rhodium clusters: molecular adsorption cluster adsorption. *Nanoscale*, **2021**, 13, 11396-11402	7.7	4
152	The unified quantum mechanical structure of tubular molecular rotors with multiple equivalent global minimum structures: the 18* -ħtase of La-[B@B]-La. *Physical Chemistry Chemical Physics*, **2021** , 23, 19146-19149	3.6	
151	B: a bilayer boron cluster. *Nanoscale*, **2021**, 13, 3868-3876	7.7	16
150	Metal-centered monocyclic carbon wheel clusters with record coordination numbers in planar species.. *RSC Advances*, **2021**, 11, 27193-27198	3.7	3
149	Transition-metal-like bonding behaviors of a boron atom in a boron-cluster boronyl complex [(⊞B)-B-BO]. *Chemical Science*, **2021**, 12, 8157-8164	9.4	4
148	Axially Chiral Cage-Like B38+ and B382+: New Aromatic Members of the Borospherene Family. *Journal of Cluster Science*, **2020**, 1	3	3

147	First-Principles Study on the Oxidation of Supported 12-Borophene. *Journal of Physical Chemistry C*, **2020**, 124, 28145-28151	3.8	6
146	A CO2-tolerant SrCo0.8Fe0.15Zr0.05O3 cathode for proton-conducting solid oxide fuel cells. *Journal of Materials Chemistry A*, **2020**, 8, 11292-11301	13	22
145	Spherical trihedral metallo-borospherenes. *Nature Communications*, **2020**, 11, 2766	17.4	20
144	Bilayer B54, B60, and B62 Clusters in a Universal Structural Pattern. *European Journal of Inorganic Chemistry*, **2020**, 2020, 3296-3301	2.3	8
143	Sea-shell-like B and B: two new axially chiral members of the borospherene family.. *RSC Advances*, **2020**, 10, 10129-10133	3.7	8
142	Improvement of solid oxide fuel cell performance by a core-shell structured catalyst using low concentration coal bed methane fuel. *International Journal of Energy Research*, **2020**, 44, 5516-5526	4.5	4
141	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. *Angewandte Chemie*, **2020**, 132, 18745-18749	3.6	6
140	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. *Angewandte Chemie - International Edition*, **2020**, 59, 18586-18590	16.4	20
139	Novel B-C binary fullerenes following the isolated BC hexagonal pyramid rule. *Journal of Molecular Modeling*, **2020**, 26, 199	2	
138	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. *Angewandte Chemie - International Edition*, **2020**, 59, 6923-6928	16.4	9
137	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. *Angewandte Chemie*, **2020**, 132, 6990-6995	3.6	9
136	Perfect cubic La-doped boron clusters La&[La@B] as the embryos of low-dimensional lanthanide boride nanomaterials.. *RSC Advances*, **2020**, 10, 12469-12474	3.7	4
135	Donor-acceptor duality of the transition-metal-like B core in core-shell-like metallo-borospherenes La&[B@B] and La&[B@B].. *RSC Advances*, **2020**, 10, 34225-34230	3.7	6
134	From inverse sandwich TaB and TaB to spherical trihedral TaB : prediction of the smallest metallo-borospherene.. *RSC Advances*, **2020**, 10, 29320-29325	3.7	7
133	Fluxional Bonds in Tubular Molecular Rotors B3-[Ta@B18] and B4-[Ta@B18]+ in 18-Electron Configurations. *Journal of Cluster Science*, **2020**, 31, 331-336	3	3
132	Probing the electronic structure of the CoB16 drum complex: Unusual oxidation state of Co *Chinese Journal of Chemical Physics*, **2019**, 32, 241-247	0.9	3
131	Exfoliation of borophenes from silver substrates assisted by Li/Mg atoms density functional theory study. *Journal of Materials Chemistry C*, **2019**, 7, 4043-4048	7.1	11
130	[La(B)La] (= 7-9): a new class of inverse sandwich complexes. *Chemical Science*, **2019**, 10, 2534-2542	9.4	42

129	Re B and Re B: New Members of the Transition-Metal-Centered Borometallic Molecular Wheel Family. *Journal of Physical Chemistry A*, **2019**, 123, 5317-5324	2.8	23
128	LaB: an inverse triple-decker lanthanide boron cluster. *Chemical Communications*, **2019**, 55, 7864-7867	5.8	25
127	Predicting two-dimensional semiconducting boron carbides. *Nanoscale*, **2019**, 11, 11099-11106	7.7	16
126	Probing the structures and bonding of size-selected boron and doped-boron clusters. *Chemical Society Reviews*, **2019**, 48, 3550-3591	58.5	90
125	B and B: chiral quasi-planar boron clusters. *Nanoscale*, **2019**, 11, 9698-9704	7.7	18
124	A strategy to reduce the impact of tar on a Ni-YSZ anode of solid oxide fuel cells. *International Journal of Energy Research*, **2019**, 43, 3038-3048	4.5	2
123	Enhanced coking resistance of Ni cermet anodes for solid oxide fuel cells based on methane on-cell reforming by a redox-stable double-perovskite Sr2MoFeO6- *International Journal of Energy Research*, **2019**, 43, 2527-2537	4.5	12
122	A solid oxide carbon fuel cell operating on pomelo peel char with high power output. *International Journal of Energy Research*, **2019**, 43, 2514-2526	4.5	5
121	A steel slag derived Boudouard reaction catalyst for improved performance of direct carbon solid oxide fuel cells. *International Journal of Energy Research*, **2019**, 43, 6970	4.5	5
120	A Supramolecular Radical Dimer: High-Efficiency NIR-II Photothermal Conversion and Therapy. *Angewandte Chemie - International Edition*, **2019**, 58, 15526-15531	16.4	97
119	A Supramolecular Radical Dimer: High-Efficiency NIR-II Photothermal Conversion and Therapy. *Angewandte Chemie*, **2019**, 131, 15672-15677	3.6	29
118	Quadruple bonding between iron and boron in the BFe(CO) complex. *Nature Communications*, **2019**, 10, 4713	17.4	26
117	Fluxional bonds in quasi-planar and half-sandwich (M = K, Rb, and Cs). *Journal of Computational Chemistry*, **2019**, 40, 1227-1232	3.5	6
116	Low-dimensional functional networks of cage-like B with effective transition-metal intercalations. *Physical Chemistry Chemical Physics*, **2019**, 21, 22611-22617	3.6	2
115	Planar B and B clusters with double-hexagonal vacancies. *Nanoscale*, **2019**, 11, 23286-23295	7.7	29
114	Probing the Fluxional Bonding Nature of Rapid Cope rearrangements in Bullvalene CH and Its Analogs CH, CH, and CBH. *Scientific Reports*, **2019**, 9, 17074	4.9	7
113	Predicting lanthanide boride inverse sandwich tubular molecular rotors with the smallest core-shell structure. *Nanoscale*, **2019**, 11, 21311-21316	7.7	10
112	Degradation of benzothiophene in diesel oil by LaZnAl layered double hydroxide: photocatalytic performance and mechanism. *Petroleum Science*, **2019**, 16, 173-179	4.4	5

111	NiB10, NiB11−, NiB12, and NiB13+: Half-Sandwich Complexes with the Universal Coordination Bonding Pattern of Plus Double Delocalization. *Journal of Cluster Science*, **2019**, 30, 115-121	3	11
110	Fluxional Bonds in Planar B , Tubular Ta@B , and Cage-Like B. *Journal of Computational Chemistry*, **2019**, 40, 966-970	3.5	14
109	Lanthanides with Unusually Low Oxidation States in the PrB and PrB Boride Clusters. *Inorganic Chemistry*, **2019**, 58, 411-418	5.1	23
108	Purified high-sulfur coal as a fuel for direct carbon solid oxide fuel cells. *International Journal of Energy Research*, **2019**, 43, 2501-2513	4.5	9
107	Electronic Structure and Bonding Situation in MO (M = Be, Mg, Ca) Rhombic Clusters. *Journal of Physical Chemistry A*, **2018**, 122, 2816-2822	2.8	21
106	Relativity-Induced Bonding Pattern Change in Coinage Metal Dimers M (M = Cu, Ag, Au, Rg). *Inorganic Chemistry*, **2018**, 57, 5499-5506	5.1	10
105	Direct Power Generation from Low Concentration Coal-Bed Gas by a Catalyst-Modified Solid Oxide Fuel Cell. *ChemElectroChem*, **2018**, 5, 1459-1466	4.3	11
104	Viable aromatic BeH stars enclosing a planar hypercoordinate boron or late transition metal. *Physical Chemistry Chemical Physics*, **2018**, 20, 7217-7222	3.6	9
103	On the Upper Limits of Oxidation States in Chemistry. *Angewandte Chemie - International Edition*, **2018**, 57, 3242-3245	16.4	37
102	Direct Operation of Solid Oxide Fuel Cells on Low-Concentration Oxygen-Bearing Coal-Bed Methane with High Stability. *Energy & Fuels*, **2018**, 32, 4547-4558	4.1	7
101	Aromatic cage-like B and B: new axially chiral members of the borospherene family. *Physical Chemistry Chemical Physics*, **2018**, 20, 15344-15349	3.6	10
100	Uranyl/12-crown-4 Ether Complexes and Derivatives: Structural Characterization and Isomeric Differentiation. *Inorganic Chemistry*, **2018**, 57, 4125-4134	5.1	5
99	Cage-like Ta@B complexes (n = 23-28, q = -1-+ 3) in 18-electron configurations with the highest coordination number of twenty-eight. *Nanoscale*, **2018**, 10, 7451-7456	7.7	15
98	Observation of highly stable and symmetric lanthanide octa-boron inverse sandwich complexes. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E6972-E6977	11.5	59
97	Charge-induced structural transition between seashell-like B and B in 18 electron configurations. *Physical Chemistry Chemical Physics*, **2018**, 20, 15330-15334	3.6	10
96	Chemical Bonding of Crystalline LnB (Ln = La-Lu) and Its Relationship with LnB Gas-Phase Complexes. *Inorganic Chemistry*, **2018**, 57, 12999-13008	5.1	39
95	High-symmetry tubular Ta@B, Ta@B, and Ta@B as embryos of boronanotubes with a transition-metal wire coordinated inside. *Physical Chemistry Chemical Physics*, **2018**, 20, 25009-25015	3.6	8
94	Simulating the effect of a triple bond to achieve the shortest main group metal-metal distance in diberyllium complexes: a computational study. *Dalton Transactions*, **2018**, 47, 14462-14467	4.3	6

93	A supramolecular radical cation: folding-enhanced electrostatic effect for promoting radical-mediated oxidation. *Chemical Science*, **2018**, 9, 5015-5020	9.4	16
92	Planar B and B clusters with a double-hexagonal vacancy: molecular motifs for borophenes. *Nanoscale*, **2017**, 9, 4550-4557	7.7	61
91	PrB : A Praseodymium-Doped Boron Cluster with a Pr Center Coordinated by a Doubly Aromatic Planar B Ligand. *Angewandte Chemie - International Edition*, **2017**, 56, 6916-6920	16.4	46
90	Preparation and Characterization of Uranium-Iron Triple-Bonded UFe(CO) and OUFe(CO) Complexes. *Angewandte Chemie - International Edition*, **2017**, 56, 6932-6936	16.4	36
89	Preparation and Characterization of Uranium Iron Triple-Bonded UFe(CO)3 and OUFe(CO)3 Complexes. *Angewandte Chemie*, **2017**, 129, 7036-7040	3.6	7
88	PrB7 A Praseodymium-Doped Boron Cluster with a PrII Center Coordinated by a Doubly Aromatic Planar -B73 Ligand. *Angewandte Chemie*, **2017**, 129, 7020-7024	3.6	12
87	A novel borophene featuring heptagonal holes: a common precursor of borospherenes. *Physical Chemistry Chemical Physics*, **2017**, 19, 19890-19895	3.6	8
86	Cage-like B clusters with the bonding pattern of + double delocalization: new members of the borospherene family. *Physical Chemistry Chemical Physics*, **2017**, 19, 10998-11003	3.6	18
85	Which Density Functional Should Be Used to Describe Protonated Water Clusters?. *Journal of Physical Chemistry A*, **2017**, 121, 3117-3127	2.8	20
84	Zigzag double-chain CBe nanoribbon featuring planar pentacoordinate carbons and ribbon aromaticity. *Journal of Materials Chemistry C*, **2017**, 5, 408-414	7.1	8
83	A Very Short Be-Be Distance but No Bond: Synthesis and Bonding Analysis of Ng-Be O -Ng' (Ng, Ng'=Ne, Ar, Kr, Xe). *Chemistry - A European Journal*, **2017**, 23, 2035-2039	4.8	34
82	A universal mechanism of the planar boron rotors B, B, B, and B: inner wheels rotating in pseudo-rotating outer bearings. *Nanoscale*, **2017**, 9, 1443-1448	7.7	26
81	Observation of a metal-centered B-Ta@B tubular molecular rotor and a perfect Ta@B boron drum with the record coordination number of twenty. *Chemical Communications*, **2017**, 53, 1587-1590	5.8	90
80	From planar boron clusters to borophenes and metalloborophenes. *Nature Reviews Chemistry*, **2017** , 1,	34.6	118
79	Crown ether complexes of actinyls: a computational assessment of AnO(15-crown-5) (An = U, Np, Pu, Am, Cm). *Dalton Transactions*, **2017**, 46, 12354-12363	4.3	23
78	A first-principles study on zigzag phosphorene nanoribbons passivated by iron-group atoms. *Physical Chemistry Chemical Physics*, **2017**, 19, 25441-25445	3.6	8
77	Structural transition in metal-centered boron clusters: from tubular molecular rotors Ta@B and Ta@B to cage-like endohedral metalloborospherene Ta@B. *Physical Chemistry Chemical Physics*, **2017**, 19, 27025-27030	3.6	27
76	Heteroborospherene clusters Ni ? B (n = 1-4) and heteroborophene monolayers Ni ? B with planar heptacoordinate transition-metal centers in B heptagons. *Scientific Reports*, **2017**, 7, 5701	4.9	13

75	B33□and B34□Aromatic Planar Boron Clusters with a Hexagonal Vacancy. *European Journal of Inorganic Chemistry*, **2017**, 2017, 4546-4551	2.3	28
74	Double-ring tubular (BO) clusters (n = 6-42) rolled up from the most stable BO double-chain ribbon in boron monoxides. *Physical Chemistry Chemical Physics*, **2017**, 19, 23213-23217	3.6	2
73	BF (n = 1-6) series: when do boron double chain nanoribbons become global minima?. *Physical Chemistry Chemical Physics*, **2017**, 19, 31655-31665	3.6	2
72	Bond-bending isomerism of AuI: competition between covalent bonding and aurophilicity. *Chemical Science*, **2016**, 7, 475-481	9.4	14
71	In situ fabrication of (Sr,La)FeO4 with CoFe alloy nanoparticles as an independent catalyst layer for direct methane-based solid oxide fuel cells with a nickel cermet anode. *Journal of Materials Chemistry A*, **2016**, 4, 13997-14007	13	50
70	From Quasi-Planar B to Penta-Ring Tubular Ca□ B: Prediction of Metal-Stabilized Ca□ B as the Embryo of Metal-Doped Boron □Nanotubes. *Scientific Reports*, **2016**, 6, 37893	4.9	6
69	Lithium-Decorated Borospherene B: A Promising Hydrogen Storage Medium. *Scientific Reports*, **2016**, 6, 35518	4.9	45
68	Relativistic Effects Break Periodicity in Group 6 Diatomic Molecules. *Journal of the American Chemical Society*, **2016**, 138, 1126-9	16.4	31
67	Saturn-like charge-transfer complexes Li&B□Li&B□, and Li&B□+: exohedral metalloborospherenes with a perfect cage-like B□ core. *Physical Chemistry Chemical Physics*, **2016**, 18, 9922-6	3.6	48
66	Probing the Electronic Structure and Chemical Bonding of Mono-Uranium Oxides with Different Oxidation States: UOx(-) and UOx (x = 3-5). *Journal of Physical Chemistry A*, **2016**, 120, 1084-96	2.8	22
65	Theoretical studies on the bonding and electron structures of a [Au3Sb6](3-) complex and its oligomers. *Dalton Transactions*, **2016**, 45, 11657-67	4.3	6
64	Endohedral Ca@B38: stabilization of a B38(2-) borospherene dianion by metal encapsulation. *Physical Chemistry Chemical Physics*, **2016**, 18, 11610-5	3.6	45
63	Multiple Dirac cones in BN co-doped □-graphyne. *Journal of Materials Chemistry C*, **2016**, 4, 7339-7344	7.1	11
62	Frontispiz: The Planar CoB18□Cluster as a Motif for Metallo-Borophenes. *Angewandte Chemie*, **2016**, 128,	3.6	1
61	The Planar CoB18 (-) Cluster as a Motif for Metallo-Borophenes. *Angewandte Chemie - International Edition*, **2016**, 55, 7358-63	16.4	71
60	A Supramolecularly Activated Radical Cation for Accelerated Catalytic Oxidation. *Angewandte Chemie - International Edition*, **2016**, 55, 8933-7	16.4	57
59	A Supramolecularly Activated Radical Cation for Accelerated Catalytic Oxidation. *Angewandte Chemie*, **2016**, 128, 9079-9083	3.6	16
58	Periodicity and Covalency of [MX2]□(M = Cu, Ag, Au, Rg; X = H, Cl, CN) Complexes. *European Journal of Inorganic Chemistry*, **2016**, 2016, 1395-1404	2.3	9

57	The Planar CoB18 Cluster as a Motif for Metallo-Borophenes. *Angewandte Chemie*, **2016**, 128, 7484-7489	3.6	24
56	Structures and chemical bonding of B3O3 (-/0) and B3O3H(-/0): A combined photoelectron spectroscopy and first-principles theory study. *Journal of Chemical Physics*, **2016**, 144, 124301	3.9	12
55	Observation and characterization of the smallest borospherene, B28(-) and B28. *Journal of Chemical Physics*, **2016**, 144, 064307	3.9	119
54	W-X-M transformations in isomerization of B39 borospherenes. *AIP Advances*, **2016**, 6, 065110	1.5	11
53	Manganese-centered tubular boron cluster - MnB16 (-): A new class of transition-metal molecules. *Journal of Chemical Physics*, **2016**, 144, 154310	3.9	84
52	Star-like superalkali cations featuring planar pentacoordinate carbon. *Journal of Chemical Physics*, **2016**, 144, 244303	3.9	19
51	Chemical bonding and dynamic fluxionality of a B15(+) cluster: a nanoscale double-axle tank tread. *Physical Chemistry Chemical Physics*, **2016**, 18, 15774-82	3.6	40
50	Cage-like B40 (+): a perfect borospherene monocation. *Journal of Molecular Modeling*, **2016**, 22, 124	2	15
49	Endohedral charge-transfer complex Ca@B37(-): stabilization of a B37(3-) borospherene trianion by metal-encapsulation. *Physical Chemistry Chemical Physics*, **2016**, 18, 14186-90	3.6	38
48	Electronic structure and characterization of a uranyl di-15-crown-5 complex with an unprecedented sandwich structure. *Chemical Communications*, **2016**, 52, 12761-12764	5.8	18
47	Competition between quasi-planar and cage-like structures in the B cluster: photoelectron spectroscopy and ab initio calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 29147-29155	3.6	71
46	Competition between drum and quasi-planar structures in RhB: motifs for metallo-boronanotubes and metallo-borophenes. *Chemical Science*, **2016**, 7, 7020-7027	9.4	78
45	Ribbon Aromaticity of Double-Chain B2n C2H2 Clusters (n = 2). *Journal of Cluster Science*, **2015**, 26, 2043-2050	3	2
44	Endohedral C3 Ca@B39(+) and C2 Ca@B39(+): axially chiral metalloborospherenes based on B39(-). *Physical Chemistry Chemical Physics*, **2015**, 17, 19690-4	3.6	30
43	Photoelectron spectroscopy of B4O4 (-): Dual 3c-4e hyperbonds and rhombic 4c-4e o-bond in boron oxide clusters. *Journal of Chemical Physics*, **2015**, 142, 134305	3.9	20
42	Cage-Like B41 (+) and B42 (2+) : New Chiral Members of the Borospherene Family. *Angewandte Chemie - International Edition*, **2015**, 54, 8160-4	16.4	87
41	A first-principles study on the B5O5 (+/0) and B5O5 (-) clusters: The boron oxide analogs of C6H5 (+/0) and CH3Cl. *Journal of Chemical Physics*, **2015**, 143, 064303	3.9	11
40	B11(-): a moving subnanoscale tank tread. *Nanoscale*, **2015**, 7, 16054-60	7.7	62

39	Periodicity, Electronic Structures, and Bonding of Gold Tetrahalides [AuX4]- (X = F, Cl, Br, I, At, Uus). *Inorganic Chemistry*, **2015**, 54, 11157-67	5.1	18
38	Endohedral and exohedral metalloborospherenes: M@B40 (M=Ca, Sr) and M&B40 (M=Be, Mg). *Angewandte Chemie - International Edition*, **2015**, 54, 941-5	16.4	105
37	Formation and Characterization of the Boron Dicarbonyl Complex [B(CO)2]□*Angewandte Chemie*, **2015**, 127, 11230-11235	3.6	50
36	Cage-Like B41+ and B422+: New Chiral Members of the Borospherene Family. *Angewandte Chemie*, **2015**, 127, 8278-8282	3.6	7
35	Formation and characterization of the boron dicarbonyl complex [B(CO)2](-). *Angewandte Chemie - International Edition*, **2015**, 54, 11078-83	16.4	86
34	Experimental and theoretical evidence of an axially chiral borospherene. *ACS Nano*, **2015**, 9, 754-60	16.7	195
33	Chemical bonding in electron-deficient boron oxide clusters: core boronyl groups, dual 3c-4e hypervalent bonds, and rhombic 4c-4e bonds. *Physical Chemistry Chemical Physics*, **2014**, 16, 7274-9	3.6	27
32	Photoelectron spectroscopy of lithium and gold alloyed boron oxide clusters: charge transfer complexes, covalent gold, hyperhalogen, and dual three-center four-electron hyperbonds. *Physical Chemistry Chemical Physics*, **2014**, 16, 5129-36	3.6	21
31	Quasi-planar aromatic B36 and B36(-) clusters: all-boron analogues of coronene. *Physical Chemistry Chemical Physics*, **2014**, 16, 18282-7	3.6	73
30	The B35 cluster with a double-hexagonal vacancy: a new and more flexible structural motif for borophene. *Journal of the American Chemical Society*, **2014**, 136, 12257-60	16.4	250
29	Observation of an all-boron fullerene. *Nature Chemistry*, **2014**, 6, 727-31	17.6	590
28	Boronyl chemistry: the BO group as a new ligand in gas-phase clusters and synthetic compounds. *Accounts of Chemical Research*, **2014**, 47, 2435-45	24.3	64
27	D(3h) [A-CE3-A]? (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	3.9	5
26	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	6
25	Covalent Bonding in Au(BO) □ and Au(BS) □. *Journal of Cluster Science*, **2013**, 24, 233-241	3	9
24	Two-dimensional carbon allotropes from graphene to graphyne. *Journal of Materials Chemistry C*, **2013**, 1, 3677	7.1	91
23	Perfectly planar boronyl boroxine D3h B6O6: a boron oxide analog of boroxine and benzene. *Journal of Chemical Physics*, **2013**, 138, 244304	3.9	39
22	Binary nature of monolayer boron sheets from ab initio global searches. *Journal of Chemical Physics* , **2013**, 138, 024701	3.9	41

21	Ribbon aromaticity in double-chain planar B(n)H2(2-) and Li2B(n)H2 nanoribbon clusters up to n = 22: lithiated boron dihydride analogues of polyenes. *Physical Chemistry Chemical Physics*, **2013**, 15, 18872-80	3.6	25
20	Photoelectron spectroscopy of aromatic compound clusters of the B12 all-boron benzene: B12Au- and B12(BO)-. *Physical Chemistry Chemical Physics*, **2013**, 15, 9646-53	3.6	39
19	Comment on "Two-dimensional boron monolayer sheets". *ACS Nano*, **2013**, 7, 879	16.7	6
18	On the structures and bonding in boron-gold alloy clusters: B6Au(n)- and B6Au(n) (n = 1-3). *Journal of Chemical Physics*, **2013**, 138, 084306	3.9	21
17	Pi and sigma double conjugations in boronyl polyboroene nanoribbons: B(n)(BO)2- and B(n)(BO)2 (n = 5-12). *Journal of Chemical Physics*, **2013**, 139, 174301	3.9	35
16	Three-chain B(6n+14) cages as possible precursors for the syntheses of boron fullerenes. *Journal of Chemical Physics*, **2013**, 139, 224307	3.9	15
15	Photoelectron spectroscopy of boron-gold alloy clusters and boron boronyl clusters: B3Au(n)(-) and B3(BO)n(-) (n = 1, 2). *Journal of Chemical Physics*, **2013**, 139, 044308	3.9	26
14	Double-chain planar D2h B4H2, C2h B8H2, and C2h B12H2: conjugated aromatic borenes. *Physical Chemistry Chemical Physics*, **2012**, 14, 14769-74	3.6	47
13	Probing the structures and chemical bonding of boron-boronyl clusters using photoelectron spectroscopy and computational chemistry: B4(BO)(n)- (n = 1-3). *Journal of Chemical Physics*, **2012**, 137, 044307	3.9	23
12	CAl2Be3(2-) and its salt complex LiCAl2Be3-: anionic global minima with planar pentacoordinate carbon. *Journal of Physical Chemistry A*, **2012**, 116, 3290-4	2.8	44
11	Deciphering the mystery of hexagon holes in an all-boron graphene sheet. *Physical Chemistry Chemical Physics*, **2011**, 13, 11575-8	3.6	122
10	Hydrogenation of B 0/12 : A Planar-to-Icosahedral Structural Transition in B12H 0/h (n = 1) Boron Hydride Clusters. *Journal of Cluster Science*, **2011**, 22, 525-535	3	17
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