

Si-Dian Li

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164
papers

5,417
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176
ext. papers

6,370
ext. citations

6.6
avg, IF

5.95
L-index

#	Paper	IF	Citations
164	Observation of an all-boron fullerene. <i>Nature Chemistry</i> , 2014 , 6, 727-31	17.6	590
163	The B35 cluster with a double-hexagonal vacancy: a new and more flexible structural motif for borophene. <i>Journal of the American Chemical Society</i> , 2014 , 136, 12257-60	16.4	250
162	Experimental and theoretical evidence of an axially chiral borospherene. <i>ACS Nano</i> , 2015 , 9, 754-60	16.7	195
161	Vibrationally resolved photoelectron spectroscopy of BO ⁻ and BO ₂ ⁻ : a joint experimental and theoretical study. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 1030-5	2.8	151
160	B ₂ (BO) ₂ (²⁻)-diboronyl diborene: a linear molecule with a triple boron-boron bond. <i>Journal of the American Chemical Society</i> , 2008 , 130, 2573-9	16.4	142
159	Deciphering the mystery of hexagon holes in an all-boron graphene sheet. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 11575-8	3.6	122
158	Observation and characterization of the smallest borospherene, B ₂₈ (⁻) and B ₂₈ . <i>Journal of Chemical Physics</i> , 2016 , 144, 064307	3.9	119
157	From planar boron clusters to borophenes and metalloborophenes. <i>Nature Reviews Chemistry</i> , 2017 , 1, 1-10	34.6	118
156	Endohedral and exohedral metalloborospherenes: M@B ₄₀ (M=Ca, Sr) and M@B ₄₀ (M=Be, Mg). <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 941-5	16.4	105
155	A Supramolecular Radical Dimer: High-Efficiency NIR-II Photothermal Conversion and Therapy. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 15526-15531	16.4	97
154	Two-dimensional carbon allotropes from graphene to graphyne. <i>Journal of Materials Chemistry C</i> , 2013 , 1, 3677	7.1	91
153	Boronyls as key structural units in boron oxide clusters: B(BO) ₂ ⁻ and B(BO) ₃ ⁻ . <i>Journal of the American Chemical Society</i> , 2007 , 129, 9254-5	16.4	91
152	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. <i>Chemical Communications</i> , 2017 , 53, 1587-1590	5.8	90
151	Probing the structures and bonding of size-selected boron and doped-boron clusters. <i>Chemical Society Reviews</i> , 2019 , 48, 3550-3591	58.5	90
150	Cage-Like B ₄₁ (+) and B ₄₂ (2+): New Chiral Members of the Borospherene Family. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 8160-4	16.4	87
149	Formation and characterization of the boron dicarbonyl complex [B(CO) ₂] ⁽⁻⁾ . <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 11078-83	16.4	86
148	Manganese-centered tubular boron cluster - MnB ₁₆ (⁻): A new class of transition-metal molecules. <i>Journal of Chemical Physics</i> , 2016 , 144, 154310	3.9	84

147	Competition between drum and quasi-planar structures in RhB: motifs for metallo-boronanotubes and metallo-borophenes. <i>Chemical Science</i> , 2016 , 7, 7020-7027	9.4	78
146	Quasi-planar aromatic B ₃₆ and B ₃₆ (-) clusters: all-boron analogues of coronene. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 18282-7	3.6	73
145	The Planar CoB ₁₈ (-) Cluster as a Motif for Metallo-Borophenes. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 7358-63	16.4	71
144	Competition between quasi-planar and cage-like structures in the B cluster: photoelectron spectroscopy and ab initio calculations. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 29147-29155	3.6	71
143	On the analogy of B-BO and B-Au chemical bonding in B ₁₁ O- and B ₁₀ Au- clusters. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 12155-61	2.8	69
142	Boronyl chemistry: the BO group as a new ligand in gas-phase clusters and synthetic compounds. <i>Accounts of Chemical Research</i> , 2014 , 47, 2435-45	24.3	64
141	B ₁₁ (-): a moving subnanoscale tank tread. <i>Nanoscale</i> , 2015 , 7, 16054-60	7.7	62
140	Planar B and B clusters with a double-hexagonal vacancy: molecular motifs for borophenes. <i>Nanoscale</i> , 2017 , 9, 4550-4557	7.7	61
139	Observation of highly stable and symmetric lanthanide octa-boron inverse sandwich complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E6972-E6977	11.5	59
138	A Supramolecularly Activated Radical Cation for Accelerated Catalytic Oxidation. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 8933-7	16.4	57
137	Simplest neutral singlet C ₂ E ₄ (E = Al, Ga, In, and Tl) global minima with double planar tetracoordinate carbons: equivalence of C ₂ moieties in C ₂ E ₄ to carbon centers in CA ₄ (2-) and CA ₅ (+). <i>Journal of Physical Chemistry A</i> , 2009 , 113, 3395-402	2.8	53
136	In situ fabrication of (Sr,Lu)FeO ₄ with CoFe alloy nanoparticles as an independent catalyst layer for direct methane-based solid oxide fuel cells with a nickel cermet anode. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 13997-14007	13	50
135	Formation and Characterization of the Boron Dicarbonyl Complex [B(CO) ₂]. <i>Angewandte Chemie</i> , 2015 , 127, 11230-11235	3.6	50
134	Saturn-like charge-transfer complexes Li ₂ B ⁻ Li ₂ B ⁺ , and Li ₂ B ⁺ : exohedral metalloborospherenes with a perfect cage-like B ₁₀ core. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 9922-6	3.6	48
133	Double-chain planar D _{2h} B ₄ H ₂ , C _{2h} B ₈ H ₂ , and C _{2h} B ₁₂ H ₂ : conjugated aromatic borenes. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 14769-74	3.6	47
132	PrB : A Praseodymium-Doped Boron Cluster with a Pr Center Coordinated by a Doubly Aromatic Planar B ₁₀ Ligand. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 6916-6920	16.4	46
131	Lithium-Decorated Borospherene B: A Promising Hydrogen Storage Medium. <i>Scientific Reports</i> , 2016 , 6, 35518	4.9	45
130	Endohedral Ca@B ₃₈ : stabilization of a B ₃₈ (2-) borospherene dianion by metal encapsulation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 11610-5	3.6	45

129	CAL ₂ Be ₃ (²⁻) and its salt complex LiCAL ₂ Be ₃ ⁻ : anionic global minima with planar pentacoordinate carbon. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3290-4	2.8	44
128	[La(β B)La] (= 7-9): a new class of inverse sandwich complexes. <i>Chemical Science</i> , 2019 , 10, 2534-2542	9.4	42
127	Binary nature of monolayer boron sheets from ab initio global searches. <i>Journal of Chemical Physics</i> , 2013 , 138, 024701	3.9	41
126	Chemical bonding and dynamic fluxionality of a B ₁₅ (+) cluster: a nanoscale double-axle tank tread. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 15774-82	3.6	40
125	Perfectly planar boronyl boroxine D _{3h} B ₆ O ₆ : a boron oxide analog of boroxine and benzene. <i>Journal of Chemical Physics</i> , 2013 , 138, 244304	3.9	39
124	Photoelectron spectroscopy of aromatic compound clusters of the B ₁₂ all-boron benzene: B ₁₂ Au- and B ₁₂ (BO) ⁻ . <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 9646-53	3.6	39
123	Chemical Bonding of Crystalline LnB (Ln = La-Lu) and Its Relationship with LnB Gas-Phase Complexes. <i>Inorganic Chemistry</i> , 2018 , 57, 12999-13008	5.1	39
122	Endohedral charge-transfer complex Ca@B ₃₇ (⁻): stabilization of a B ₃₇ (³⁻) borospherene trianion by metal-encapsulation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14186-90	3.6	38
121	On the Upper Limits of Oxidation States in Chemistry. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 3242-3245	16.4	37
120	Preparation and Characterization of Uranium-Iron Triple-Bonded UFe(CO) and OUFe(CO) Complexes. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 6932-6936	16.4	36
119	Pi and sigma double conjugations in boronyl polyboroene nanoribbons: B(n)(BO) ₂ ⁻ and B(n)(BO) ₂ (n = 5-12). <i>Journal of Chemical Physics</i> , 2013 , 139, 174301	3.9	35
118	A Very Short Be-Be Distance but No Bond: Synthesis and Bonding Analysis of Ng-Be O -Ng' (Ng, Ng'=Ne, Ar, Kr, Xe). <i>Chemistry - A European Journal</i> , 2017 , 23, 2035-2039	4.8	34
117	Bridging μ -BO in B ₂ (BO) ₃ (⁻) and B ₃ (BO) ₃ (⁻) clusters: boronyl analogs of boranes. <i>ChemPhysChem</i> , 2011 , 12, 2549-53	3.2	34
116	T(d) B(BO) ₄ (⁻): a tetrahedral boron oxide cluster analogous to boron hydride T(d) BH ₄ (⁻). <i>Journal of Physical Chemistry A</i> , 2009 , 113, 2561-4	2.8	33
115	Relativistic Effects Break Periodicity in Group 6 Diatomic Molecules. <i>Journal of the American Chemical Society</i> , 2016 , 138, 1126-9	16.4	31
114	Endohedral C ₃ Ca@B ₃₉ (⁺) and C ₂ Ca@B ₃₉ (⁺): axially chiral metalloborospherenes based on B ₃₉ (⁻). <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 19690-4	3.6	30
113	A Supramolecular Radical Dimer: High-Efficiency NIR-II Photothermal Conversion and Therapy. <i>Angewandte Chemie</i> , 2019 , 131, 15672-15677	3.6	29
112	Planar B and B clusters with double-hexagonal vacancies. <i>Nanoscale</i> , 2019 , 11, 23286-23295	7.7	29

111	B33□ and B34□ Aromatic Planar Boron Clusters with a Hexagonal Vacancy. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 4546-4551	2.3	28
110	Chemical bonding in electron-deficient boron oxide clusters: core boronyl groups, dual 3c-4e hypervalent bonds, and rhombic 4c-4e bonds. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 7274-9	3.6	27
109	Structural transition in metal-centered boron clusters: from tubular molecular rotors Ta@B and Ta@B to cage-like endohedral metalloborospherene Ta@B. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 27025-27030	3.6	27
108	A universal mechanism of the planar boron rotors B ₃ , B ₄ , B ₅ , and B ₆ : inner wheels rotating in pseudo-rotating outer bearings. <i>Nanoscale</i> , 2017 , 9, 1443-1448	7.7	26
107	Quadruple bonding between iron and boron in the BFe(CO) complex. <i>Nature Communications</i> , 2019 , 10, 4713	17.4	26
106	Photoelectron spectroscopy of boron-gold alloy clusters and boron boronyl clusters: B ₃ Au(n)(-) and B ₃ (BO)n(-) (n = 1, 2). <i>Journal of Chemical Physics</i> , 2013 , 139, 044308	3.9	26
105	LaB: an inverse triple-decker lanthanide boron cluster. <i>Chemical Communications</i> , 2019 , 55, 7864-7867	5.8	25
104	Ribbon aromaticity in double-chain planar B(n)H ₂ (2-) and Li ₂ B(n)H ₂ nanoribbon clusters up to n = 22: lithiated boron dihydride analogues of polyenes. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 18872-80	3.6	25
103	The Planar CoB ₁₈ □ Cluster as a Motif for Metallo-Borophenes. <i>Angewandte Chemie</i> , 2016 , 128, 7484-7489	3.6	24
102	Re□ B and Re□ B: New Members of the Transition-Metal-Centered Borometallic Molecular Wheel Family. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 5317-5324	2.8	23
101	Crown ether complexes of actinyls: a computational assessment of AnO(15-crown-5) (An = U, Np, Pu, Am, Cm). <i>Dalton Transactions</i> , 2017 , 46, 12354-12363	4.3	23
100	Probing the structures and chemical bonding of boron-boronyl clusters using photoelectron spectroscopy and computational chemistry: B ₄ (BO)(n)- (n = 1-3). <i>Journal of Chemical Physics</i> , 2012 , 137, 044307	3.9	23
99	Lanthanides with Unusually Low Oxidation States in the PrB and PrB Boride Clusters. <i>Inorganic Chemistry</i> , 2019 , 58, 411-418	5.1	23
98	A CO ₂ -tolerant SrCo _{0.8} Fe _{0.15} Zr _{0.05} O ₃ □ cathode for proton-conducting solid oxide fuel cells. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 11292-11301	13	22
97	Probing the Electronic Structure and Chemical Bonding of Mono-Uranium Oxides with Different Oxidation States: UO _x (-) and UO _x (x = 3-5). <i>Journal of Physical Chemistry A</i> , 2016 , 120, 1084-96	2.8	22
96	Electronic Structure and Bonding Situation in MO (M = Be, Mg, Ca) Rhombic Clusters. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 2816-2822	2.8	21
95	Photoelectron spectroscopy of lithium and gold alloyed boron oxide clusters: charge transfer complexes, covalent gold, hyperhalogen, and dual three-center four-electron hyperbonds. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 5129-36	3.6	21
94	On the structures and bonding in boron-gold alloy clusters: B ₆ Au(n)- and B ₆ Au(n) (n = 1-3). <i>Journal of Chemical Physics</i> , 2013 , 138, 084306	3.9	21

93	Which Density Functional Should Be Used to Describe Protonated Water Clusters?. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 3117-3127	2.8	20
92	Photoelectron spectroscopy of B ₄ O ₄ ⁽⁻⁾ : Dual 3c-4e π -hyperbonds and rhombic 4c-4e σ -bond in boron oxide clusters. <i>Journal of Chemical Physics</i> , 2015 , 142, 134305	3.9	20
91	Spherical trihedral metallo-borospherenes. <i>Nature Communications</i> , 2020 , 11, 2766	17.4	20
90	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 18586-18590	16.4	20
89	Star-like superalkali cations featuring planar pentacoordinate carbon. <i>Journal of Chemical Physics</i> , 2016 , 144, 244303	3.9	19
88	Cage-like B clusters with the bonding pattern of π - π double delocalization: new members of the borospherene family. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 10998-11003	3.6	18
87	B and B: chiral quasi-planar boron clusters. <i>Nanoscale</i> , 2019 , 11, 9698-9704	7.7	18
86	Periodicity, Electronic Structures, and Bonding of Gold Tetrahalides [AuX ₄] ⁻ (X = F, Cl, Br, I, At, Uus). <i>Inorganic Chemistry</i> , 2015 , 54, 11157-67	5.1	18
85	Electronic structure and characterization of a uranyl di-15-crown-5 complex with an unprecedented sandwich structure. <i>Chemical Communications</i> , 2016 , 52, 12761-12764	5.8	18
84	Hydrogenation of B _{0/n} : A Planar-to-Icosahedral Structural Transition in B ₁₂ H _{0/n} (n = 1B) Boron Hydride Clusters. <i>Journal of Cluster Science</i> , 2011 , 22, 525-535	3	17
83	Predicting two-dimensional semiconducting boron carbides. <i>Nanoscale</i> , 2019 , 11, 11099-11106	7.7	16
82	A Supramolecularly Activated Radical Cation for Accelerated Catalytic Oxidation. <i>Angewandte Chemie</i> , 2016 , 128, 9079-9083	3.6	16
81	B: a bilayer boron cluster. <i>Nanoscale</i> , 2021 , 13, 3868-3876	7.7	16
80	A supramolecular radical cation: folding-enhanced electrostatic effect for promoting radical-mediated oxidation. <i>Chemical Science</i> , 2018 , 9, 5015-5020	9.4	16
79	Cage-like Ta@B complexes (n = 23-28, q = -1+3) in 18-electron configurations with the highest coordination number of twenty-eight. <i>Nanoscale</i> , 2018 , 10, 7451-7456	7.7	15
78	Three-chain B(6n+14) cages as possible precursors for the syntheses of boron fullerenes. <i>Journal of Chemical Physics</i> , 2013 , 139, 224307	3.9	15
77	Cage-like B ₄₀ ⁽⁺⁾ : a perfect borospherene monocation. <i>Journal of Molecular Modeling</i> , 2016 , 22, 124	2	15
76	Bond-bending isomerism of Au ₁ : competition between covalent bonding and aurophilicity. <i>Chemical Science</i> , 2016 , 7, 475-481	9.4	14

75	Fluxional Bonds in Planar B , Tubular Ta@B , and Cage-Like B. <i>Journal of Computational Chemistry</i> , 2019 , 40, 966-970	3.5	14
74	Heteroborospherene clusters Ni _n B (n = 1-4) and heteroborophene monolayers Ni _n B with planar heptacoordinate transition-metal centers in EB heptagons. <i>Scientific Reports</i> , 2017 , 7, 5701	4.9	13
73	PrB7@A Praseodymium-Doped Boron Cluster with a PrIII Center Coordinated by a Doubly Aromatic Planar B7@B73 Ligand. <i>Angewandte Chemie</i> , 2017 , 129, 7020-7024	3.6	12
72	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. <i>International Journal of Energy Research</i> , 2019 , 43, 2527-2537	4.5	12
71	Structures and chemical bonding of B3O3 (-/0) and B3O3H(-/0): A combined photoelectron spectroscopy and first-principles theory study. <i>Journal of Chemical Physics</i> , 2016 , 144, 124301	3.9	12
70	Exfoliation of borophenes from silver substrates assisted by Li/Mg atoms. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 4043-4048	7.1	11
69	A first-principles study on the B5O5 (+/0) and B5O5 (-) clusters: The boron oxide analogs of C6H5 (+/0) and CH3Cl. <i>Journal of Chemical Physics</i> , 2015 , 143, 064303	3.9	11
68	Direct Power Generation from Low Concentration Coal-Bed Gas by a Catalyst-Modified Solid Oxide Fuel Cell. <i>ChemElectroChem</i> , 2018 , 5, 1459-1466	4.3	11
67	Multiple Dirac cones in BN co-doped B-graphyne. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 7339-7344	7.1	11
66	M-X-M transformations in isomerization of B39 borospherenes. <i>AIP Advances</i> , 2016 , 6, 065110	1.5	11
65	NiB10, NiB11, NiB12, and NiB13+: Half-Sandwich Complexes with the Universal Coordination Bonding Pattern of Plus Double Delocalization. <i>Journal of Cluster Science</i> , 2019 , 30, 115-121	3	11
64	Relativity-Induced Bonding Pattern Change in Coinage Metal Dimers M (M = Cu, Ag, Au, Rg). <i>Inorganic Chemistry</i> , 2018 , 57, 5499-5506	5.1	10
63	Aromatic cage-like B and B: new axially chiral members of the borospherene family. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 15344-15349	3.6	10
62	Charge-induced structural transition between seashell-like B and B in 18 electron configurations. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 15330-15334	3.6	10
61	Expanded Inverse-Sandwich Complexes of Lanthanum Borides: LaB and LaB. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 2622-2630	2.8	10
60	Predicting lanthanide boride inverse sandwich tubular molecular rotors with the smallest core-shell structure. <i>Nanoscale</i> , 2019 , 11, 21311-21316	7.7	10
59	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 6923-6928	16.4	9
58	Formation and Characterization of a BeOBeC Multiple Radical Featuring a Quartet Carbyne Moiety. <i>Angewandte Chemie</i> , 2020 , 132, 6990-6995	3.6	9

57	Viable aromatic BeH stars enclosing a planar hypercoordinate boron or late transition metal. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 7217-7222	3.6	9
56	Covalent Bonding in Au(BO) \square and Au(BS) \square . <i>Journal of Cluster Science</i> , 2013 , 24, 233-241	3	9
55	Periodicity and Covalency of [MX ₂] \square (M = Cu, Ag, Au, Rg; X = H, Cl, CN) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 1395-1404	2.3	9
54	Purified high-sulfur coal as a fuel for direct carbon solid oxide fuel cells. <i>International Journal of Energy Research</i> , 2019 , 43, 2501-2513	4.5	9
53	A novel borophene featuring heptagonal holes: a common precursor of borospherenes. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 19890-19895	3.6	8
52	Zigzag double-chain CBe nanoribbon featuring planar pentacoordinate carbons and ribbon aromaticity. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 408-414	7.1	8
51	Bilayer B ₅₄ , B ₆₀ , and B ₆₂ Clusters in a Universal Structural Pattern. <i>European Journal of Inorganic Chemistry</i> , 2020 , 2020, 3296-3301	2.3	8
50	Sea-shell-like B and B: two new axially chiral members of the borospherene family.. <i>RSC Advances</i> , 2020 , 10, 10129-10133	3.7	8
49	A first-principles study on zigzag phosphorene nanoribbons passivated by iron-group atoms. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 25441-25445	3.6	8
48	High-symmetry tubular Ta@B, Ta@B, and Ta@B as embryos of \square boronanotubes with a transition-metal wire coordinated inside. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25009-25015	3.6	8
47	Preparation and Characterization of Uranium-Iron Triple-Bonded UFe(CO) ₃ \square and OUF ₂ (CO) ₃ \square Complexes. <i>Angewandte Chemie</i> , 2017 , 129, 7036-7040	3.6	7
46	Direct Operation of Solid Oxide Fuel Cells on Low-Concentration Oxygen-Bearing Coal-Bed Methane with High Stability. <i>Energy & Fuels</i> , 2018 , 32, 4547-4558	4.1	7
45	Cage-Like B ₄₁₊ and B ₄₂₂₊ : New Chiral Members of the Borospherene Family. <i>Angewandte Chemie</i> , 2015 , 127, 8278-8282	3.6	7
44	From inverse sandwich TaB and TaB to spherical trihedral TaB : prediction of the smallest metallo-borospherene.. <i>RSC Advances</i> , 2020 , 10, 29320-29325	3.7	7
43	Probing the Fluxional Bonding Nature of Rapid Cope rearrangements in Bullvalene CH and Its Analogs CH, CH, and CBH. <i>Scientific Reports</i> , 2019 , 9, 17074	4.9	7
42	First-Principles Study on the Oxidation of Supported \square 12-Borophene. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 28145-28151	3.8	6
41	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Single-Atom Catalysts. <i>Angewandte Chemie</i> , 2020 , 132, 18745-18749	3.6	6
40	From Quasi-Planar B to Penta-Ring Tubular Ca \square B: Prediction of Metal-Stabilized Ca \square B as the Embryo of Metal-Doped Boron \square Nanotubes. <i>Scientific Reports</i> , 2016 , 6, 37893	4.9	6

39	Theoretical studies on the bonding and electron structures of a [Au ₃ Sb ₆](3-) complex and its oligomers. <i>Dalton Transactions</i> , 2016 , 45, 11657-67	4.3	6
38	Planar D _{2h} B ₂₆ H ₈ , D _{2h} B ₂₆ H ₈ 2+, and C _{2h} B ₂₆ H ₆ : Building Blocks of Stable Boron Sheets with Twin-Hexagonal Holes. <i>Journal of Cluster Science</i> , 2013 , 24, 1127-1137	3	6
37	Comment on "Two-dimensional boron monolayer sheets". <i>ACS Nano</i> , 2013 , 7, 879	16.7	6
36	Donor-acceptor duality of the transition-metal-like B core in core-shell-like metallo-borosphenes La@[B@B] and La@[B@B].. <i>RSC Advances</i> , 2020 , 10, 34225-34230	3.7	6
35	Fluxional bonds in quasi-planar and half-sandwich (M = K, Rb, and Cs). <i>Journal of Computational Chemistry</i> , 2019 , 40, 1227-1232	3.5	6
34	Simulating the effect of a triple bond to achieve the shortest main group metal-metal distance in diberyllium complexes: a computational study. <i>Dalton Transactions</i> , 2018 , 47, 14462-14467	4.3	6
33	Uranyl/12-crown-4 Ether Complexes and Derivatives: Structural Characterization and Isomeric Differentiation. <i>Inorganic Chemistry</i> , 2018 , 57, 4125-4134	5.1	5
32	A solid oxide carbon fuel cell operating on pomelo peel char with high power output. <i>International Journal of Energy Research</i> , 2019 , 43, 2514-2526	4.5	5
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