Hua-Jin Zhai

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3157620/publications.pdf

Version: 2024-02-01

209 papers	16,072 citations	15466 65 h-index	17055 122 g-index
232 all docs	232 docs citations	232 times ranked	6058 citing authors

#	Article	IF	Citations
1	Au20: A Tetrahedral Cluster. Science, 2003, 299, 864-867.	6.0	1,091
2	Observation of an all-boron fullerene. Nature Chemistry, 2014, 6, 727-731.	6.6	724
3	Hydrocarbon analogues of boron clusters â€" planarity, aromaticity and antiaromaticity. Nature Materials, 2003, 2, 827-833.	13.3	650
4	On the Electronic and Atomic Structures of Small AuN- (N = 4â^'14) Clusters:â€‰ A Photoelectron Spectroscopy and Density-Functional Study. Journal of Physical Chemistry A, 2003, 107, 6168-6175.	1.1	598
5	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. Coordination Chemistry Reviews, 2006, 250, 2811-2866.	9.5	588
6	Planar-to-tubular structural transition in boron clusters: B20 as the embryo of single-walled boron nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 961-964.	3.3	490
7	A concentric planar doubly Ï€-aromatic B19â^' cluster. Nature Chemistry, 2010, 2, 202-206.	6.6	481
8	Hepta- and Octacoordinate Boron in Molecular Wheels of Eight- and Nine-Atom Boron Clusters: Observation and Confirmation. Angewandte Chemie - International Edition, 2003, 42, 6004-6008.	7.2	477
9	Experimental Observation and Confirmation of Icosahedral W@Au12 and Mo@Au12 Molecules. Angewandte Chemie - International Edition, 2002, 41, 4786-4789.	7.2	325
10	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, 12257-12260.	6.6	298
11	All-boron analogues of aromatic hydrocarbons: B17â^' and B18â^'. Journal of Chemical Physics, 2011, 134, 224304.	1.2	283
12	A Photoelectron Spectroscopic and Theoretical Study of B₁₆^{â^'} and B₁₆^{2â^'}: An All-Boron Naphthalene. Journal of the American Chemical Society, 2008, 130, 7244-7246.	6.6	264
13	Facile preparation of polypyrrole/graphene oxide nanocomposites with large areal capacitance using electrochemical codeposition forÂsupercapacitors. Journal of Power Sources, 2014, 263, 259-267.	4.0	235
14	Experimental and Theoretical Evidence of an Axially Chiral Borospherene. ACS Nano, 2015, 9, 754-760.	7.3	228
15	Electronic structure and chemical bonding of B5â^' and B5 by photoelectron spectroscopy andab initiocalculations. Journal of Chemical Physics, 2002, 117, 7917-7924.	1.2	222
16	All-Metal Antiaromatic Molecule: Rectangular Al44- in the Li3Al4- Anion. Science, 2003, 300, 622-625.	6.0	219
17	Electronic Structure, Isomerism, and Chemical Bonding in B7-and B7. Journal of Physical Chemistry A, 2004, 108, 3509-3517.	1.1	201
18	Observation of d-Orbital Aromaticity. Angewandte Chemie - International Edition, 2005, 44, 7251-7254.	7.2	197

#	Article	IF	Citations
19	Structure and Bonding in B6-and B6:Â Planarity and Antiaromaticity. Journal of Physical Chemistry A, 2003, 107, 1359-1369.	1.1	193
20	Photoelectron Spectroscopy and ab Initio Study of B3-and B4-Anions and Their Neutrals. Journal of Physical Chemistry A, 2003, 107, 9319-9328.	1.1	183
21	Aromaticity and antiaromaticity in transition-metal systems. Physical Chemistry Chemical Physics, 2008, 10, 257-267.	1.3	183
22	Probing the Electronic Structure and Band Gap Evolution of Titanium Oxide Clusters (TiO2)n- (n =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3022-3026.	6.6	178
23	B₂(BO)₂²⁻ Diboronyl Diborene:â€‰ A Linear Molecule with a Triple Boronâ^'Boron Bond. Journal of the American Chemical Society, 2008, 130, 2573-2579.	6.6	163
24	Vibrationally Resolved Photoelectron Spectroscopy of BO-and BO2-:Â A Joint Experimental and Theoretical Study. Journal of Physical Chemistry A, 2007, 111, 1030-1035.	1.1	160
25	Molecular Wheel B82- as a New Inorganic Ligand. Photoelectron Spectroscopy and ab Initio Characterization of LiB8-. Inorganic Chemistry, 2004, 43, 3552-3554.	1.9	150
26	Observation and characterization of the smallest borospherene, B28â^' and B28. Journal of Chemical Physics, 2016, 144, 064307.	1.2	141
27	Icosahedral gold cage clusters: M@Au[sub 12][sup â^'] (M=V, Nb, and Ta). Journal of Chemical Physics, 2004, 121, 8369.	1.2	137
28	[SiAu4]: Aurosilane. Angewandte Chemie - International Edition, 2004, 43, 2125-2129.	7.2	130
29	Î'â€…Aromaticity in [Ta3O3]â^'. Angewandte Chemie - International Edition, 2007, 46, 4277-4280.	7.2	130
30	Endohedral and Exohedral Metalloborospherenes: M@B₄₀ (M=Ca, Sr) and M&B₄₀ (M=Be, Mg). Angewandte Chemie - International Edition, 2015, 54, 941-945.	7.2	130
31	Al62- â^' Fusion of Two Aromatic Al3- Units. A Combined Photoelectron Spectroscopy and ab Initio Study of M+[Al62-] (M = Li, Na, K, Cu, and Au). Journal of the American Chemical Society, 2002, 124, 11791-11801.	6.6	124
32	Probing the Interactions of O₂ with Small Gold Cluster Anions (Au_n^{â^'}, n = 1â^'7): Chemisorption vs Physisorption. Journal of the American Chemical Society, 2010, 132, 4344-4351.	6.6	124
33	Gold Apes Hydrogen. The Structure and Bonding in the Planar B7Au2- and B7Au2 Clusters. Journal of Physical Chemistry A, 2006, 110, 1689-1693.	1.1	120
34	Electronic structure of chromium oxides, CrOnâ^' and CrOn (n=1â€“5) from photoelectron spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2001, 115, 7935-7944.	1.2	115
35	Electronic Structure and Chemical Bonding in MOn-and MOnClusters (M = Mo, W;n= 3â^'5):Â A Photoelectron Spectroscopy and ab Initio Study. Journal of the American Chemical Society, 2004, 126, 16134-16141.	6.6	110
36	Doping Golden Buckyballs: Cu@Au16â^' and Cu@Au17â^' Cluster Anions. Angewandte Chemie - International Edition, 2007, 46, 2915-2918.	7.2	110

#	Article	IF	Citations
37	Probing the Electronic Structure of Early Transition-Metal Oxide Clusters:â€‰ Polyhedral Cages of (V₂O₅)_n⁻ (n = 2â˜’4) and (M₂O₅)₂⁻ (M = Nb, Ta). Journal of the American Chemical Society, 2007, 129, 13270-13276.	6.6	109
38	Cageâ€Like B₄₁⁺ and B₄₂²⁺: New Chiral Members of the Borospherene Family. Angewandte Chemie - International Edition, 2015, 54, 8160-8164.	7.2	105
39	Photoelectron spectroscopy andab initiostudy of the doubly antiaromatic B62â˜’ dianion in the LiB6â˜’ cluster. Journal of Chemical Physics, 2005, 122, 054313.	1.2	103
40	Unique CO Chemisorption Properties of Gold Hexamer:â€‰ Au6(CO)n- (n = 0â˜’3). Journal of the American Chemical Society, 2005, 127, 12098-12106.	6.6	102
41	Probing the Electronic and Structural Properties of Chromium Oxide Clusters (CrO₃)_n^{â˜’} and (CrO₃)_n (n = 1â€“5): Photoelectron Spectroscopy and Density Functional Calculations. Journal of the American Chemical Society, 2008, 130, 5167-5177.	6.6	99
42	Boronyls as Key Structural Units in Boron Oxide Clusters:â€‰ B(BO)₂⁻ and B(BO)₃⁻. Journal of the American Chemical Society, 2007, 129, 9254-9255.	6.6	98
43	Probing the electronic structure of early transition metal oxide clusters: Molecular models towards mechanistic insights into oxide surfaces and catalysis. Chemical Physics Letters, 2010, 500, 185-195.	1.2	98
44	Probing the Electronic Structure and Aromaticity of Pentapnictogen Cluster Anions Pn5-(Pn = P, As,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Chemistry A, 2002, 106, 5600-5606.	1.1	94
45	Quasi-planar aromatic B₃₆and B₃₆^{â˜’}clusters: all-boron analogues of coronene. Physical Chemistry Chemical Physics, 2014, 16, 18282.	1.3	91
46	Chemisorption sites of CO on small gold clusters and transitions from chemisorption to physisorption. Journal of Chemical Physics, 2005, 122, 051101.	1.2	89
47	Competition between quasi-planar and cage-like structures in the B₂₉^{â˜’}cluster: photoelectron spectroscopy and ab initio calculations. Physical Chemistry Chemical Physics, 2016, 18, 29147-29155.	1.3	85
48	A highly flexible solid-state supercapacitor based on the carbon nanotube doped graphene oxide/polypyrrole composites with superior electrochemical performances. Organic Electronics, 2016, 37, 197-206.	1.4	84
49	On the Structure and Chemical Bonding of Tri-Tungsten Oxide Clusters W3On- and W3On (n = 7â˜’10):â€‰ W3O8 As A Potential Molecular Model for O-Deficient Defect Sites in Tungsten Oxides. Journal of Physical Chemistry A, 2006, 110, 85-92.	1.1	83
50	Coaxial Tripleâ€Layered versus Helical Be₆B₁₁^{â˜’} Clusters: Dual Structural Fluxionality and Multifold Aromaticity. Angewandte Chemie - International Edition, 2017, 56, 10174-10177.	7.2	83
51	An All-Metal Aromatic Sandwich Complex [Sb₃Au₃Sb₃]^{3â€“}. Journal of the American Chemical Society, 2015, 137, 10954-10957.	6.6	82
52	Superior performance of highly flexible solid-state supercapacitor based on the ternary composites of graphene oxide supported poly(3,4-ethylenedioxythiophene)-carbon nanotubes. Journal of Power Sources, 2016, 323, 125-133.	4.0	82
53	Electronic structure and chemical bonding of divanadium-oxide clusters (V2Ox, x=3â€“7) from anion photoelectron spectroscopy. Journal of Chemical Physics, 2002, 117, 7882-7888.	1.2	80
54	Structural and electronic properties of small titanium clusters: A density functional theory and anion photoelectron spectroscopy study. Journal of Chemical Physics, 2003, 118, 2116-2123.	1.2	79

#	Article	IF	Citations
55	On the Analogy of Bâ˜BO and Bâ˜Au Chemical Bonding in B₁₁O^{â˜} and B₁₀Au^{â˜} Clusters. Journal of Physical Chemistry A, 2010, 114, 12155-12161.	1.1	76
56	Planar B₃₈^{â˜}and B₃₇^{â˜}clusters with a double-hexagonal vacancy: molecular motifs for borophenes. Nanoscale, 2017, 9, 4550-4557.	2.8	76
57	Gold as hydrogen: Structural and electronic properties and chemical bonding in Si3Au3+â•0â•â˜ and comparisons to Si3H3+â•0â•â˜. Journal of Chemical Physics, 2006, 125, 133204.	1.2	75
58	Photoelectron Spectroscopy of Doubly and Singly Charged Group VIB Dimetalate Anions:â€‰ M2O72-, MMâ€˜O72-, and M2O7- (M, Mâ€˜ = Cr, Mo, W). Journal of Physical Chemistry A, 2005, 109, 10512-10520.	1.1	73
59	Probing the Electronic Structure and Chemical Bonding of Gold Oxides and Sulfides in AuO_n^{â˜} and AuS_n^{â˜} (n = 1, 2). Journal of the American Chemical Society, 2008, 130, 9156-9167.	6.6	72
60	B₁₁^{â˜}: a moving subnanoscale tank tread. Nanoscale, 2015, 7, 16054-16060.	2.8	72
61	Boronyl Chemistry: The BO Group as a New Ligand in Gas-Phase Clusters and Synthetic Compounds. Accounts of Chemical Research, 2014, 47, 2435-2445.	7.6	71
62	Experimental and Computational Studies of Alkali-Metal Coinage-Metal Clusters. Journal of Physical Chemistry A, 2006, 110, 4244-4250.	1.1	70
63	Electronic and Structural Evolution and Chemical Bonding in Ditungsten Oxide Clusters:Â W2On-and W2On(n= 1â˜6). Journal of Physical Chemistry A, 2005, 109, 6019-6030.	1.1	67
64	Peculiar Antiaromatic Inorganic Molecules of Tetrapnictogen in Na+Pn4-(Pn = P, As, Sb) and Important Consequences for Hydrocarbons. Inorganic Chemistry, 2002, 41, 6062-6070.	1.9	66
65	Experimental and Theoretical Characterization of Superoxide Complexes [W2O6(O2â˜)] and [W3O9(O2â˜)]: Models for the Interaction of O2 with Reduced W Sites on Tungsten Oxide Surfaces. Angewandte Chemie - International Edition, 2006, 45, 657-660.	7.2	66
66	Photoelectron spectroscopy of pentaatomic tetracoordinate planar carbon molecules: CAl3Siâ˜ and CAl3Geâ˜. Chemical Physics Letters, 2002, 357, 415-419.	1.2	65
67	Competition between linear and cyclic structures in monochromium carbide clusters CrCnâ˜ and CrCnâ€Š(n=2â€“8): A photoelectron spectroscopy and density functional study. Journal of Chemical Physics, 2004, 120, 8996-9008.	1.2	64
68	Quantum theory of concerted electronic and nuclear fluxes associated with adiabatic intramolecular processes. Physical Chemistry Chemical Physics, 2015, 17, 29421-29464.	1.3	64
69	Lithium-Decorated Borospherene B40: A Promising Hydrogen Storage Medium. Scientific Reports, 2016, 6, 35518.	1.6	64
70	Structural and Electronic Properties of Reduced Transition Metal Oxide Clusters, M₃O₈and M₃O₈^{â˜}(M = Cr, W), from Photoelectron Spectroscopy and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2009, 113, 11273-11288.	1.1	60
71	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.	1.3	58
72	Enhanced electrochemical performances of polypyrrole/carboxyl graphene/carbon nanotubes ternary composite for supercapacitors. Electrochimica Acta, 2018, 290, 1-11.	2.6	58

#	Article	IF	Citations
73	Structural and electronic properties of iron monoxide clusters FenO and FenOâ^'â€Š(n=2â€“6): A combined photoelectron spectroscopy and density functional theory study. Journal of Chemical Physics, 2003, 119, 11135-11145.	1.2	55
74	Probing the Electronic and Structural Properties of the Niobium Trimer Cluster and Its Mono- and Dioxides: Nb₃O_n^{â^'} and Nb₃O_n (n = 0â^'2). Journal of Physical Chemistry A, 2009, 113, 3866-3875.	1.1	55
75	Peculiar Allâ€Metal Ïƒâ€Aromaticity of the [Au₂Sb₁₆]^{4â^'} Anion in the Solid State. Angewandte Chemie - International Edition, 2016, 55, 15344-15346.	7.2	52
76	Chemisorption-induced Structural Changes and Transition from Chemisorption to Physisorption in Au₆(CO)_n^{â^'} (n = 4â^'9). Journal of Physical Chemistry C, 2008, 112, 11920-11928.	1.5	51
77	Endohedral Ca@B₃₈: stabilization of a B₃₈^{2â^'}borospherene dianion by metal encapsulation. Physical Chemistry Chemical Physics, 2016, 18, 11610-11615.	1.3	50
78	Stoichiometric and Oxygen-Rich M₂O_n^{â^'}and M₂O_n(M = Nb, Ta;n= 5â^'7) Clusters: Molecular Models for Oxygen Radicals, Diradicals, and Superoxides. Journal of the American Chemical Society, 2011, 133, 3085-3094.	6.6	49
79	Multiple Aromaticity and Antiaromaticity in Silicon Clusters. ChemPhysChem, 2004, 5, 1885-1891.	1.0	48
80	Structural Evolution, Sequential Oxidation, and Chemical Bonding in Tritantalum Oxide Clusters: Ta3Onâ^' and Ta3On (n = 1â^'8). Journal of Physical Chemistry A, 2009, 113, 9804-9813.	1.1	48
81	Photoelectron spectroscopy of aromatic compound clusters of the B12 all-boron benzene: B12Auâ^' and B12(BO)â^'. Physical Chemistry Chemical Physics, 2013, 15, 9646.	1.3	48
82	Petal-shaped poly(3,4-ethylenedioxythiophene)/sodium dodecyl sulfate-graphene oxide intercalation composites for high-performance electrochemical energy storage. Journal of Power Sources, 2014, 272, 203-210.	4.0	48
83	Chemical bonding and dynamic fluxionality of a B₁₅⁺cluster: a nanoscale double-axle tank tread. Physical Chemistry Chemical Physics, 2016, 18, 15774-15782.	1.3	48
84	Thiazole-based ratiometric fluorescence pH probe with large Stokes shift for intracellular imaging. Sensors and Actuators B: Chemical, 2016, 233, 566-573.	4.0	48
85	B26â^': The smallest planar boron cluster with a hexagonal vacancy and a complicated potential landscape. Chemical Physics Letters, 2017, 683, 336-341.	1.2	48
86	Electronic and structural evolution ofConclusters(n=1â€“108)by photoelectron spectroscopy. Physical Review B, 2001, 64, .	1.1	47
87	On the Electronic Structure and Chemical Bonding in the Tantalum Trimer Cluster. Journal of Physical Chemistry A, 2008, 112, 10962-10967.	1.1	47
88	Vibrationally Resolved Photoelectron Spectroscopy of Di-Gold Carbonyl Clusters Au₂(CO)_n^{â^'} (n = 1â^'3): Experiment and Theory. Journal of Physical Chemistry A, 2010, 114, 1247-1254.	1.1	47
89	Probing the electronic properties of dichromium oxide clusters Cr2Onâ^' (n=1â€“7) using photoelectron spectroscopy. Journal of Chemical Physics, 2006, 125, 164315.	1.2	46
90	Observation of Au[sub 2]H[sup â^'] impurity in pure gold clusters and implications for the anomalous Au-Au distances in gold nanowires. Journal of Chemical Physics, 2004, 121, 8231.	1.2	45

#	Article	IF	Citations
91	Probing the electronic and structural properties of doped aluminum clusters: MAl12â^' (M=Li, Cu, and) Tj ETQq1 1 0.784314 rgBT /Overl	1.2	45
92	On the Electronic and Structural Properties of Tri-Niobium Oxide Clusters Nb₃O_n^{â^'} (n = 3â^'8): Photoelectron Spectroscopy and Density Functional Calculations. Journal of Physical Chemistry A, 2010, 114, 5958-5966.	1.1	45
93	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.	1.3	45
94	On the Chemical Bonding of Gold in Auro-Boron Oxide Clusters AunBO-(n= 1â^'3). Journal of Physical Chemistry A, 2007, 111, 1648-1658.	1.1	44
95	Dynamic Mg₂B₈ Cluster: A Nanoscale Compass. Chemistry - an Asian Journal, 2017, 12, 2899-2903.	1.7	44
96	Photoelectron spectroscopy of Tinâ^' clusters (n=1â€“130). Journal of Chemical Physics, 2003, 118, 2108-2115.	1.2	43
97	Perfectly planar boronyl boroxine D3h B6O6: A boron oxide analog of boroxine and benzene. Journal of Chemical Physics, 2013, 138, 244304.	1.2	43
98	Planar or tetrahedral? A ternary 17-electron CBe₅H₄⁺ cluster with planar pentacoordinate carbon. Chemical Communications, 2020, 56, 8305-8308.	2.2	42
99	B₃₃^{â€“} and B₃₄^{â€“}: Aromatic Planar Boron Clusters with a Hexagonal Vacancy. European Journal of Inorganic Chemistry, 2017, 2017, 4546-4551.	1.0	41
100	Star-Like CBe₅Au₅⁺ Cluster: Planar Pentacoordinate Carbon, Superalkali Cation, and Multifold (Ï€ and Ï*f*) Aromaticity. Journal of Physical Chemistry A, 2018, 122, 1138-1145.	1.1	41
101	s-dhybridization and evolution of the electronic and magnetic properties in small Co and Ni clusters. Physical Review B, 2002, 65, .	1.1	40
102	Electronic and Structural Evolution of Monoiron Sulfur Clusters, FeSn- and FeSn (n = 1â^'6), from Anion Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2003, 107, 2821-2828.	1.1	40
103	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.	1.2	40
104	Bridging Î·²â€BO in B₂(BO)₃^{â^'} and B₃(BO)₃^{â^'} Clusters: Boronyl Analogs of Boranes. ChemPhysChem, 2011, 12, 2549-2553.	1.0	39
105	A comparative study on long and short carbon nanotubes-incorporated polypyrrole/poly(sodium) Tj ETQq1 1 0.784314 rgBT /Overlock 1 Metals, 2015, 209, 405-411.	2.1	39
106	Photoelectron spectroscopy of mono-niobium carbide clusters NbCnâ^'(n=2â€“7): Evidence for a cyclic to linear structural transition. Journal of Chemical Physics, 2001, 115, 5170-5178.	1.2	37
107	Structural and Electronic Properties of Reduced Transition Metal Oxide Clusters, M₄O₁₀ and M₄O₁₀^{â€“} (M = Cr, W), from Photoelectron Spectroscopy and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2012, 116, 5256-5271.	1.1	36
108	A universal mechanism of the planar boron rotors B₁₁^{â^'}, B₁₃⁺, B₁₅⁺, and B₁₉^{â^'}: inner wheels rotating in pseudo-rotating outer bearings. Nanoscale, 2017, 9, 1443-1448.	2.8	35

#	Article	IF	Citations
109	Enhanced supercapacitive behaviors of poly(3,4-ethylenedioxythiophene)/ graphene oxide hybrids prepared under optimized electropolymerization conditions. Electrochimica Acta, 2021, 372, 137861.	2.6	35
110	Cu3C4-:Â A New Sandwich Molecule with Two Revolving C22-Units. Journal of Physical Chemistry A, 2005, 109, 562-570.	1.1	32
111	Photoelectron spectroscopy of boron-gold alloy clusters and boron boronyl clusters: B3Aunâ^' and B3(BO)nâ^' (n = 1, 2). Journal of Chemical Physics, 2013, 139, 044308.	1.2	32
112	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.	1.3	31
113	Endohedral C₃Ca@B₃₉⁺and C₂Ca@B₃₉⁺: axially chiral metalloborospherenes based on B₃₉^{â^'}. Physical Chemistry Chemical Physics, 2015, 17, 19690-19694.	1.3	31
114	Boron-based binary Be₆B₁₀^{2â^'} cluster: three-layered aromatic sandwich, electronic transmutation, and dynamic structural fluxionality. Physical Chemistry Chemical Physics, 2018, 20, 22719-22729.	1.3	30
115	Evolution of the electronic properties of small Ninâ^'â€Š(n=1â€“100) clusters by photoelectron spectroscopy. Journal of Chemical Physics, 2002, 117, 9758-9765.	1.2	29
116	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.	1.3	29
117	Why nanoscale tank treads move? Structures, chemical bonding, and molecular dynamics of a doped boron cluster B₁₀C. Nanoscale, 2017, 9, 9310-9316.	2.8	29
118	Sandwich-type Na₆B₇^{â^'} and Na₈B₇⁺ clusters: charge-transfer complexes, four-fold Ï€/Ïƒ aromaticity, and dynamic fluxionality. Physical Chemistry Chemical Physics, 2019, 21, 18338-18345.	1.3	29
119	Star-like superalkali cations featuring planar pentacoordinate carbon. Journal of Chemical Physics, 2016, 144, 244303.	1.2	28
120	The [(Al₂O₃)₂]^{â^'} Anion Cluster: Electron Localizationâ€“Delocalization Isomerism. ChemPhysChem, 2009, 10, 2410-2413.	1.0	27
121	A facile approach to improve the electrochemical properties of polyaniline-carbon nanotube composite electrodes for highly flexible solid-state supercapacitors. International Journal of Hydrogen Energy, 2018, 43, 18339-18348.	3.8	27
122	Probing the structures and chemical bonding of boron-boronyl clusters using photoelectron spectroscopy and computational chemistry: B4(BO)nâ^' (n = 1â€“3). Journal of Chemical Physics, 2012, 137, 044307.	1.2	26
123	On the structures and bonding in boron-gold alloy clusters: B6Aunâ^' and B6Aun (n = 1â^'3). Journal of Chemical Physics, 2013, 138, 084306.	1.2	24
124	Monohafnium Oxide Clusters HfO_n^{â€“} and HfO_n (n = 1â€“6): Oxygen Radicals, Superoxides, Peroxides, Diradicals, and Triradicals. Journal of Physical Chemistry A, 2013, 117, 1042-1052.	1.1	23
125	Photoelectron spectroscopy of B4O4â^': Dual 3c-4e Ï€ hyperbonds and rhombic 4c-4e o-bond in boron oxide clusters. Journal of Chemical Physics, 2015, 142, 134305.	1.2	23
126	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.	1.3	22

#	Article	IF	Citations
127	B₃₁^{â^'} and B₃₂^{â^'}: chiral quasi-planar boron clusters. Nanoscale, 2019, 11, 9698-9704.	2.8	22
128	Ternary CBe₄Au₄ cluster: a 16-electron system with quasi-planar tetracoordinate carbon. Physical Chemistry Chemical Physics, 2018, 20, 6299-6306.	1.3	20
129	Planar Pentacoordinate versus Tetracoordinate Carbons in Ternary CBe₄Li₄ and CBe₄Li₄^{2â€“} Clusters. Journal of Physical Chemistry A, 2018, 122, 8370-8376.	1.1	20
130	Peculiar Allâ€Metal Ïƒâ€Aromaticity of the [Au₂Sb₁₆]^{4â^'} Anion in the Solid State. Angewandte Chemie, 2016, 128, 15570-15572.	1.6	19
131	Ternary 12-electron CBe₃X₃⁺ (X = H, Li, Na, Cu, Ag) clusters: planar tetracoordinate carbons and superalkali cations. Physical Chemistry Chemical Physics, 2019, 21, 22048-22056.	1.3	17
132	Coaxial Tripleâ€Layered versus Helical Be₆B₁₁^{â^'} Clusters: Dual Structural Fluxionality and Multifold Aromaticity. Angewandte Chemie, 2017, 129, 10308-10311.	1.6	17
133	Planar pentacoordinate carbon in a sulphur-surrounded boron wheel: the global minimum of CB₅S₅⁺. Chemical Communications, 2022, 58, 2552-2555.	2.2	17
134	On the electronic structure and conflicting d-orbital aromaticity in the Re3O3â^' cluster. RSC Advances, 2012, 2, 2707.	1.7	16
135	Cage-like B40 +: a perfect borospherene monocation. Journal of Molecular Modeling, 2016, 22, 124.	0.8	16
136	Adjust the electrochemical performances of graphene oxide nanosheets-loaded poly(3,4-ethylenedioxythiophene) composites for supercapacitors with ultralong cycle life. Journal of Materials Science: Materials in Electronics, 2016, 27, 2773-2782.	1.1	16
137	Boron-based inorganic heterocyclic clusters: electronic structure, chemical bonding, aromaticity, and analogy to hydrocarbons. Physical Chemistry Chemical Physics, 2019, 21, 20523-20537.	1.3	16
138	A dual-doped strategy to enhance the electrochemical performances of electropolymerized polyaniline electrodes for flexible energy storage. Materials Chemistry and Physics, 2020, 240, 122259.	2.0	16
139	In Search of Covalently Bound Tetra- and Penta-Oxygen Species:Â A Photoelectron Spectroscopic and Ab Initio Investigation of MO4-and MO5-(M = Li, Na, K, Cs). Journal of the American Chemical Society, 2002, 124, 6742-6750.	6.6	15
140	On the electronic structure of mono-rhenium oxide clusters: and ReOn (n=3,4). Chemical Physics Letters, 2011, 512, 49-53.	1.2	15
141	Mechanically exfoliated graphite paper with layered microstructures for enhancing flexible electrochemical energy storage. Inorganic Chemistry Frontiers, 2022, 9, 1920-1930.	3.0	15
142	Planar dicyclic B6S6, B6S6â^', and B6S62â^' clusters: Boron sulfide analogues of naphthalene. Journal of Chemical Physics, 2015, 142, 014302.	1.2	14
143	A first-principles study on the B5O5+/0 and B5O5â^' clusters: The boron oxide analogs of C6H5+/0 and CH3Cl. Journal of Chemical Physics, 2015, 143, 064303.	1.2	14
144	Structures and chemical bonding of B3O3â^'/0 and B3O3Hâ^'/0: A combined photoelectron spectroscopy and first-principles theory study. Journal of Chemical Physics, 2016, 144, 124301.	1.2	14

#	Article	IF	Citations
145	Concentric dual Ï€ aromaticity in bowl-like B₃₀cluster: an all-boron analogue of corannulene. Physical Chemistry Chemical Physics, 2016, 18, 23304-23311.	1.3	14
146	A niobium-necked cluster [As₃Nb(As₃Sn₃)]^{3â^'}with aromatic Sn₃^{2â^'}. Dalton Transactions, 2016, 45, 3874-3879.	1.6	14
147	Divide and Stack Up: Boronâ€Based Sandwich Cluster as a Subnanoscale Propeller. Chemistry - an Asian Journal, 2019, 14, 2945-2949.	1.7	14
148	Starting a subnanoscale tank tread: dynamic fluxionality of boron-based B₁₀Ca alloy cluster. Nanoscale Advances, 2019, 1, 735-745.	2.2	14
149	Boronâ€Based Chiral Helix Be₆B₁₀^{2â^'} and Be₆B₁₁^{â^'} Clusters: Structures, Chemical Bonding, and Formation Mechanism. Chemistry - an Asian Journal, 2020, 15, 1094-1104.	1.7	14
150	Remarkably enhanced performances of polyaniline/electrochemically surface-treated graphite electrodes with optimal charge transfer pathways for flexible supercapacitor application. Journal of Power Sources, 2018, 402, 311-319.	4.0	13
151	Bare and ligand protected planar hexacoordinate silicon in SiSb₃M₃⁺ (M = Ca, Sr, Ba) clusters. Chemical Science, 2022, 13, 8045-8051.	3.7	13
152	Sequential Oxidation of the Cubane [4Feâ^'4S] Cluster from [4Feâ^'4S]-to [4Feâ^'4S]3+in Fe4S4Ln-Complexes. Journal of the American Chemical Society, 2004, 126, 8413-8420.	6.6	12
153	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.	1.1	12
154	On the nature of chemical bonding in the all-metal aromatic [Sb₃Au₃Sb₃]^{3â^'} sandwich complex. Physical Chemistry Chemical Physics, 2016, 18, 13423-13431.	1.3	12
155	High performance flexible supercapacitor based on electropolymerized poly(3,4-ethylenedioxythiophene) grown on superficial expansion-treated graphite. Organic Electronics, 2018, 63, 149-158.	1.4	12
156	Boron-based ternary Rb₆Be₂B₆ cluster featuring unique sandwich geometry and a naked hexagonal boron ring. Physical Chemistry Chemical Physics, 2020, 22, 20043-20049.	1.3	12
157	Cageâ€Like B₄₁⁺ and B₄₂²⁺: New Chiral Members of the Borospherene Family. Angewandte Chemie, 2015, 127, 8278-8282.	1.6	11
158	On the structure and bonding in the B₄O₄⁺cluster: a boron oxide analogue of the 3,5-dehydrophenyl cation with p and s double aromaticity. Physical Chemistry Chemical Physics, 2015, 17, 29697-29706.	1.3	11
159	Ternary B₂X₂H₂(X = O and S) rhombic clusters and their potential use as inorganic ligands in sandwich-type (B₂X₂H₂)₂Ni complexes. Physical Chemistry Chemical Physics, 2015, 17, 16798-16804.	1.3	11
160	Rapid preparation of the hybrid of MnO 2 dispersed on graphene nanosheets with enhanced supercapacitive performance. Electrochimica Acta, 2016, 215, 339-345.	2.6	11
161	On the nature of bonding in binary Be2O2and Si2O2clusters: rhombic four-center four-electron Ï€ and Ïƒ bonds. Physical Chemistry Chemical Physics, 2016, 18, 9594-9601.	1.3	11
162	Nature of Bonding in Bowlâ€Like B₃₆ Cluster Revisited: Concentric (6Ï€+18Ï€) Double Aromaticity and Reason for the Preference of a Hexagonal Hole in a Central Location. Chemistry - an Asian Journal, 2018, 13, 1148-1156.	1.7	11

#	Article	IF	Citations
163	Planar Tricyclic B₈O₈ and B₈O₈^{â€“} Clusters: Boron Oxide Analogues of s-Indacene C₁₂H₈. Journal of Physical Chemistry A, 2018, 122, 2297-2306.	1.1	11
164	A simple strategy to prepare polyaniline nanorods by surfactant-assisted electropolymerization for remarkably improved supercapacitive performances. Organic Electronics, 2019, 69, 98-105.	1.4	11
165	Transition-metal-like bonding behaviors of a boron atom in a boron-cluster boronyl complex [(Î·⁷-B₇)-B-BO]^{â^’}. Chemical Science, 2021, 12, 8157-8164.	3.7	11
166	The high-capacity hydrogen storage of B6Ca2 and B8Ca2 inverse sandwiches. International Journal of Hydrogen Energy, 2021, 46, 24225-24232.	3.8	10
167	Boosting the electrochemical capacitive properties of polypyrrole using carboxylated graphene oxide as a new dopant. Journal of Materials Science: Materials in Electronics, 2018, 29, 7893-7903.	1.1	9
168	A designer 32-electron superatomic CBe8H12 cluster: coreâ€“shell geometry, octacoordinate carbon, and cubic aromaticity. New Journal of Chemistry, 2020, 44, 7286-7292.	1.4	9
169	[Sb4Au4Sb4]2â^’: A designer all-metal aromatic sandwich. Journal of Chemical Physics, 2016, 145, 044308.	1.2	8
170	Promoted supercapacitive performances of electrochemically synthesized poly(3,4-ethylenedioxythiophene) incorporated with manganese dioxide. Journal of Materials Science: Materials in Electronics, 2018, 29, 3935-3942.	1.1	8
171	Planar B₃S₂H₃^{â^’}and B₃S₂H₃clusters with a five-membered B₃S₂ring: boronâ€“sulfur hydride analogues of cyclopentadiene. Physical Chemistry Chemical Physics, 2016, 18, 21412-21420.	1.3	7
172	Chemical Bonding and Ïƒ-Aromaticity in Charged Molecular Alloys: [Pd2As14]4â^’ and [Au2Sb14]4â^’ Clusters. Scientific Reports, 2017, 7, 791.	1.6	7
173	Wheel-like, elongated, circular, and linear geometries in boron-based C_nB_{7â^’n}(n = 0â€“7) clusters: structural transitions and aromaticity. Physical Chemistry Chemical Physics, 2017, 19, 24284-24293.	1.3	7
174	Planar tetracoordinate carbon molecules with 14 valence electrons: examples of CBe₄M_n^{nâ^’2} (M = Li, Au; n = 1â€“3) clusters. New Journal of Chemistry, 2020, 44, 18293-18302.	1.4	7
175	A strategy to boost electrochemical properties of the graphene oxideâ€“poly(3,4-ethylenedioxythiophene) composites for supercapacitor electrodes. Journal of Materials Science, 2018, 53, 5216-5228.	1.7	6
176	Anchoring a bow-shaped boron single chain in binary Be6B7â^’ cluster: hybrid octagonal ring, multifold Ï€/Ïƒ aromaticity, and dual electronic transmutation. Physical Chemistry Chemical Physics, 2020, 22, 25574-25583.	1.3	6
177	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.	1.2	5
178	Boronyl as a terminal ligand in boron oxide clusters: hexagonal ring C_{2v}B₆O₄and ethylene-like D_{2h}B₆O₄^{â^’/2â^’}. Physical Chemistry Chemical Physics, 2015, 17, 19929-19935.	1.3	5
179	Pentagonal five-center four-electron Ï€ bond in ternary B₃N₂H₅ cluster: an extension of the concept of three-center four-electron Ï‰ bond. Physical Chemistry Chemical Physics, 2017, 19, 2479-2486.	1.3	5
180	B₁₂F_n^{0/â^’}(n= 1â€“6) series: when do boron double chain nanoribbons become global minima?. Physical Chemistry Chemical Physics, 2017, 19, 31655-31665.	1.3	5

#	Article	IF	Citations
181	Structures and bonding of B 4 O 5 and B 4 O 5 â^' clusters: Emergence of boroxol ring and competition between rhombic B 2 O 2 and hexagonal B 3 O 3 cores. International Journal of Quantum Chemistry, 2019, 119, e25907.	1.0	5
182	Facile preparation of polyaniline-carbon nanotube hybrid electrodes and dependence of their supercapacitive properties on degree of carboxylation of carbon nanotubes. Journal of Nanoparticle Research, 2020, 22, 1.	0.8	5
183	An effective approach to prepare three-dimensional porous manganese dioxide electrodes by surfactant assisted electrosynthesis for improved supercapacitive properties. Journal of Materials Science: Materials in Electronics, 2017, 28, 13983-13989.	1.1	4
184	Boron-based Be₂B₅^{+/0/â^'} alloy clusters: inverse sandwiches with pentagonal boron ring and reduction-induced structural transformation to molecular wheel structure. New Journal of Chemistry, 2021, 45, 4675-4682.	1.4	4
185	Au20: A Tetrahedral Cluster.. ChemInform, 2003, 34, no.	0.1	3
186	On the Nature of Bonding in Synthetic Charged Molecular Alloy [P7ZnP7]4â€“ Cluster and Its Relevant [P7]3â€“ Zintl Ion. ACS Omega, 2018, 3, 11958-11965.	1.6	3
187	Are all planar and quasi-planar boron clusters aromatic? Counter examples of island or global Ï€ antiaromaticity from chemical bonding analysis. Physical Chemistry Chemical Physics, 2020, 22, 25084-25094.	1.3	3
188	Concentric Inner 2Ï€/6Ïƒ and Outer 10Ï€/14Ïƒ Aromaticity Underlies the Dynamic Structural Fluxionality of Planar B₁₉^{â€“} Wankel Motor Cluster. Journal of Physical Chemistry A, 2021, 125, 5022-5030.	1.1	3
189	Ternary 14-electron XB₂Be₂ (X = Si, Ge, Sn, Pb) clusters: a planar tetracoordinate silicon (ptSi) system and its ptGe/Sn/Pb congeners. Physical Chemistry Chemical Physics, 2022, 24, 7068-7076.	1.3	3
190	The unique sandwich K₆Be₂B₆H₆ cluster with a real borozene B₆H₆ core. RSC Advances, 2022, 12, 8617-8623.	1.7	3
191	Structures and chemical bonding of boron-based B₁₂O and B₁₁Au clusters. A counterexample in boronyl chemistry. Physical Chemistry Chemical Physics, 2022, 24, 10952-10961.	1.3	3
192	On the Electronic and Atomic Structures of Small AuN- (N = 4â€”14) Clusters: A Photoelectron Spectroscopy and Density-Functional Study.. ChemInform, 2003, 34, no.	0.1	2
193	Can Synthetic Allâ€Metal Cluster Compound Support Multifold (Ï€ and Ïƒ) Aromaticity and dâ€Orbital Aromaticity?. Chinese Journal of Chemistry, 2019, 37, 126-130.	2.6	2
194	Cycling stability depends closely on scan rate: the case of polyaniline supercapacitor electrodes. Soft Materials, 2020, , 1-5.	0.8	2
195	Electronic and Structural Evolution of Monoiron Sulfur Clusters, FeS-n and FeSn (n = 1â€”6) from Anion Photoelectron Spectroscopy.. ChemInform, 2003, 34, no.	0.1	1
196	Chapter 3 Probing the unique size-dependent properties of small Au clusters, Au alloy clusters, and CO-chemisorbed Au clusters in the gas phase. Chemical Physics of Solid Surfaces, 2007, , 91-150.	0.3	1
197	A photoelectron spectroscopy and quantum chemical study on ternary Alâ€“Bâ€“O clusters: Al_nBO₂^{â^'} and Al_nBO₂ (n = 2, 3). Physical Chemistry Chemical Physics, 2018, 20, 5200-5209.	1.3	1
198	In search of the smallest boroxolâ€type heterocyclic ring system: Planar hexagonal B 3 S 3 + cluster with double 6Ï€/2Ïƒ aromaticity. International Journal of Quantum Chemistry, 2020, 120, e26229.	1.0	1

#	Article	IF	Citations
199	Obvious enhancement in electrochemical capacitive properties for poly(3,4-ethylenedioxythiophene) electrodes prepared under optimized conditions. Journal of Materials Science: Materials in Electronics, 2021, 32, 10078-10088.	1.1	1
200	Boron Oxide B5O6â˜ Cluster as a Boronyl-Based Inorganic Analog of Phenolate Anion. Frontiers in Chemistry, 2022, 10, 868782.	1.8	1
201	Structure and Bonding in B6- and B6: Planarity and Antiaromaticity.. ChemInform, 2003, 34, no.	0.1	0
202	Hepta- and Octacoordinate Boron in Molecular Wheels of Eight- and Nine-Atom Boron Clusters: Observation and Confirmation.. ChemInform, 2004, 35, no.	0.1	0
203	Electronic Structure, Isomerism, and Chemical Bonding in B7- and B7. ChemInform, 2004, 35, no.	0.1	0
204	[SiAu4]: Aurosilane.. ChemInform, 2004, 35, no.	0.1	0
205	Molecular Wheel B2-8 as a New Inorganic Ligand. Photoelectron Spectroscopy and ab initio Characterization of LiB-8.. ChemInform, 2004, 35, no.	0.1	0
206	Sequential Oxidation of the Cubane [4Feâ€”4S] Cluster from [4Feâ€”4S]- to [4Feâ€”4S]3+ in Fe4S4L-n Complexes.. ChemInform, 2004, 35, no.	0.1	0
207	Electronic Structure and Chemical Bonding in MOn- and MOn Clusters (M: Mo, W; n = 3?5): A Photoelectron Spectroscopy and ab initio Study.. ChemInform, 2005, 36, no.	0.1	0
208	Observation of d-Orbital Aromaticity.. ChemInform, 2006, 37, no.	0.1	0
209	Chemical Bonding in Transition Metal Nitride Os3N3+ Cluster: 6Ï€ Inorganic Benzene and Î?2Î*1Î*1 Aromaticity. ACS Omega, 2018, 3, 17083-17091.	1.6	0