

Yue-Wen Mu

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Observation of an all-boron fullerene. <i>Nature Chemistry</i> , 2014, 6, 727-731.	13.6	724
2	O-coordinated W-Mo dual-atom catalyst for pH-universal electrocatalytic hydrogen evolution. <i>Science Advances</i> , 2020, 6, eaba6586.	10.3	263
3	Cage-like B_{41}^{+} and B_{42}^{2+} : New Chiral Members of the Borospherene Family. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 8160-8164.	13.8	105
4	A DFT based method for calculating the surface energies of asymmetric MoP facets. <i>Applied Surface Science</i> , 2018, 427, 357-362.	6.1	81
5	Planar B_{38}^{\sim} and B_{37}^{\sim} clusters with a double-hexagonal vacancy: molecular motifs for borophenes. <i>Nanoscale</i> , 2017, 9, 4550-4557.	5.6	76
6	Chemical Functionalization of GaN Monolayer by Adatom Adsorption. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20911-20916.	3.1	65
7	Lithium-Decorated Borospherene B ₄₀ : A Promising Hydrogen Storage Medium. <i>Scientific Reports</i> , 2016, 6, 35518.	3.3	64
8	Saturn-like charge-transfer complexes $Li_4 \& B_{36}$, $Li_5 \& B_{36}^{+}$, and $Li_6 \& B_{36}^{2+}$: exohedral metalloborospherenes with a perfect cage-like $B_{36}^{4\sim}$ core. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 9922-9926.	2.8	58
9	Endohedral $Ca@B_{38}$: stabilization of a $B_{38}^{2\sim}$ borospherene dianion by metal encapsulation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11610-11615.	2.8	50
10	Structures and magnetic properties of $SinMn^{\sim}$ ($n=1\sim 15$) clusters. <i>Journal of Chemical Physics</i> , 2009, 130, 164514.	3.0	46
11	Graphitic-N highly doped graphene-like carbon: A superior metal-free catalyst for efficient reduction of CO ₂ . <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120510.	20.2	46
12	Binary nature of monolayer boron sheets from <i>ab initio</i> global searches. <i>Journal of Chemical Physics</i> , 2013, 138, 024701.	3.0	44
13	N-Doped amorphous MoS_x for the hydrogen evolution reaction. <i>Nanoscale</i> , 2019, 11, 11217-11226.	5.6	43
14	B_{48}^{\sim} : a bilayer boron cluster. <i>Nanoscale</i> , 2021, 13, 3868-3876.	5.6	43
15	Scalable Production of Freestanding Few-Layer B_{12} -Borophene Single Crystalline Sheets as Efficient Electrocatalysts for Lithium-Sulfur Batteries. <i>ACS Nano</i> , 2021, 15, 17327-17336.	14.6	40
16	Structural transition in metal-centered boron clusters: from tubular molecular rotors $Ta@B_{21}$ and $Ta@B_{22}^{+}$ to cage-like endohedral metalloborospherene $Ta@B_{22}^{\sim}$. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27025-27030.	2.8	38
17	Ribbon aromaticity in double-chain planar BnH_{2n}^{\sim} and Li_2BnH_2 nanoribbon clusters up to $n = 22$: lithiated boron dihydride analogues of polyenes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18872.	2.8	31
18	Endohedral $C_3@B_{39}^{+}$ and $C_2@B_{39}^{+}$: axially chiral metalloborospherenes based on B_{39}^{\sim} . <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19690-19694.	2.8	31

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19	Predicting two-dimensional semiconducting boron carbides. <i>Nanoscale</i> , 2019, 11, 11099-11106.	5.6	29
20	Structures and magnetic properties of Pd clusters (Pd _n) ⁺ clusters (n = 1-10) with the bonding pattern of T _h symmetry. <i>Physical Review A</i> , 2011, 84, 043407.	2.5	28
21	Cage-like B ₃₉ ⁺ clusters with the bonding pattern of I _h + I _h double delocalization: new members of the borospherene family. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10998-11003.	2.8	23
22	Cage-like Ta@B _q n 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.	5.6	23
23	Fluxional Bonds in Planar B ₁₉ ⁺ , Tubular Ta@B ₂₀ ⁺ , and Cage-like B ₃₉ ⁺ . <i>Journal of Computational Chemistry</i> , 2019, 40, 966-970.	3.3	23
24	Structures and magnetic properties of Si _n Ni (n = 1-17) clusters. <i>Computational and Theoretical Chemistry</i> , 2009, 916, 139-146.	1.5	21
25	Two-dimensional gradient Ag nanoparticle assemblies: multiscale fabrication and SERS applications. <i>Nanotechnology</i> , 2010, 21, 495601.	2.6	21
26	Strain-induced metal-semimetal transition of Be ₂ monolayer. <i>RSC Advances</i> , 2015, 5, 11392-11396.	3.6	19
27	Predicting lanthanide boride inverse sandwich tubular molecular rotors with the smallest core-shell structure. <i>Nanoscale</i> , 2019, 11, 21311-21316.	5.6	19
28	Heteroborospherene clusters Ni _n B ₄₀ (n = 1-4) and heteroborophene monolayers Ni ₂ B ₁₄ with planar heptacoordinate transition-metal centers in C _{7v} heptagons. <i>Scientific Reports</i> , 2017, 7, 5701.	3.3	16
29	CoP/RGO-Pd Hybrids with Heterointerfaces as Highly Active Catalysts for Ethanol Electrooxidation. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 28903-28914.	8.0	16
30	Exfoliation of borophenes from silver substrates assisted by Li/Mg atoms: a density functional theory study. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4043-4048.	5.5	15
31	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.	2.0	15
32	Prediction of freestanding semiconducting bilayer borophenes. <i>Nano Research</i> , 2022, 15, 5752-5757.	10.4	15
33	Boosting capacitive performance of nitrogen-doped carbon by atomically dispersed iron. <i>Journal of Power Sources</i> , 2022, 532, 231335.	7.8	15
34	Multiple Dirac cones in BN co-doped $\hat{1}^2$ -graphyne. <i>Journal of Materials Chemistry C</i> , 2016, 4, 7339-7344.	5.5	14
35	Aromatic cage-like B ₃₄ and B ₃₅ ⁺ : new axially chiral members of the borospherene family. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15344-15349.	2.8	13
36	First-Principles Study on the Oxidation of Supported $\hat{1}^2$ -Borophene. <i>Journal of Physical Chemistry C</i> , 2020, 124, 28145-28151.	3.1	13

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37	A novel borophene featuring heptagonal holes: a common precursor of borospherenes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19890-19895.	2.8	12
38	Charge-induced structural transition between seashell-like B_{29}^{+} and B_{29}^{+} in 18 π -electron configurations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15330-15334.	2.8	12
39	Cage-like B_{41}^{+} and B_{42}^{2+} : New Chiral Members of the Borospherene Family. <i>Angewandte Chemie</i> , 2015, 127, 8278-8282.	2.0	11
40	$W-X$ transformations in isomerization of B_{39}^{+} borospherenes. <i>AIP Advances</i> , 2016, 6, .	1.3	11
41	A first-principles study on zigzag phosphorene nanoribbons passivated by iron-group atoms. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25441-25445.	2.8	11
42	Zigzag double-chain C_{60} Be nanoribbon featuring planar pentacoordinate carbons and ribbon aromaticity. <i>Journal of Materials Chemistry C</i> , 2017, 5, 408-414.	5.5	10
43	Sea-shell-like B_{31}^{+} and B_{32} : two new axially chiral members of the borospherene family. <i>RSC Advances</i> , 2020, 10, 10129-10133.	3.6	10
44	High-symmetry tubular $Ta@B_{18}^{3+}$, $Ta_2@B_{18}$, and $Ta_2@B_{27}^{+}$ as embryos of I_h -boronanotubes with a transition-metal wire coordinated inside. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25009-25015.	2.8	9
45	Perfect cubic La-doped boron clusters La_6 & $[La@B_{24}]^{+0}$ as the embryos of low-dimensional lanthanide boride nanomaterials. <i>RSC Advances</i> , 2020, 10, 12469-12474.	3.6	9
46	Probing into the crystal plane effect on the reduction of I_h - Fe_2O_3 in CO by Operando Raman spectroscopy. <i>Journal of Fuel Chemistry and Technology</i> , 2021, 49, 1558-1566.	2.0	9
47	Visualizing Topological Insulating Bi_2Te_3 Quintuple Layers on SiO_2 -Capped Si Substrates and Its Contrast Optimization. <i>Journal of Nanoscience and Nanotechnology</i> , 2011, 11, 7042-7046.	0.9	8
48	Fluxional bonds in quasi-planar and half-sandwich ($M = K, Rb, \text{ and } Cs$). <i>Journal of Computational Chemistry</i> , 2019, 40, 1227-1232.	3.3	8
49	From Quasi-Planar B_{56} to Penta-Ring Tubular $Ca@B_{56}$: Prediction of Metal-Stabilized $Ca@B_{56}$ as the Embryo of Metal-Doped Boron I_h -Nanotubes. <i>Scientific Reports</i> , 2016, 6, 37893.	3.3	7
50	Comment on "Two-Dimensional Boron Monolayer Sheets". <i>ACS Nano</i> , 2013, 7, 879-879.	14.6	6
51	Stuffing Enhances the Stability of Medium-Sized $(GaAs)_n$ Clusters. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12835-12840.	3.1	5
52	Low-dimensional functional networks of cage-like B_{40} with effective transition-metal intercalations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22611-22617.	2.8	5
53	Fluxional Bonds in Tubular Molecular Rotors $B_3-[Ta@B_{18}]$ and $B_4-[Ta@B_{18}]^{+}$ in 18-Electron Configurations. <i>Journal of Cluster Science</i> , 2020, 31, 331-336.	3.3	5
54	Axially Chiral Cage-Like B_{38}^{+} and B_{382}^{+} : New Aromatic Members of the Borospherene Family. <i>Journal of Cluster Science</i> , 2020, , 1.	3.3	5

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55	Ribbon Aromaticity of Double-Chain B _{2n} C _{2H₂} Clusters (n=9): A First Principle Study. Journal of Cluster Science, 2015, 26, 2043-2050.	3.3	4
56	K(CO) ₈ and Rb(CO) ₈ : Cube-Like Alkali Octacarbonyls Satisfying the 18-Electron Rule. Journal of Cluster Science, 2019, 30, 621-626.	3.3	4
57	La@[La ₅ B ₃₀]O ₂ : endohedral trihedral metallo-borosphenes with spherical aromaticity. Physical Chemistry Chemical Physics, 2022, 24, 3918-3923.	2.8	4
58	The microstructure and magnetic behavior of Co nanostructured film prepared by energetic cluster beam deposition. European Physical Journal D, 2009, 52, 163-166.	1.3	3
59	Structures and electronic properties of stoichiometric hydrogenated aluminum clusters. European Physical Journal D, 2010, 57, 197-205.	1.3	3
60	Double-ring tubular (B _{2O₂}) _n 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.	2.8	3
61	Structures and polarizabilities of medium-sized Ga _n As _m clusters. Chemical Physics Letters, 2011, 511, 97-100.	2.6	2
62	(C ₆ H ₆ Cr) _n & B ₄₀ (n=1-6): Exohedral Borospherene Complexes with Cage-like B ₄₀ as an Effective Ligand with Multiple Coordination Sites. Journal of Cluster Science, 2020, 31, 1363-1369.	3.3	2
63	Compression-induced crimping of boron nanotubes from borophenes: a DFT study. Physical Chemistry Chemical Physics, 2022, 24, 14566-14572.	2.8	2
64	Magnetolectric response analysis of the piezoelectric/piezomagnetic thin-film heterostructure derived by low energy cluster beam deposition. , 2008, , .		1
65	Using phosphorus-doped molybdenum sulfide with (1 0 0)-facet-exposed and enlarged interlayer spacing to enhance hydrogen evolution. Journal of Electroanalytical Chemistry, 2021, 897, 115545.	3.8	1
66	Smart nanostructure derived by low energy cluster beam deposition. , 2009, , .		0
67	The optical band-gap changing of Cu doped ZnO nanostructured film. , 2009, , .		0
68	First-principles calculations of the structural, electronic and magnetic properties of B _n N _{20-n} (n =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.3	0
69	Novel B-C binary fullerenes following the isolated B ₄ C ₃ hexagonal pyramid rule. Journal of Molecular Modeling, 2020, 26, 199.	1.8	0