

Boron/Carbon Analogy: Planar Borophenes, Cage-Like Borospherenes, Boron Nanotubes, and Their Metal-Doped Heteronanostructures

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Abstract

Boron-based nanomaterials have attracted considerable attention in recent years. We present herein the latest combined experimental and theoretical investigations on cage-like borospherenes B_n^q ($q=n-40$, $n=36-42$), metal-doped heteroborospherenes $Ni_n \in B_{40}$ ($n=1-6$), planar borophenes, metal-doped $Ni_2 \in B_{14}$ heteroborophenes, tubular molecular rotors $B_2-Ta@B_{18}^-$, $B_3-Ta@B_{18}$, and $B_4-Ta@B_{18}^+$, and the tubular to cage-like structural transition in metal-centered boron clusters at $Ta@B_{22}^-$ which is the smallest axially chiral endohedral metalloborospherene with the record coordination number of $CN=22$. These nanostructures which are dominated with the double-chain chemistry of boron exhibit unique structural fluctuations due to the bonding fluctuations originated from the electron deficiency of the systems. Boron double chains (BDCs) appear to be equivalent to carbon single chains (CSCs) in these boron nanostructures. Boron-based nanostructures possess properties complementary to carbon nanostructures and may find wide applications in catalysis, energy-storage, and electronics materials.

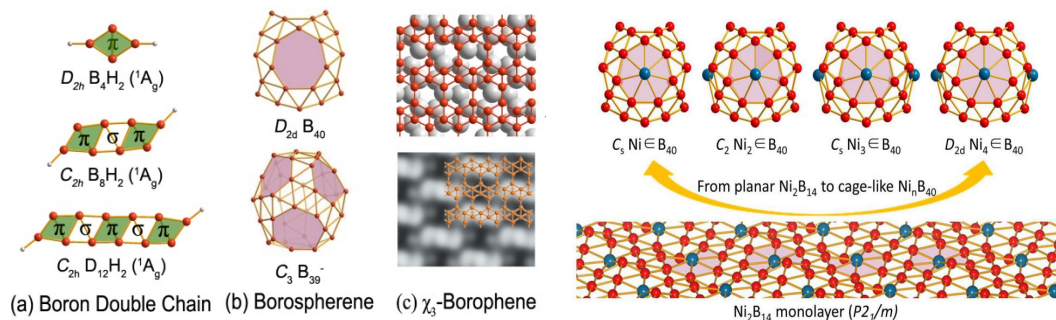


Fig.1 Borospherenes and borophenes composed of interwoven boron double chains **Fig.2** Heteroborospherenes and heteroborophenes

References

1. H.J. Zhai, J. Li, S.D. Li, L. S. Wang et al, *Nat. Chem.*, 2014, **6**, 727–731.
2. Q. Chen, H. J. Zhai, S. D. Li, L.S. Wang et al, *ACS Nano*, 2015, **9**, 754–760.
3. H. Bai, H. J. Zhai, S. D. Li et al, *Angew. Chem. Int. Ed.*, 2014, **54**, 941–945;
4. W.L. Li, J. Li. S. D, Li, L.S. Wang et al, *Chem. Comm.*, 2017, **53**, 1587-1590.
5. H. R. Li, S. D. Li et al, *Sci. Reports*, 2017, **7**, 5701.
6. H. R. Li, S. D. Li et al, *Phys. Chem. Chem. Phys.*, 2017, DOI: 10.1039/C7CP05179D.