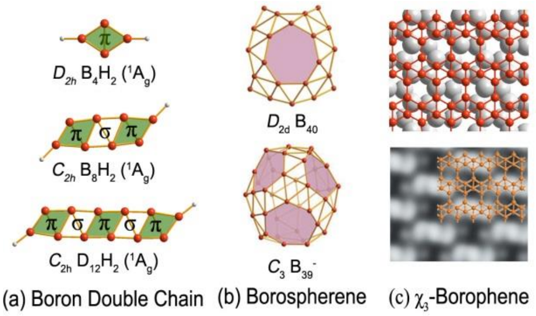
Planar Borophenes, Cage-Like Borospherenes, Boron Nanotubes, and Their Metal-Doped Heteronanostructures with the highest coordination numbers in chemistry

Si-Dian Li
Institute of Molecular Science, Shanxi University, P. R. China
(Email: lisidian@sxu.edu.cn)

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 boronanostructures. Boron-based nanostructures possess properties complementary to carbon nanostructures and may find wide applications in catalysis, energy-storage, and electronics materials.



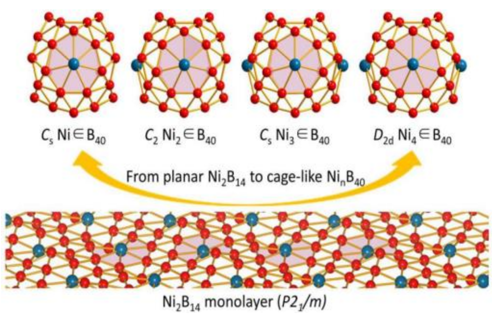


Fig.1 Borospherenes and borophenes composed of interwoven boron double chains **Fig.2** Heteroborospherenes and heteroborophenes

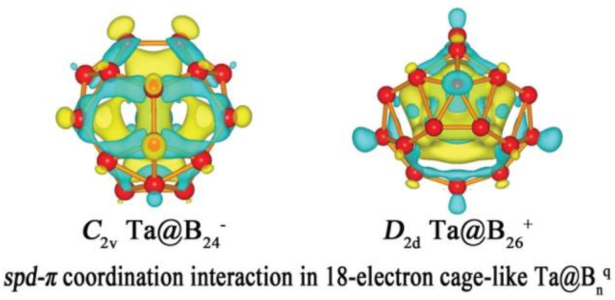


Fig.2 Electron density difference map of C_{2v} Ta@B_{24}^- and D_{2d} Ta@B_{26}^+, with regions of increased and decreased electron densities indicated in yellow and blue, respectively.

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