Nanoclusters of Boron and Metal Borides

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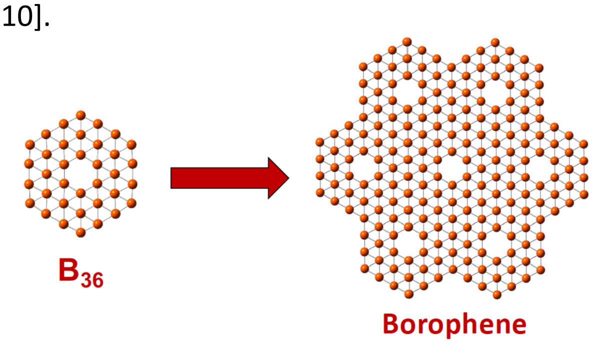
Photoelectron spectroscopy in combination with computational chemistry has shown that bare boron clusters possess planar structures [1], in contrast to that of bulk boron, which is dominated by three-dimensional polyhedral building blocks. The propensity for planarity has been found to be a result of both σ and π electron delocalization over the molecular plane [2]. The B_{36} cluster was found to have a highly stable planar structure with a central hexagonal vacancy, providing the first experimental evidence that single-atom boron-sheets with hexagonal vacancies (borophenes) are viable [3]. Borophenes have since been synthesized and characterized on inert substrates, forming a new class of synthetic 2D materials [4,5]. We have found that the B_{48}^{-} cluster possesses a bilayer structure [6], suggesting the feasibility of bilayer borophenes. Boron forms important bulk boride materials with most metals in the periodic table. Many transition-metal borides are superhard materials, while lanthanide borides are essential magnetic materials. Metal boride clusters are ideal systems to probe the metal-boron bonding in boride materials. We have observed that transition-metal atoms can be doped into the plane of boron clusters, indicating the possibility of metallo-borophenes [7]. However, lanthanide-doped boron clusters form half-sandwich complexes [8], inverse-sandwich complexes [9], as well as novel lanthanide boron cages [10].



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