

Analysis of the electron density features of boron clusters and effects of doping

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Boron atomic clusters show several interesting and unusual size-dependent features due to the small covalent radius, electron deficiency, and higher than carbon coordination number of boron atoms. These include aromaticity and a diverse array of structures such as quasi-planar, ring or tubular shaped and fullerene-like. In the present work, we analyze features of the computed electron density distributions of a large number of boron clusters of different sizes and different types to discern trends in the bonding and stability of these clusters, and to predict the effects of doping by other atoms.