

Abstract Submitted
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Why Boron clusters are Planar? KIRAN BOGGAVARAPU, ANIL KANDALAM, McNeese State University — The origin of the unusual stability of planar and quasi-planar B₁₂ and B₁₃⁺ clusters is explored. Our results demonstrate that in B₁₂ and B₁₃⁺ clusters a $6\pi-6\sigma_{delo}-6\sigma_{3ring}$ trifurcation leads to the triple aromaticity, which is unique to these clusters. Most importantly, the H-L gaps of these clusters are strongly dependent on the strength of the interaction between the inner- and the outer-rings, which make up these clusters. Furthermore, the similarities and the differences between B₁₂ and other stable boron species, B₁₀ and B₁₄ clusters are also discussed. The implication of the current analysis is discussed with respect to Carbon, Silicon and Aluminum clusters.

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