DFT STUDY OF NEUTRAL $B_{12}H_n$ ($n \leq 12$), $AlB_{12}H_n$ ($n \leq 13$) CLUSTERS AND CHARGED CLUSTERS OF $[B_{12}H_{12}]^q$, $[AlB_{12}H_{12}]^q$, $[AlB_{12}H_{13}]^q$ ($q = \pm 1, \pm 2$)

Mustafa Böyükata[1] and Ziya B. Güvenç[2]

[1]Department of Physics, Bozok University, 66200 Yozgat, Turkey
[2]Department of Electronics and Communication Engineering., Çankaya University, 06530 Ankara, Turkey

---

Abstract: Density Functional Theory (DFT) with B3LYP / 6-311++g** level has been performed to investigate the electronic structures of cage $B_{12}H_n$ for up to $n=\leq 12$ and $AlB_{12}H_n$ for up to $n \leq 13$. Moreover, the computations has been extended to the charged clusters of $[B_{12}H_{12}]^q$, $[AlB_{12}H_{12}]^q$ and $[AlB_{12}H_{13}]^q$ ($q= \pm 1$ and ± 2). Their enegetics and structural analysis have been done. Cage form of B_{12} is stable against to hydrogen adsorptions.

Keywords: DFT, Boron, Hydrogen.
