Exploring electonic Structure and Spectral Properties of Nitrogen-Doped Boron Clusters BnN with n=10-20.

Cheng-Hong Deng[1], Zheng-wen Long[1], Yue-Ju Yang[2], and Shi-Xiong Li[2]

[1]Guizhou University
[2]Guizhou Education University

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Abstract

For a better understanding the effects of nitrogen atom doping on boron clusters, we investigated adopting the ABCluster global search technique and CALYPSO approach combined with density functional theory the lowest energy structures, bonding, electrons delocalization and spectral properties of neutral nitrogen-doped boron clusters, the size of which varies from 10 to 20. The results of its calculations are displayed the global minimum of these clusters are plane or quasi plane structures at n= 11, 13, 15-20, the bowl-like structures at n= 10, 12 and the boat-shaped structure at n=14. It is found that B20N is most stable of all structures. Natural population analysis (NPA) indicates that boron atoms sectional electrons transfer to doped nitrogen atoms. Electron localization Orbital Function (LOL) and Electron Localization Function (ELF) analysis indicate there are strong covalent bonds between doped N atons and B atoms for clusters BnN(n=10-20). In addition, under the same isosurface, the isosurface of B10N is the thickest, indicating that it has the most electrons and the strongest delocalization. Infrared and Raman spectra show that clusters BnN(n=10-20) have a great deal of characteristic peaks, and the strongest IR peaks and Raman peaks are situated at different positions, which can be used to identify the clusters structures and make comparative analysis with future experiments. Electronic absorption spectrum analysis shows that the first absorption peak of these clusters is located in the visible band. The study provides theoretical guidance and basis for the development of novel boron-based nanomaterials.

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