DFT investigation for low-energy structures of 22- atom and 23-atom Boron Clusters

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Motivation

Since the advent of carbon nanotubes, boron nanoparticles have been of high interest due to the similar electrochemical properties of boron and carbon. The hope is that boron nanoparticles will have a similar structure to carbon and produce desirable properties for various applications. Previous studies have also shown certain boron nanoparticles ranging in size from 19 to 24 atoms prefer a planar or a double ring structure. At present, nanoparticles with 22 and 23 atoms have have not been verified.

Software & Methodology

The main method that were used to look for these stable structures was Density Functional Theory. Density functional Theory solves the Schrodinger equation using electron density rather than the position of each electron.

$$\widehat{H}\Psi(r_1, r_2, ..., r_N) = E\Psi(r_1, r_2, ..., r_N)$$

$$\Downarrow$$

$$\widehat{H}\rho(r) = E\rho(r)$$

This significantly decreases the computation time needed to solve the equation. This is done by transforming it from an equation of 3N variables where N is the total number of electrons in the system to an equation of just three variables. Density functional theory is implemented using software called Naval Research Laboratory Molecular Orbital Library (NRLMOL). The structures that are studied come from a list of around 200 possible structures.

Results

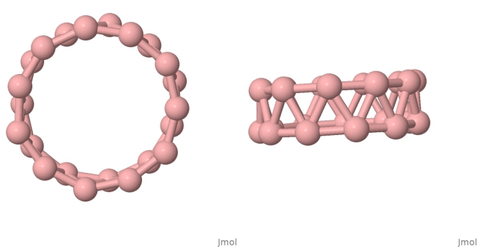

Figure 1. Ring structure for B22 neutral, anion, and cation nanoparticles.

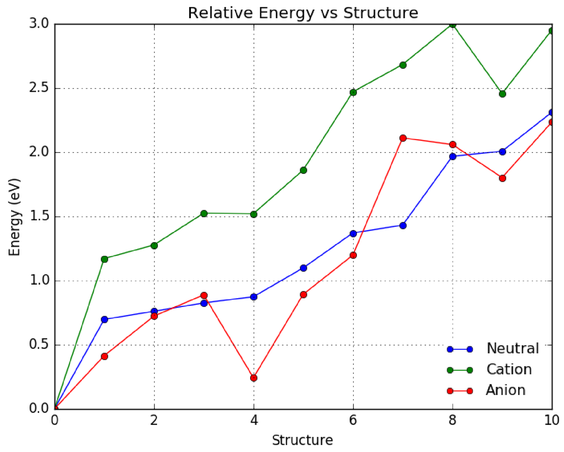

Figure 2. Relative energy for each B22 cluster.

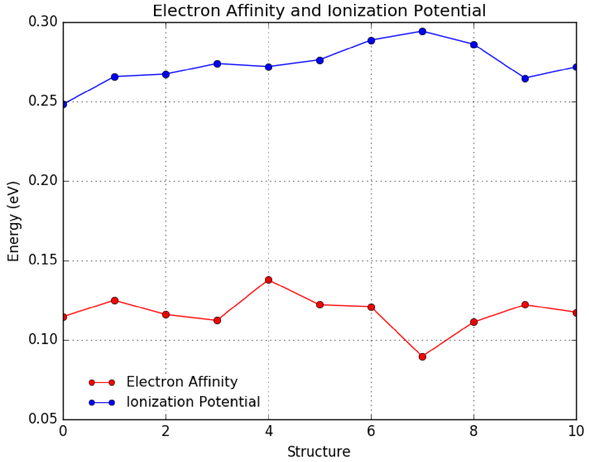

Figure 3. Electron affinity and ionization potential for B22

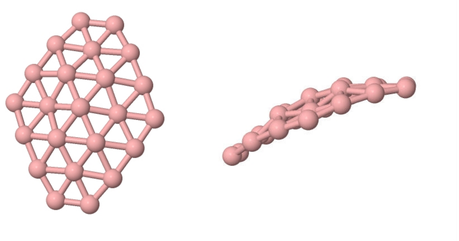

Figure 4. Planar structure for B23 neutral, anion, and cation nanoparticles.

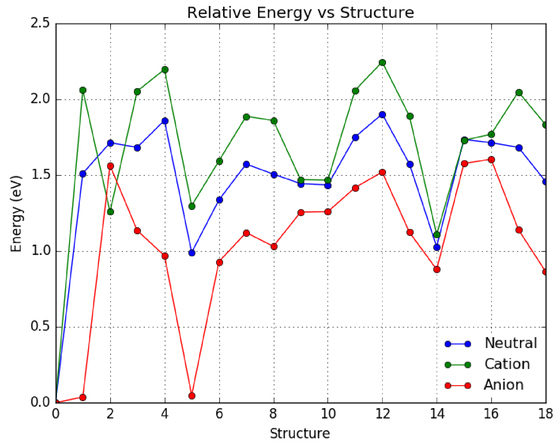

Figure 5. Relative energy for each B23 cluster.

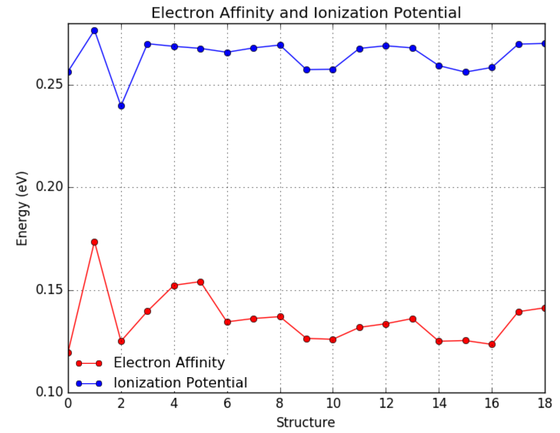

Figure 6. Electron affinity and ionization potential for B23

Summary

Our calculations show that B22 clusters prefer a double ring structure. This was found to be the same regardless of the overall charge on the cluster. The same can be said for B23 clusters, except the preferred structure is planar. These structures and energies will now be used to find properties of each cluster.

Future Work

Simulations of B23 are ongoing. We are investigating many properties, including the dipole energy, vibrational energy, and infrared absorption intensity.

References

Hikmat BC, Tunna Baruah, and Rajendra R. Zope. "Low-lying planar isomers of neutral and charged B22 clusters." J. Phys B: At. Mol. Opt. Phys. 45, 225101 (2012).