# Systematic Study on the Structure of Mixed Boron-Carbon Clusters via Density Functional Tight Binding and Density Functional Theory

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**Abstract**

The extended version of Modified Basin Hopping (EMBH) was used to study the lowest energy structures (LESes) for mixed boron-carbon (BC) clusters, $B_xC_y$ $(3 \leq x+y \leq 10)$. This is a two-stage calculation where in the first stage, MBH was used to generate random structures and these structures were optimized using Density Functional Tight Binding (DFTB). The structure that has the lowest energy is used as an input to the second stage calculation. This input structure was continuously modified and optimized using Density Functional Theory (DFT). As DFTB is computationally more efficient than DFT, using DFTB to first screen through the PES has reduced the time needed in the second stage DFT calculation in locating the LESes. For the study at DFTB level, new set of B-B, C-C, B-C and C-B Slater-Koster (SK) parameters were created. The LESes generated using MBH/DFTB matched or mimicked 27 out of 41 LESes or low-lying isomers (LLIs) reported at DFT level. The results improved after second stage MBH/DFT calculation. Only 5 out of 41 structures studied matched or mimicked the LESes or LLIs reported at DFT level by previous publications. This may be due to the ability of DFT to treat the valence electron more accurately. These results show reasonable agreement to the observation made by previous studies. The LESes for $B_3C_6$, $B_3C_7$ and $B_9C_1$ which were not reported by previous publications, were predicted in this study. In carbon-rich $B_3C_6$ and $B_3C_7$, there LES generated does not show multicoordinate structure while in the boron-rich $B_9C_1$, it was predicted to have $C_1$ structure, similar to the LLI of $B_{10}$ cluster that had $C_{2v}$ structure. The EMBH method is shown to be efficient and effective method for locating the LES. DFTB has shown to be an efficient method to screen through the potential energy surface and eliminate some high energy structures. This reduces the computational time for the entire EMBH process for locating the LES.

Keywords: DFTB; DFT; mixed boron-carbon clusters; lowest energy structure; global minimum search