INVESTIGATION OF THE STRUCTURE AND STABILITY OF BORON-CARBON CLUSTERS USING THE DFT METHOD

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Knowledge of ground state atomic configurations and the stability of B_nC_m clusters yields insights into the structural foundations and explains a wide range of facts about such interesting objects as boron-carbon nanoclusters, nanowires, films and crystals, which may be used as H_2 and N_2 gas nanosensors, quantum dots, thermoelectric energy converters, etc..[1] Using evolutionary algorithm USPEX and ab initio calculations, the optimal atomic structures of boron-carbon clusters B_nC_m in wide range of compositions (n, $m = 0 - 12$) were predicted. We constructed a map based on our data to illustrate the structural differences among clusters. Furthermore, we investigated the stability of clusters using the following criteria: second-order energy difference (Δ^2E), fragmentation energy (E_{frag}). Based on these criteria, we constructed maps, which demonstrate the existence of the "ridges" and "islands" of stability, corresponding to the most stable "magic" clusters. For each of the clusters, we checked multiplicities up to 4 and identified that some of them in ground state have multiplicity 3. Using the obtained data, we constructed a map of magnetic moments for the clusters. We also determined HOMO-LUMO gaps for each of the clusters. We have found unique clusters that can serve as building blocks, as well as intermediates in the chemical reactions of synthesizing complex nano-sized B-C formations.

References

[1] S.J. Lu, *B8C10: A C2v planar polycyclic structure bridged by the central strong CC bond and strengthened by the aromaticity.* Chemical Physics Letters, **801**, p.139715, 2022.