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INTERACTION OF BORON CLUSTERS WITH OXYGEN: A DFT STUDY[1] KAMRON SALAVITABAR, West Chester Univeristy of Pennsylvania, KIRAN BOGGAVARAPU, McNeese State University, ANIL KANDALAM, West Chester Univeristy of Pennsylvania — A controlled combustion involving aluminum nanoparticles has often been the focus of studies in the field of solid fuel propellants. However very little focus has been given to the study of boron nanoparticles in controlled combustion. In contrast to aluminum nanoclusters, boron nanoclusters (B_n) are known to exhibit a planar geometries even at the size of $n = 19 - 20$, and thus offer a greater surface area for interaction with oxygen. Earlier experimental studies have shown that boron nanoclusters exhibit different reactivity with oxygen depending on their size and charge. In this poster, we present our recent density functional theory based results, focusing on the reactivity patterns of neutral and negatively charged B_5 cluster with O_n, where $n = 1 - 5$; and B_6 cluster with O_n ($n = 1 - 2$). The effect of charge on the reactivity of boron cluster, variation in the stability of product clusters, i e., neutral and negatively charged B_5O_n ($n = 1 - 5$) and B_6O_n ($n = 1 - 2$) are also examined.

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