

Abstract Submitted  
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**Quantum chemistry modeling of  $B_nN_2$  clusters formation in reaction between small  $B_n$  clusters ( $n=2-4$ ) and  $N_2$  molecule for boron nitride nanotubes synthesis.**<sup>1</sup> YURI BARSUKOV, Peter the Great St.Petersburg Polytechnic University, IGOR KAGANOVICH, OMESH DWIVEDI, SIERRA JUBIN, STEPHANE ETHIER, Princeton Plasma Physics Laboratory — We study precursors for the boron nitride nanotubes (BNNTs) formation that can effectively convert molecular nitrogen into boron nitride. The data have been obtained by using a DFT (density function theory) method with unrestricted WB97X-D functional with 6-311+G(2dp) basis set. Using quantum chemistry methods, we discovered that formation of linear BNB<sub>n</sub>, cyclo-BNB<sub>n</sub>B and cyclo-BNB<sub>n</sub>B<sub>2</sub> species from  $B_n$  ( $n=2-4$ ) and  $N_2$  proceeds through sequential steps, and activation barrier of the rate-limited step is near 1.1 eV for all considered  $B_n$  clusters. On the other hand, the highest barrier towards dissociation of BNB<sub>n</sub>, cyclo-BNB<sub>n</sub>B and cyclo-BNB<sub>n</sub>B<sub>2</sub> species on  $B_n$  and  $N_2$  increases and equals 2.5, 4.8 and 5.6 eV respectively. Thus, based on our calculations we can conclude that  $N_2$  is able to react with small  $B_n$  clusters producing new  $B_nN_2$  clusters with BN bonds, and these  $B_nN_2$  clusters can be accumulated in the gas phase even at high temperature providing contribution in the BNNTs growth.

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