Abstract Submitted
for the GEC20 Meeting of
The American Physical Society

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.[1] YURI BARSUKOV, Saint-Petersburg Polytechnic University, Saint Petersburg, Russia, IGOR KAGANOVICH, OMESH DWIVEDI, SIERRA JUBIN, STEPHANE ETHIER, Princeton Plasma Physics Laboratory, Princeton NJ — 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 BNBN, cyclo-BNBNB and cyclo-$BNBNB_2$ 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 BNBN, cyclo-BNBNB and cyclo-$BNBNB_2$ 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.

[1]This research was performed at the Princeton Collaborative Low Temperature Plasma Research Facility (PCRF) at PPPL, and supported by the US DOE under contract DE-AC02-09CH11466

Yuri Barsukov
Saint-Petersburg Polytechnic University, Saint Petersburg, Russia

Date submitted: 15 Jun 2020 Electronic form version 1.4