Abstract Submitted
for the DPP16 Meeting of
The American Physical Society

**Computer Simulation of Synthesis of Boron-Nitride Nanostructures**[1] PREDRAG KRSTIC, LONGTAO HAN, State Univ of NY- Stony Brook — Synthesis of boron-nitride fullerenes, nano-cocoons and nano-cages by self-organization of BN molecules in a high-temperature plasma is simulated with the DFT tight-binding method. No boron nano-cluster or catalytic nanoparticles are needed to initiate this process. By varying the plasma temperature, incoming flux of BN molecule, and the total time of growth, we can simulate growth of $sp^2$ cages of various shape, size and quality. Role of hydrogen in the syntheses is also considered, with the simulation of HBNH and $H_2BNH_2$ molecules as feedstock.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Material Sciences and Engineering Division.

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Date submitted: 18 Jul 2016 Electronic form version 1.4