

Abstract Submitted
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Synthesis of boron-nitride nanocages and fullerenes in a BN plasma¹ 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 using the DFT tight-binding method. No boron nano-cluster or catalysts nano-particle are needed to initiate this process. By varying the plasma temperature and the BN density, as well as the time of growth we can simulate growth of the sp^2 cages of various shape, size and quality. Role of hydrogen in HBNH and H_2BNH_2 synthesis is also considered.

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