Abstract Submitted
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Quantum-mechanical simulations of the synthesis of boron-nitride nano-structures in a hot, high-pressure plasma[1] PREDRAG KRSTIC, LONGTAO HAN, Stony Brook University — The clusterization and anglomeration of boron-nitride nano-structures in a hot, high-pressure plasma was simulated on nanosecond time scale using quantum-classical molecular dynamics (QCMD). Eleven different atomic and molecular precursor systems of boron, nitrogen and hydrogen were used, with more than 1500 atoms at temperatures in range 1500 to 6000 K. Several various mechanisms for the nanotube growth, as well as the optimal temperatures (around 2000K) and optimal choice of precursors (containing BN diatomics within the precursor molecular structure) for growth of nanocages, nanoflakes and diamond-like structures were identified1. The quantum-mechanical component of the QCMD was based on the density-functional tight-binding (DFTB) quantum mechanics in conjunction with a divide-and-conquer (DC) linear scaling algorithm, as implemented in the DC-DFTB-K code2. 1Predrag Krstic, Longtao Han, Stephen Irle and Hiromi Nakai, Chemical Science 9, 3803 (2018). 2 Y.Nishizawa, Y. Nishimura, M. Kobayashi, S. Irle and H. Nakai, J. Comput. Chem. 37, 1983 (2016).

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