Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Energy landscape of fullerene materials: A comparion of boron to boron nitride and carbon[1] SANDIP DE, University of Basel, Basel, Switzerland — After the discovery of the C60 fullerene some 25 years ago, many more hollow and endohedrally doped structures made out of various elements have been proposed theoretically. However, since no other fullerenes have been synthesized up to date, the question arises whether experimentalists have just not yet found a way to synthesize these theoretically predicted fullerenes, or whether they do not exist at all in nature. Following the theoretical discovery of the B_{80} fullerene by Szwacki et al, various other fullereneand stuffed fullerene structures were proposed but none of them could be synthesized in the laboratory yet. Using the minima hopping global geometry optimization method on the density functional potential energy surface we show that the energy landscape of boron clusters is glass like. Medium size boron clusters exhibit many structures which are lower in energy than the cages. This is in contrast to carbon and boron nitride systems which can be clearly identified as structure seekers. The differences in the potential energy landscape explain why carbon and boron nitride systems are found in nature whereas pure boron fullerenes have not been found. We thus present a methodology which can make predictions on the feasibility of the synthesis of new nano structures.

[1]Indi-swiss research grant., Swiss national foundation, cscs swiss national super computer

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Date submitted: 23 Nov 2011 Electronic form version 1.4