Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Maximizing the bandgap of BCN nanoribbons RAISI BALDEZ, PAULO PIQUINI, ALEX SCHMIDT, Universidade Federal de Santa Maria, MARCELO KURODA, Auburn University — Carbon and boron-nitride based compounds share many electronic and structural features. This fact permits mixed carbon-boron-nitride compounds to be easily synthesized without significant structural changes. Further, the partially ionic character of the boron-nitrogen bonds allow to modify the electronics of carbon based materials, introducing a variability that can be used to tune the electronic properties according to the boron and nitrogen contents. Graphene and graphene nanoribbons have emerged as promising materials for electronic applications, due to the high mobility of its charge carriers. In this work we use the genetic algorithm approach to search for configurations with variable B, C and N contents that maximize the band gap of $B_xC_yN_z$ nanoribbons. Different stoichiometries are analyzed and the structural patterns that lead to the maximal band gaps are presented.

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Date submitted: 14 Nov 2014 Electronic form version 1.4