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Electronic and Structural Properties of Graphene Dots in h-BN

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A major challenge for graphene-based applications is the creation of a tunable electronic band gap as would be present for traditional semiconductor alloys. Since hexagonal boron nitride has a very similar structure to graphene, it is a natural candidate to modify the electronic structure of graphene by forming a hybrid phase sheet containing domains of graphene and hexagonal boron nitride, as has been done experimentally. Here we investigate the properties of such hybrid sheets by using pseudopotential-density functional theory implemented in real space. We find for a graphene dot comparable in size to those observed in experiment, the band gap of the sheet is not significantly modified. Moreover, when the size of graphene dot decreases below $\sim$13Å, strong structural instabilities of the graphene domain occur.

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