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Electronic structure of flattened boron nitride nanotubes: first-principles DFT study

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Summary

Boron nitride nanotubes (BNNTs) have been found to be truly electrically insulating regardless of their diameters, chiralities and number of shells. On the other hand, a recent experimental work on multi-walled BNNTs has shown that electrical transport properties of the BNNTs change from insulating to semiconducting through a bending deformation. However, deformation-induced electrical effects in BNNTs have not been fully clarified yet. In the present work, HOMO-LUMO energy gaps of (5,0), (13,0), (21,0) single-walled BNNTs (SWBNNTs) and (5,0)@(13,0), (13,0)@(21,0) double-walled BNNTs (DWBNNTs) under flattening deformation have been investigated using first-principles density functional calculations. The LUMO energies of the three SWBNNTs decrease with increasing flattening deformation, while the HOMO energies hardly change, resulting in monotonic decrease in the energy gaps. The same is equally true of the (13,0)@(21,0) DWBNNT, but it exhibits more rapid decrease in the energy gap than the SWBNNTs. In contrast, the energy gap of the (5,0)@(13,0) DWBNNT firstly increases and then decreases. These facts indicate that the electronic structure of flattened BNNTs is affected by interaction between the inner and outer tubes in the BNNTs.

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