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Energetics and electronic structure of double-walled boron nanotubes HUI TANG, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Single-walled boron nanotubes have been studied extensively since their first successful fabrication in experiments. On the other hand, double-walled or multi-walled boron nanotubes have not yet been discussed in literature. Here, using density functional theory, we present a stable semiconducting two-dimensional double-layered boron sheet, which is 0.14 eV/atom more stable than the most stable single-layered α-sheet [1]. This double-layered sheet is stabilized due to the formation of inter-layer bonds. We show that double-walled boron nanotubes made from this double-layered sheet are all semiconducting. These double-walled nanotubes are more stable than single-walled ones for large nanotubes, but become less energetically favorable when the tube radius is smaller than 20 Å due to their large curvature energies. To reduce the large curvature energies, we construct double-walled nanotubes whose inner and outer walls have different number of atoms around their circumference. The resulting nanotubes are more stable than single-walled ones for all radii.

[1] H. Tang, and S. Ismail-Beigi, PRL 99, 115501 (2007).

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