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Possible Precursors for Boron Nanotubes: A Novel Bonding Picture in Boron Sheets and Nanotubes HUI TANG, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Boron nanotubes (BNTs) have attracted a great deal of attention due to their unique properties: unlike carbon nanotubes (CNTs), all BNTs are predicted to be metallic regardless of chirality or radii. Based on density functional theory, we present a class of boron sheets, composed of mixtures of triangular and hexagonal motifs, that are more stable than any sheet-structures considered to date and thus are more likely to be the precursors of atomically thin BNTs [1]. We describe a picture of the nature of the bonding in these sheets which clarifies their stability. We further point out that our bonding picture, which focuses on the balance of two-center and three-center bonding, is crucial for the stability of other boron nanostructures. We also discuss BNTs made from our new boron sheets.
[1] H. Tang and S. Ismail-Beigi, Phys. Rev. Lett. 99, 115501 (2007).

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