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Self-doping in Boron Nanostructures[1] HUI TANG, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Boron nanotubes have attracted much attention since their first fabrication in experiments. Boron nanotubes with large radii ($R \geq 10$ Å) are predicted to be metallic with large densities of states at their Fermi energies, which may provide excellent conducting systems for one-dimensional electronics. In previous work [1], we have shown a class of stable boron sheets, composed of mixtures of triangular and hexagonal motifs, that are likely to be the precursors of boron nanotubes. These sheets are stabilized by a balance of 2-center and 3-center bonding. Here, using density functional theory and Maximally Localized Wannier Functions, we show that adding a boron atom to a boron sheet is equivalent to doping the boron sheet with all three valence electrons of the added atom. Based on this self-doping picture, we propose a simple counting scheme to construct stable boron nanostructures, e.g. from corresponding carbon ones. We also apply this knowledge to study Mg-doped boron sheets and discuss the possible stable structures of MgB_2 nanotubes. [1] H. Tang, and S. Ismail-Beigi, Phys. Rev. Lett. 99, 115501 (2007).

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