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Boron Nanotubes: Characterization Through Theory ABHISHEK SINGH, ARTA SADRZADEH, Department of Mechanical Engineering and Materials Science, Rice University, Houston, Tx 77005, BORIS YAKOBSON, Department of Mechanical Engineering and Materials Science Rice University, and Department of Chemistry, Rice University, Houston Tx 77005 — Boron nanotubes have been believed to be metallic irrespective of diameter and chirality, as apposed to carbon nanotubes (CNTs), which could be both metallic and semiconducting. However, the separation of metallic and semiconducting CNTs is still a challenging task, which eventually, plagues their applications. Using first principle calculations, we investigate mechanical and electronic properties of the BNTs and show that BNTs could also be semiconducting. We discus the origin of semiconductivity in BNTs. Prospect of having only metallic BNTs is a great advantage over CNTs, however, having semiconducting BNTs could make them applicable in electronics, sensing and optoelectronics.

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