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Boron Nanotubes and Boron Sheets – New Perspectives for Nanotechnology JENS KUNSTMANN, Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany, ALEXANDER QUANDT, Institut fuer Physik der Universitaet Greifswald, Domstrasse 10a, 17489 Greifswald, Germany — We report about a recent ab initio study of boron nanotubes (BNTs). The latter were first predicted by theory, and have recently been synthesized experimentally. To understand the basic properties of BNTs, we have derived a structure model for an extended boron sheet (i.e. a boron analogue of a single graphene sheet) as a possible structural precursor of boron nanotubes. This sheet has a puckered structure, high stiffness, and anisotropic bonding properties. Puckering turns out to be the key mechanism for stabilizing sp sigma bonds lying along the armchair direction of the sheet. The BNTs have puckered surfaces as well, and their chiral angles are defined in a range from 0 to 90 degree. We show that all ideal boron nanotubes are metallic, irrespective of their radii and chiral angles, and discuss the possible existence of helical currents in chiral BNTs. Furthermore we show that strain energies of BNTs depend on their radii AND on their chiral angles. This unique property could be the basis of a new structure control mechanism in nanotechnology that permits to make nanotubes of a specified type, only. Zigzag nanotubes for example seem to have very little strain energy, if any. Therefore they should be highly susceptible to structural collapses, and might not exist at all.

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