

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Bonding in boron: building high-pressure phases from boron sheets JENS KUNSTMANN, Dresden University of Technology, Dresden, Germany, LILIA BOERI, Max Planck Institute for Solid State Research, Stuttgart, Germany, JENS KORTUS, TU Bergakademie Freiberg, Freiberg, Germany — We present the results of a study of the high pressure phase diagram of elemental boron, using full-potential density functional calculations. We show that at high pressures ($P \gtrsim 100$ GPa) boron crystallizes in quasi-layered bulk phases, characterized by in-plane multicenter bonds and out-of-plane unidimensional sigma bonds. These structures are all metallic, in contrast to the low-pressure icosahedral ones, which are semiconducting. We show that the structure and bonding of layered bulk phases can be easily described in terms of single puckered boron sheets [1]. Our results bridge the gap between boron nanostructures and bulk phases.

[1] Kunstmann et al., Phys. Rev. B 74, 035413 (2006).

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Date submitted: 02 Nov 2009

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