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Structural transition and mechanical properties of one dimensional boron ribbons and chains from first principles MINGJIE LIU, VASILII I. ARTYUKHOV, BORIS I. YAKOBSON, Department of Materials Science and NanoEngineering, Rice University, Houston, TX — The past decade has brought great progress in fabrication and characterization of single-atom chains of carbon (carbyne). Very recently novel atomic chain compositions such as BN and CsI were reported. The extreme and unusual properties of such 1D materials[1,2] motivate the search for other possible compositions with interesting behaviors. We use first-principles calculations to uncover the rich structural and mechanical properties of 1D boron. While the ground state structure of linear boron is a two-atoms-wide ribbon, tension can unravel it into a single-atom string structure. We analyze the mechanical and electronic properties of these two "phases" and study the thermodynamics and kinetics of transition between them using static first-principles calculations and semiempirical (DFTB) molecular dynamics. The interesting properties of 1D boron nanostructures make them an attractive system for experimental investigations.

[1]M. Liu *et al.*, *ACS Nano* 7, 10075 (2013)
[2]V. I. Artyukhov, M. Liu, and B. I. Yakobson, *Nano Lett.* 14, 4224 (2014)

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