

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

One-dimensional atomic chains: rich physics in simple structures

MINGJIE LIU, VASILII I. ARTYUKHOV, BORIS I. YAKOBSON, Department of Materials Science and NanoEngineering, Rice University, Houston, TX — Carbyne—1D polymorph of carbon—has been hypothesized since 1960's, however reproducible techniques of fabricating long carbon chains and measuring their properties have arrived only in the last decade. More recently, 1D chains of other compositions have been fabricated, such as CsI and BN. Here we report our first-principles studies of the properties of carbyne, which shows extreme mechanical performance¹ as well as strongly strain-sensitive electronic properties.² We also study 1D nanostructures of boron which shows a reversible tension-driven transition from metallic ribbons to insulating atomic chains with an unusual antiferromagnetic ground state.³

¹M. Liu *et al.*, *ACS Nano* 7, 10075 (2013)

²V. I. Artyukhov, M. Liu, and B. I. Yakobson, *Nano Lett.* 14, 4224 (2014)

³V. I. Artyukhov, M. Liu, and B. I. Yakobson, in preparation

Vasilii I. Artyukhov
Department of Materials Science and NanoEngineering, Rice University

Date submitted: 14 Nov 2014

Electronic form version 1.4