

## Accepted Manuscript

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PII: S2352-4316(16)30147-X

DOI: <http://dx.doi.org/10.1016/j.eml.2016.10.011>

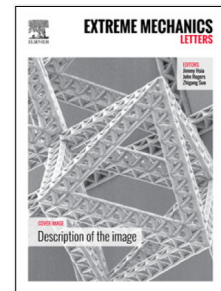
Reference: EML 232

To appear in: *Extreme Mechanics Letters*

Received date: 12 July 2016

Revised date: 24 October 2016

Accepted date: 30 October 2016



Please cite this article as: V. Sorkin, Y.W. Zhang, Effect of edge passivation on the mechanical properties of phosphorene nanoribbons, *Extreme Mechanics Letters* (2016), <http://dx.doi.org/10.1016/j.eml.2016.10.011>

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# Effect of Edge Passivation on the Mechanical Properties of Phosphorene Nanoribbons

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## Abstract

Using density functional tight binding simulations, we studied the edge structures, edge elastic properties, deformation and failure behavior of phosphorene nanoribbons (PNRs) with edges passivated by hydrogen atoms. Two primary types of edge, that is, arm-chair (AC) and zig-zag (ZZ), were examined. It was found that edge relaxation primarily occurred within three atomic rows near the passivated edges, in the form of alteration in bond length and angle. The edge passivation was able to lessen the edge relaxation and reduce the edge stresses and elastic moduli. For AC PNRs under tension, three deformation stages were identified: linear elastic, bond rotation and bond stretching. At  $\epsilon \approx 0.5$ , intra-row bonds fracture in a double-row-wise manner in the interior of the sample, leading to fragmentation of AC PNRs. For ZZ PNRs under tension, inter-row bonds are stretched directly. At  $\epsilon \approx 0.18$ , a fraction of the inter-row bonds break randomly, leading to the failure of ZZ PNRs. Interestingly, the edge passivation increases both the failure strain ( $\Delta\epsilon/\epsilon \approx 80\%$ ) and strength ( $\Delta\sigma/\sigma \approx 26\%$ ) of ZZ PNRs significantly, but the failure strain ( $\Delta\epsilon/\epsilon \approx 2\%$ ) and strength ( $\Delta\sigma/\sigma \approx 5\%$ ) of AC PNRs only slightly.

*Keywords: passivated phosphorene nanoribbons, edge stress, edge elastic moduli, failure, DFTB calculations*

## 1. Introduction

Phosphorene, a two-dimensional (2D) layer of black phosphorus, has provoked a significant interest due to its direct band-gap semiconducting feature [1–6]. At first, multi-layer phosphorene was attained by mechanical exfoliation [1,7,8], and then monolayer phosphorene through plasma thinning [9]. Phosphorene is a very appealing addition to existing 2D materials, such as graphene [10,11], boron nitride [12–14], and transition metal dichalcogenides [15–18] since it is ideally suitable for field-effect transistors [19–24]. Furthermore, phosphorene has a comparatively high direction-dependent carrier mobility [22,25–34] and highly anisotropic thermomechanical

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