

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Remarkably low-energy one-dimensional fault line defects in single-layered phosphorene ALOYSIUS SOON, WOOSUN JANG, KISUNG KANG, Department of Materials Science and Engineering, Yonsei University — Systematic engineering of atomic-scale low-dimensional defects in two-dimensional nanomaterials is a promising way to modulate the electronic properties of these nanomaterials. Defects at interfaces such as grain boundaries and line defects can often be detrimental to technologically important nanodevice operations and thus a fundamental understanding of how such one-dimensional defects may have an influence on its physio-chemical properties is pivotal to optimizing their device performance. In this study [1], using density-functional theory, we investigate the temperature-dependent energetics and electronic structure of a single-layered phosphorene with various fault line defects. We have generated different line defect models based on a fault method, rather than the conventional rotation method. This has allowed us to study and identify new low-energy line defects, and we show how these low-energy line defects could well modulate the electronic band gap energies of single-layered two-dimensional phosphorene – offering a range of metallic to semiconducting properties in these newly proposed low-energy line defects in phosphorene. [1] A. Soon et al. *Nanoscale*, DOI 10.1039/C5NR05605E (2015)

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Date submitted: 04 Nov 2015

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