

Accepted Manuscript

Anisotropic mechanical properties and strain tuneable band-gap in single-layer SiP, SiAs, GeP and GeAs

Bohayra Mortazavi, Timon Rabczuk

PII: S1386-9477(18)30438-7

DOI: [10.1016/j.physe.2018.06.011](https://doi.org/10.1016/j.physe.2018.06.011)

Reference: PHYSE 13182

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

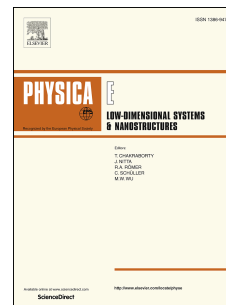
Received Date: 22 March 2018

Revised Date: 7 June 2018

Accepted Date: 13 June 2018

Please cite this article as: B. Mortazavi, T. Rabczuk, Anisotropic mechanical properties and strain tuneable band-gap in single-layer SiP, SiAs, GeP and GeAs, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.06.011.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Anisotropic mechanical properties and strain tuneable band-gap in single-layer SiP, SiAs, GeP and GeAs

Bohayra Mortazavi^{*,1} and Timon Rabczuk^{#,2}

¹*Institute of Structural Mechanics, Bauhaus-Universität Weimar, Marienstr. 15, D-99423 Weimar, Germany.*

²*College of Civil Engineering, Department of Geotechnical Engineering, Tongji University, Shanghai, China.*

Abstract

Group IV–V-type two-dimensional (2D) materials, such as GeP, GeAs, SiP and SiAs with anisotropic atomic structures, have recently attracted remarkable attention due to their outstanding physics. In this investigation, we conducted density functional theory simulations to explore the mechanical responses of these novel 2D systems. In particular, we explored the possibility of band-gap engineering in these 2D structures through different mechanical loading conditions. First-principles results of uniaxial tensile simulations confirm anisotropic mechanical responses of these novel 2D structures, with considerably higher elastic modulus, tensile strength and stretchability along the zigzag direction as compared with the armchair direction. Notably, the stretchability of considered monolayers along the zigzag direction was found to be slightly higher than that of the single-layer graphene and h-BN. The electronic band-gaps of energy minimized single-layer SiP, SiAs, GeP and GeAs were estimated by HSE06 method to be 2.58 eV, 2.3 eV, 2.24 eV and 1.98 eV, respectively. Our results highlight the strain tuneable band-gap character in single-layer SiP, SiAs, GeP and GeAs and suggest that various mechanical loading conditions can be employed to finely narrow the electronic band-gaps in these structures.

Keywords: 2D materials; first-principles; mechanical; band-gap; simulations;

*Corresponding author (Bohayra Mortazavi): bohayra.mortazavi@gmail.com

Tel: +49 157 8037 8770; Fax: +49 364 358 4511; #Timon.rabczuk@uni-weimar.de

Download English Version:

<https://daneshyari.com/en/article/7933148>

Download Persian Version:

<https://daneshyari.com/article/7933148>

[Daneshyari.com](https://daneshyari.com)