Accepted Manuscript

Title: Tunable electronic and optical behaviors of two-dimensional germanium carbide

Author: Zhuo Xu Yangping Li Chenxi Li Zhengtang Liu



Please cite this article as: Z. Xu, C. Li, Z. Liu, Tunable electronic and optical behaviors of two-dimensional germanium carbide, *Applied Surface Science* (2016), http://dx.doi.org/10.1016/j.apsusc.2016.01.136

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.



Tunable electronic and optical behaviors of two-dimensional germanium carbide

Zhuo Xu¹, Yangping Li¹, Chenxi Li, Zhengtang Liu

(State Key Laboratory of Solidification Processing, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an 710072, China)

Abstract

The electronic and optical properties of two-dimensional graphene-like germanium carbide (2D-GeC) are calculated using first-principle calculation based on density functional theory. Monolayer GeC has a direct band gap of 2.19 eV. The imaginary part of the dielectric function shows a wide energy range of absorption spectrum for monolayer GeC. Tunable band structures are found for monolayer GeC through in-plane strain. In addition, the band structures and optical properties of bilayer GeC under strain along the c axis are analyzed. Multilayer GeC exhibits a direct band gap like monolayer GeC, and new options of interband transitions are found between layers. The results suggest that 2D-GeC could be a good candidate for optoelectronic such as light-emitting diodes, photodiodes, and solar cells.

Key words: two-dimensional germanium carbide; density-functional theory; electronic properties; optical properties; bilayer GeC.

¹ Corresponding author.

E-mail: xuzhuo1022@mail.nwpu.edu.cn, liyp@nwpu.edu.cn

Download English Version:

https://daneshyari.com/en/article/5347879

Download Persian Version:

https://daneshyari.com/article/5347879

Daneshyari.com