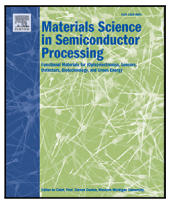
Materials Science in Semiconductor Processing 186 (2025) 109055

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp



High stability Janus structures of two dimensional Fe_3GeTe_2 monolayer by first-principles investigations

Nguyen T. Hiep [a,b], Dinh T. Khan [c], Le T.P. Thao [c,*], Cuong Q. Nguyen [a,b], Bui D. Hoi [d], Huynh V. Phuc [e,*], Nguyen N. Hieu [a,b]

[a] Institute of Research and Development, Duy Tan University, Da Nang, Viet Nam
[b] Faculty of Natural Sciences, Duy Tan University, Da Nang, Viet Nam
[c] Faculty of Physics, University of Science and Education, The University of Da Nang, Da Nang, Viet Nam
[d] Faculty of Physics, University of Education, Hue University, Hue, Viet Nam
[e] Division of Physics, School of Education, Dong Thap University, Cao Lanh, Viet Nam

ARTICLE INFO

Keywords:
Janus structures
Electronic characteristics
Spin-polarization
DFT method

ABSTRACT

In line with ongoing efforts on discovering new materials for the utilization in advanced nanotechnologies, in the present work, based on the original Fe_3GeTe_2 material, two-dimensional Janus Fe_3GeXTe (X = S and Se) monolayers are constructed and analyzed by using first-principles calculations. All three monolayers of Fe_3GeTe_2, Fe_3GeSTe, and $Fe_3GeSeTe$ exhibit hexagonal structures with good dynamical stability. No negative frequency is observed in the phonon dispersion spectra. During the *ab initio* molecular dynamics simulation at room temperature, the Fe_3GeXTe structures are predicted to be thermally stable without any reconstruction/fracture, suggesting the high thermal stability of these systems. In addition, the Fe_3GeXTe monolayers show high negative cohesive energy of about −5 eV/atom and the obtained elastic constants satisfy the Born and Huang condition. Their Young's modulus and Poisson's ratio exhibit isotropic elastic behaviors due to the isotropic structures. These results confirm that the Fe_3GeXTe monolayers are energetically and mechanically stable for experimental synthesis. Especially, the electronic properties of our studied structures are explored for applications in electronic devices. The Fe_3GeXTe monolayers show a metallic nature for both the spin-up and spin-down cases. The projected density of states reveals that the Fe_3GeTe_2, Fe_3GeSTe, and $Fe_3GeSeTe$ are magnetic materials due to their different spin-up and-down configurations. The results of our study can provide more information for the Janus Fe_3GeXTe materials and stimulate future experimental studies for practical applications in magnetic and electronic devices.

1. Introduction

The exploration of two-dimensional (2D) Janus materials has opened a new era in materials science. The 2D Janus nanomaterials such as metal dichalcogenides [1,2], transition metal monochalcogenides [3,4], transition metal oxides [5], MXenes [6], black phosphorous [7], and bismuthene [8], are emerging as promising candidates for innovative materials due to their broken mirror symmetry structures. These 2D materials show extraordinary electronic [9,10], thermodynamic [4,11], catalytic [12,13], magnetic [14,15], optical [16], and mechanical [17,18] behaviors for various applications.

Recently, the discovery of Fe_3GeTe_2 intrinsic ferromagnetic monolayer has stimulated more research studies on this interesting material for rare-earth-free magnets. Some research groups have investigated and reported the properties of Fe_3GeTe_2. For instance, Zhao et al. presented 2D ternary intrinsic magnetic compounds including the Fe_3GeTe_2 and its family by using high throughput first-principles calculations. The Fe_3GeTe_2 had good stability with a low formation energy of −0.15 eV/atom. It also exhibited a metal phase and high magnetic transition temperature of 110 K from the Monte Carlo simulation [19]. In another report, the Fe_3GeTe_2 was found to have high magnetic anisotropy energy of 3.0 meV/f.u which was higher than the other reported $Cr_2Ge_2Te_6$ and CrI_3 ferromagnetic semiconductors. Besides, the Fe_3GeTe_2 exhibited large magnetic circular dichroism on the magneto-optical spectra, leading to a high Faraday rotation angle of −156°/μm and large Kerr rotation angle of 2.7°. This indicates the promising applications of the Fe_3GeTe_2 in high-density magnetic-data-storage and nano magneto-optical devices [20]. By hole doping, Park and co-workers controlled the magnetic anisotropy of the Fe_3GeTe_2 material. The DFT calculation results showed that the electronic band structure was changed due to the effects of spin–orbit coupling, which

* Corresponding authors.
E-mail addresses: ltpthao@ued.udn.vn (L.T.P. Thao), hvphuc@dthu.edu.vn (H.V. Phuc).

https://doi.org/10.1016/j.mssp.2024.109055
Received 17 June 2024; Received in revised form 24 October 2024; Accepted 25 October 2024