Chemical Physics 594 (2025) 112660

Contents lists available at ScienceDirect

Chemical Physics

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

Novel Janus Co_3GeXTe (X = S, Se) monolayers with high structural stability: First-principles predictions

Nguyen T. Hiep [a,b], Vo Q. Nha [c], Le D. Hieu [c], Bui D. Hoi [d,*], Nguyen P.Q. Anh [e], Huynh V. Phuc [f], Cuong Q. Nguyen [a,b], Nguyen N. Hieu [a,b]

[a] Institute of Research and Development, Duy Tan University, Da Nang, 550000, Viet Nam
[b] Faculty of Natural Sciences, Duy Tan University, Da Nang, 550000, Viet Nam
[c] School of Engineering and Technology, Hue University, Hue, Viet Nam
[d] Faculty of Physics, University of Education, Hue University, Hue, Viet Nam
[e] Faculty of Electronics and Telecommunications, Saigon University, 273 An Duong Vuong St, Ward 2, District 5, Ho Chi Minh city, Viet Nam
[f] Division of Physics, School of Education, Dong Thap University, Cao Lanh, Viet Nam

ARTICLE INFO

Keywords:
Two-dimensional Janus material
Structural stability
Electronic properties
Density functional theory

ABSTRACT

This study attempts to construct two-dimensional (2D) Janus Co_3GeXTe (X = S and Se) monolayers from the original Co_3GeTe_2 based on first-principles predictions for new magnetic materials. The optimized Co_3GeTe_2, Co_3GeSTe, and $Co_3GeSeTe$ configurations show hexagonal structures with honeycomb lattices from Co and Te atoms. Then their stabilities are investigated to evaluate the feasibility of synthesizing the Co_3GeXTe materials by experiments. From the phonon dispersion spectra, all three monolayers expose eighteen positive phonon modes without any imaginary frequency. This implies that the Co_3GeXTe structures are dynamically stable. Only small total energy fluctuations and no structure fracture/reconstruction are observed after the *ab initio* molecular dynamics tests, revealing the high thermal stability of the Co_3GeXTe systems. Besides, the Co_3GeXTe monolayers have high negative E_{coh} of about −5 eV/atom and the C_{11}, C_{12}, and C_{66} elastic constants obey the condition of Born and Huang for mechanical stability. According to the Poisson's ratio and Young's modulus polar diagrams, the isotropic elastic properties are found in all three Co_3GeTe_2, Co_3GeSTe, and $Co_3GeSeTe$ monolayers. The obtained evidence indicates the good stabilities of the Co_3GeXTe structures for experimental synthesis. Moreover, we utilize different approaches for the Co_3GeXTe band structure calculations to explore the electronic properties. The results show metallic behaviors of the Co_3GeXTe materials for both spin-up and spin-down configurations. The differences of spin-up and spin-down configurations in the projected density of states demonstrate that the Co_3GeXTe are magnetic materials. Hence, our findings offer new Janus Co_3GeXTe magnetic materials and stimulate further studies for electronic and magnetic applications of these Co_3GeXTe materials.

1. Introduction

Since the discovery of graphene, many kinds of two-dimensional (2D) nanomaterials have been found and reported including bismusthene [1], black phosphorous [2], MXenes [3], transition metal oxides [4], transition metal monochalcogenides [5,6], and metal dichalcogenides [7,8]. Notably, the 2D Janus materials with asymmetric structures caused an out-of-plane electric field, leading to their unique physical and chemical behaviors. Therefore, these 2D materials have gained considerable interest for applications in various fields, such as optics [9,10], electronics [11,12], optoelectronics [13,14], magnetics [15–17] piezoelectricity [18,19], photocatalysis [20,21].

Due to the intense studies on exploring 2D materials, the 2D magnetic material family is also extending. The 2D chromium triiodide (CrI_3) monolayer was first reported as an Ising ferromagnet by using magneto-optical Kerr effect microscopy. Compared with the bulk crystal, the Curie temperature of CrI_3 monolayer was lower, indicating the low coupling between layers. Remarkably, the magnetization was suppressed by bilayer CrI_3 from a metamagnetic effect, while the interlayer ferromagnetism in trilayer CrI_3 was restored as in the bulk crystal [22]. Gong et al. used scanning magneto-optic Kerr microscopy and found an almost perfect 2D Heisenberg $Cr_2Ge_2Te_6$ ferromagnet. With extremely small fields of less than 0.3 tesla, they could control the paramagnetic and ferromagnetic states as transition temperature. They also

* Correspondence to: Faculty of Physics, University of Education, Hue University, Hue, Viet Nam.
E-mail addresses: buidinhhoi@hueuni.edu.vn (B.D. Hoi), hvphuc@dthu.edu.vn (H.V. Phuc), hieunn@duytan.edu.vn (N.N. Hieu).

https://doi.org/10.1016/j.chemphys.2025.112660
Received 13 December 2024; Received in revised form 10 February 2025; Accepted 11 February 2025
Available online 26 February 2025