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Optical manifestation of buckled configurations in graphene-like materials

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ABSTRACT

In the present study, the effects of the configuration buckling on dielectric function of silicene, germanene and stanene are investigated. The behavior of the optical absorption spectrum and the refractive index dispersion are studied using the density functional theory in terms of incident photon energy at different buckling heights. The results show that for a fixed bond length, increasing the unit cell buckling height, increases the absorption and the refractive index in silicene and germanene but decreases in stanene. In addition, the absorption peaks shift toward the longer wavelengths (red shift) in the case of silicene and germanene by increasing the buckling height. For clear understanding of the mentioned results, the behavior of the optical absorption spectrum and refractive index dispersion at different buckling heights are studied within the present work. In the case of the silicene and germanene reduction of the band gap with increasing the buckling height could be regarded as the origin of this red shift. Meanwhile unlike the silicene and germanene, band-structure reshaping in stanene could explain the stanene blue shift as a result of the buckling height increment.

1. Introduction

Nowadays, there are many review and scientific articles about graphene-like materials [1]. After the discovery of the graphene in 2004 [2,3], research in two-dimensional structures of the group IV elements of the periodic table has accelerated further.

Generally, two-dimensional material with a honeycomb structure [4] and its unusual electrical, optical and mechanical properties are attracting topics for researchers to challenge [3]. These challenges, such as optimizing production and cost-effectiveness, presence or absence of the energy band gap, study the composition graphene-like materials and its impact on other elements of the physical features are already on going. Despite of the major differences between the two-dimensional allotropes of the group IV elements, such as graphene, silicene, germanene and stanene they have also some similar properties and characteristics [5,6]. Silicene, germanene, and stanene [7] have attracted considerable attention in recent years since the discovery of graphene [8]. Meanwhile silicon is the most used material in the manufacture of diodes, transistors, integrated circuits and other semiconductor devices. However, from the application point of view silicene and

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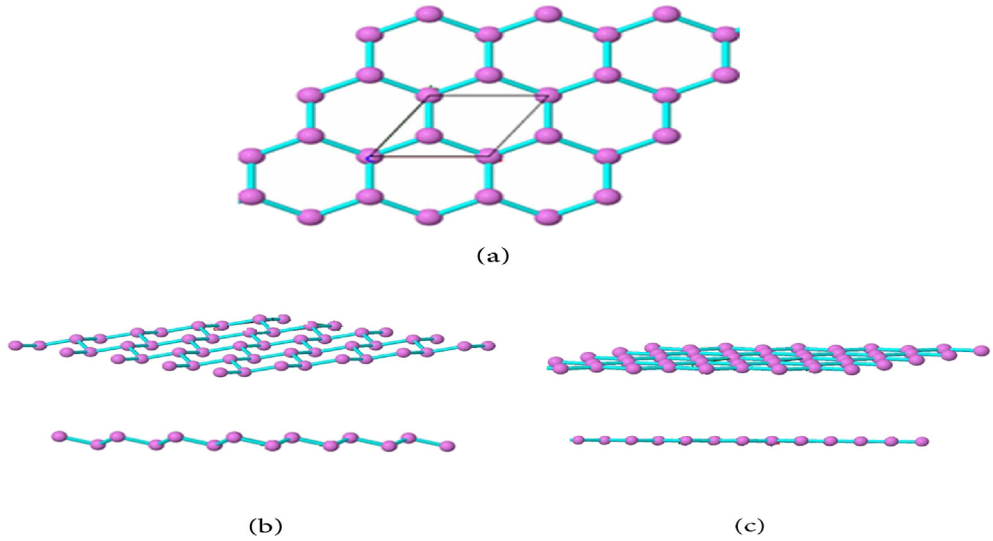

Fig. 1. (a).2-D hexagonal structure, (b). Buckled structure, (c). Planner structure.

other graphene-like materials deserve more attention to be industrially applicable. Both silicene and germanene have four valence electrons as the other elements of the IV group.

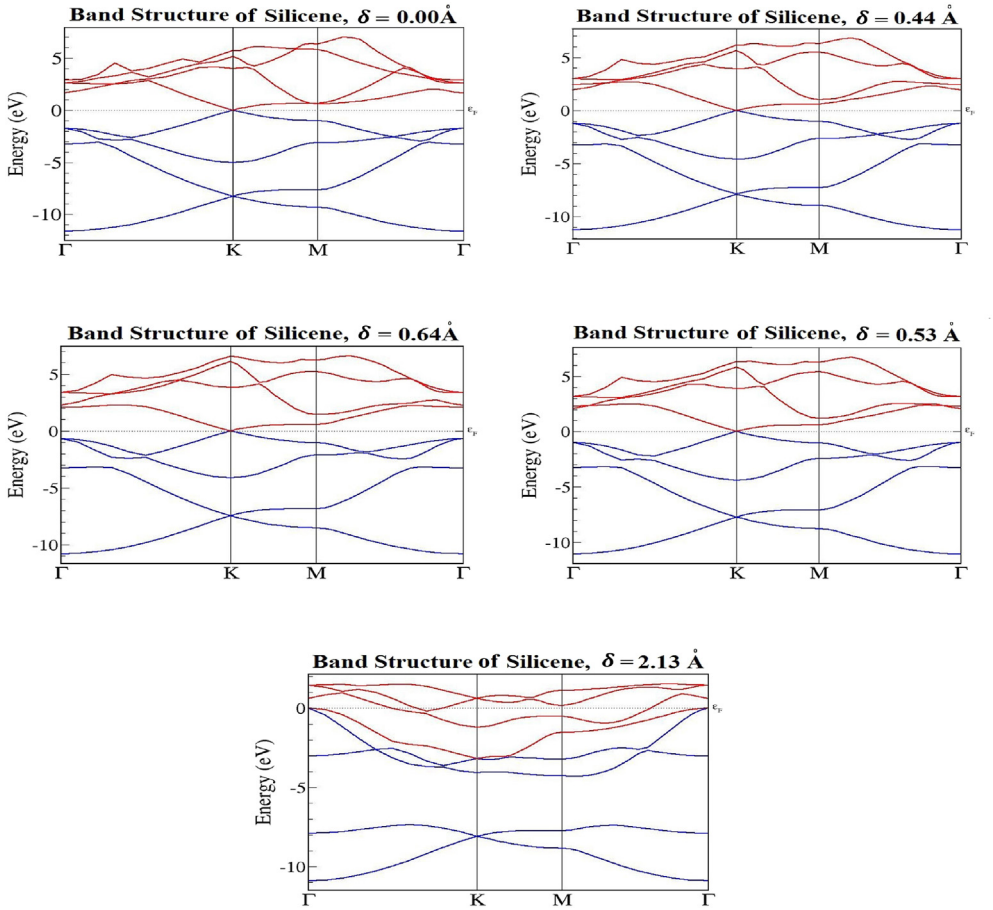

Fig. 2. Band structure of different buckled silicene configurations within the DFT-LDA method.