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PII: S0040-6090(18)30205-0
DOI: doi:10.1016/j.tsf.2018.03.061
Reference: TSF 36565

To appear in: *Thin Solid Films*

Received date: 2 August 2017
Revised date: 12 March 2018
Accepted date: 20 March 2018

Please cite this article as: Sake Wang, Jin Yu , Tuning electronic properties of silicane layers by tensile strain and external electric field: A first-principles study. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Tsf(2017), doi:10.1016/j.tsf.2018.03.061

Tuning electronic properties of silicane layers by tensile strain and external electric field: A first-principles study

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Abstract

The structural and electronic properties of silicane layers and bulk, the effects of a biaxial tensile strain and an external electric field (E-field) on the electronic properties of silicane monolayer and bilayer are investigated using density functional theory computations with the van der Waals (vdW) correction. It is demonstrated that the weak vdW interaction between silicane layers can efficiently tune the electronic properties of silicane multilayers. The silicane multilayers (up to 5) are indirect bandgap semiconductors whose bandgap slightly decreases with the number of layers, whereas bulk silicane is a direct bandgap semiconductor. The bandgaps of both silicane monolayer and bilayer can be flexibly modulated by applying a biaxial tensile strain, and indirect-direct transition occurs when the biaxial tensile strain reaches +4% and +2%, respectively. Besides, the bandgaps of the silicane monolayer and bilayer can also be continuously modulated by an external E-field, with an indirect-direct transition observed when its magnitude reaches 0.5 and 0.7 V/Å, respectively. A larger E-field can trigger a semiconductor-metal transition at approximately 0.8 V/Å for both silicane monolayer and bilayer. Our results provide rather effective and flexible approaches to tune the electronic properties of silicane layers for application in silicane-based electronic and optoelectronic devices.

1. Introduction

Silicene [1,2], the silicon analog of graphene, is a two-dimensional (2D) crystal with a hexagonal lattice structure. A number of experiments have realized the epitaxial growth of silicene on some metal substrates, such as Ag [1–7], Ir [8] and ZrB_2 thin films [9]. As reported by early theoretical works, silicene is a zero-bandgap semimetal, similar to graphene. Silicene also exhibits linear energy dispersion behavior around the Fermi level at the *K* point, which can lead to high carrier mobility [1,10]. Some fantastic features, such as a quantum spin Hall effect [11,12], giant magnetoresistance [13] and multiple topological interface states [14] have been predicted for monolayer silicene. Despite its outstanding electronic properties and effective integration with current silicon-based microelectronics, silicene cannot be used in many fields, such as field-effect transistors (FETs), because its zero bandgap restricts the achievability of on-off current ratio. Hence, some effective strategies should be adopted to open a bandgap in silicene.

Doping [15–24], adsorption [25–29] and functionalization [30,31] are three effective approaches to tuning the electronic and magnetic properties of 2D materials. For silicene, chemical functionalization [32–47] is a pretty effective technique for tuning its properties. For instance, the electronic and magnetic properties of silicene can be well tuned by half-hydrogenation, as reported by many theoretical [41,42] and experimental works [43,44]. An extreme example, which had previously been investigated by many theoretical works [40,45,46] is silicane (fully hydrogenated silicene). It is an indirect semiconductor with a bandgap of 2.94 eV (by Heyd-Scuseria-Ernzerhof (HSE06)) [47]. Potential applications such as high-performance FET [48], optoelectronic devices [49] and even

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