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Review

Silicene on Ag(111): Geometric and electronic structures of a new honeycomb material of Si



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ABSTRACT

Silicene, a two-dimensional honeycomb sheet consisting of Si atoms, has attracted much attention as a new low-dimensional material because it gains various fascinating characteristics originating from the combination of Dirac fermion features with spin–orbit coupling. The novel properties such as the quantum spin Hall effect and the compatibility with the current Si device technologies have fueled competition to realize the silicene. This review article focuses on the geometric and electronic structures of silicene grown on Ag(111) investigated by scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and density functional theory (DFT) calculations. The silicene on Ag(111) takes locally-buckled structure in which the Si atoms are displaced perpendicularly to the basal plane. As a result, several superstructures such as 4×4 , $\sqrt{13} \times \sqrt{13}R13.9^\circ$, $4/\sqrt{3} \times 4/\sqrt{3}$, and etc. emerge. The atomic arrangement of the 4×4 silicene has been determined by STM, DFT calculations and LEED dynamical analysis, while the other superstructures remain to be fully-resolved. In the 4×4 silicene, Si atoms are arranged to form a buckled honeycomb structure where six Si atoms of 18 Si atoms in the unit cell are displaced vertically. The displacements lead to the vertical shift of the substrate Ag atoms, indicating the non-negligible coupling at the interface between the silicene layer and the substrate. The interface coupling significantly modifies the electronic structure of the

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4×4 silicene. No Landau level sequences were observed by scanning tunneling spectroscopy (STS) with magnetic fields applied perpendicularly to the sample surface. The DFT calculations showed that the π and π^* bands derived from the Si $3p_z$ are hybridized with the Ag electronic states, leading to the drastic modification in the band structure and then the absence of Dirac fermion features together with the two-dimensionality in the electronic states. These findings demonstrate that the strong coupling at the interface causes the symmetry breaking for the 4×4 silicene and as a result the disappearance of Dirac fermion features. The geometric and electronic structures of other superstructures are also discussed.

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Contents

1. Introduction	2
2. Geometric and electronic structures of freestanding silicene	3
3. Geometric structure of silicene on Ag(111)	5
3.1. 4×4 structure	6
3.2. $\sqrt{13} \times \sqrt{13}R13.9^\circ$ structure	9
3.3. $4/\sqrt{3} \times 4/\sqrt{3}$ structure	10
3.4. Other superstructures	11
4. Electronic structure of silicene on Ag(111)	11
4.1. 4×4 structure	12
4.2. $4/\sqrt{3} \times 4/\sqrt{3}$ structure	15
5. Summary and outlook	16
Acknowledgements	17
References	17

1. Introduction

The elements in the 14th group are invaluable in periodic table. Carbon (C), reacting with various elements such as hydrogen, nitrogen, oxygen and etc., generates tremendous number of compounds, some of which are indispensable as fundamental building blocks for all living organisms on the globe. Silicon (Si) and germanium (Ge) are used in the heart of every electronic device to provide solid foundation to our highly-networked information society. These elements take the common valence electronic configuration described as $(ns)^2(np)^2$ where n is the principal quantum number, leading to similar properties as a result of the formation of hybrid orbitals by promoting one of the ns electrons to the empty np orbital. In their bulk, each atom bonds with the nearest neighbors, crystalizing into the three-dimensional diamond structure through the sp^3 hybrid network. When the framework is distorted locally, the amorphous phases appear. The structural features are common to C, Si and Ge. The most striking difference is that C atoms stably form into a two-dimensional (2D) honeycomb lattice called as graphene, which appears as graphite in nature. In contrast, the counterpart materials of Si and Ge, which are called silicene and germanene, respectively, do not exist in nature.

With great success of graphene [1–3], 2D materials, especially, 2D honeycomb lattice materials [4–7], have gathered lots of attention. Actually, the history of silicene and germanene predates the discovery of graphene. Takeda and Shiraishi [8] investigated the energetic stability of silicene and germanene with first principles density functional theory (DFT) calculations in 1994. This is the first report on the freestanding silicene and germanene as far as we know. Note that the terms “silicene”

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