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Two-dimensional silicon carbide structure under uniaxial strains, electronic and bonding analysis

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ABSTRACT

Based on Density Functional Theory (DFT) calculations, the narrowed band gap of two-dimensional (2D) SiC planar structure was investigated under uniaxial strains applied along the zigzag and armchair directions. 2D SiC structure exhibits an indirect band gap in its pristine state which undergoes towards direct band gap at −10.35% compressive zigzag strain and vanishes below −16.87% leading to its metallization. The unidirectional strain, applied along the zigzag direction, induces the closure of Si—C—Si bond angle bending from 120° to 99° promoting the increase of the ionic character of the disynaptic (Si—C) atomic basin while reducing the covalent character observed in the pristine structure as revealed by electron localization function (ELF). Additionally, the strain imposed along the zigzag direction, promotes the appearance of weak interactions in regions where there is no absence of strain by means of non-covalent interactions (NCI) index. These non-covalent interactions promote the stability of 2D SiC planar structure under strain regime as recently observed in its three dimensional counterpart (3C SiC). Our structural-electronic-bonding analysis shows that the band gap engineering can be monitored by unidirectional strain regime optimizing the narrowed band gap opening potential routes on the band gap engineering of 2D semiconductor materials with applications in the new generation of electronic devices.

1. Introduction

The great success of graphene has encouraged the fast development of novel two-dimensional (2D) materials, which have received considerable attention owing to their intriguing properties [1–5]. Focusing on the electronic properties, several 2D semiconductor materials have a direct finite band gap in their monolayer structure making them promising candidates for optoelectronic devices [6,7]. This family of 2D materials sustains strain regimes making their electronic properties particularly feasible to module by using engineering strain protocol [8]. The concept of engineering strain has been demonstrated mostly in transition-metal dichalcogenides (TMDs) compounds as a powerful technique for tuning physical and chemical properties [9,10]. The engineering strain properties of 2D materials also represent an engaging research area for the next-generation electronics. Nonetheless, such materials and research directions remain elusive for many other applications of 2D materials [11,12].

For ranking 2D materials, two classes can be distinguished (i) inherently layered materials bounded by van der Waals interactions such as TMDs among others, and (ii) those with non-planar covalent bonding in their bulk form such as the remaining group-IV elements (Si, Ge, Sn and Pb) [13]. It should be noted that unlike graphene, silicene (Si) exhibits a chair-like distortion of the hexagonal rings, resulting in an out-of-plane corrugation. Although it exists a structural analogy between graphene and silicene, the greater covalent bonding leads to the sp^3 hybridization (bulk phases) in silicon carbide (SiC) compounds. Bulk SiC has many exceptional physical properties such as high strength and high thermal conductivity. Thus, it is widely used in micro-electrochemical systems as well as in high-temperature, high-frequency and high-power electronic devices [14,15]. In contrast, less attention has been put on SiC based systems such as: monolayer of few-layers SiC [16] or on few carbon-rich SiC monolayers with particular

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stoichiometry (see for example: SiC_3 [17], g-SiC_2 [18], pt-SiC_3 [19] and buckled tetragonal t-SiC [20]). Computational based studies have shown that monolayer SiC is a semiconductor material with a band gap around 4.86 eV (using ab initio many body calculations by using GW quasiparticle corrections [21]) and 2.5 eV (using generalized gradient approximation (GGA) [22]). Monolayer or few-layer 2D SiC can be depicted simply as silicene/graphene in which half the atoms are replaced by the chemically similar carbon/silicon atoms. Recently a comprehensive structural search on the 2D Si_xC_{1-x} sheet with $0 < x < 1$ by using cluster expansion method together with density functional theory (DFT) calculations have revealed that the ground state structures of 2D Si_xC_{1-x} have high thermodynamic stability[23]. This study, described as a band gap engineering by composition analysis, reported Si_xC_{1-x} sheets with a rich variety of electronic properties depending on composition. On the other hand, atomic resolution scanning transmission electron microscopy observations have provided the first direct experimental finding over the existence of 2D SiC [24,16]. The ground state of 2D SiC was indeed completely planar with sp^2 hybridization of the Si−C bonds but, the large charge transfer from Si to C and the preference of Si for sp^3 hybridization renders the layer chemically reactive and unstable in bilayers. Additionally, structural predictions of 2D SiC recently reported have shown that the structure with composition Si:C = 1:1 with an alternatingly occupied hexagonal lattice is the only 2D structure found so far in the Si/C system that is thermodynamically stable with respect to decomposition intro graphene and silicene [25].

Most experimental works conducted by moissanite anvil cell experiments [10] and first principles calculations showed that applying strain on mono-layer or bi-layer compounds yields in the most of cases: to an electronic transition to semi-metal of metallic phase. For example in [26] 1L-MoS_2 mono-layer has been investigated under different strain regimes and demonstrates that directional pressure clearly induces direct to indirect band-gap transition at 23 GPa, and a semiconductor-to-semi-metal one at 68 GPa. Additionally, Wang et al. [27] studied the WS_2 under uniaxial in-plane strain, and related the change of light emission and lattice vibration of the CVD-grown mono-layer WS_2 to the effect of the applied strain. This wide knowledge of band gap engineering by strain on 2D TMDs contrasts with the lack on the strain effect on other families of 2D materials such as the 2D SiC planar structure reported herein. In this context only the mechanical stability a set of 2D SiC sheets has been investigated under uniaxial tension in the armchair and zigzag directions [28,29].

Therefore, it exists a demand in the literature of studies to understand the band gap modulation under uniaxial compression regimes. Motivated by recent experimental developments and theoretical investigations explained earlier on 2D SiC monolayer structure, we carried out here a systematic study based on density functional theory (DFT) calculations with the challenge of shedding light on the band gap engineering by using zigzag and armchair in-plain strain regime. This study compiles an accurate analysis of structural, electronic, bonding properties on 2D SiC which could be relevant for experimentalists in the design of electronic devices. On another side, Morales Garcia et al. [10] making an ab initio investigation of the 2D dichalcogenide compounds, have demonstrated that it is possible to modulate the gap of 2D structures by applying an out-of-plane compression by bringing two parallel planes closer together so that a weak van der Waals interaction can occur between these two planes. The authors have shown that this interaction is responsible to the metallization of the compound. Also, they have emphasized that the application of compression in the plane does not affect the monolayer but the out-of-plane does. However, the case of planar system was not discussed; due to the role of sp^2 geometry and the important role of neighboring atoms, this latter could involves different mechanism under in plane strains.

2. Computational details and models

Our computer atomistic simulations are based on Density Functional Theory (DFT) [30] as implemented in the (SIESTA) (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code [31]. Where the Kohn-Sham equations are solved self-consistently while expanding the valence electronic wave functions in a basis set of numerical atomic orbitals and adopting norm conserving pseudopotentials to describe the interaction of valence electrons with core electrons and nuclei. In the present calculations, 2s and 2p orbitals of both carbon and silicon atoms were explicitly included in the valence band and their wave functions were described by a linear combinations of double zeta polarized atomic orbitals. Soft Trouiller-Martins pseudopotentials [32] were used to account for core electrons. Our basis functions have a finite range corresponding to an energy shift of 0.01 Ry. This was set by applying a soft confining potential, as described by Junquera et al. [33], which allows to get rid of instabilities during structural relaxations. Exchange and correlations were treated within the Generalized Gradient Approximation (GGA), where the Perdew Burke Ernzerhof (PBE) functional was adopted [34]. Part of overlap and hamiltonian integrals were evaluated in the real space over grids whose the fineness corresponds to mesh cut-off of 500Ry. The Brillouin zone was sampled by using $1 \times 8 \times 8$ Monkhorst-Pack grids [35]. Structural optimizations were achieved by using the conjugate gradients algorithm and equilibrium structures were obtained when the forces and stresses were well below 0.01 eV/Å and 0.05 GPa, respectively. It must be mentioned that dispersion correction was also considered including the Grimme's correction (D2) [36]. Note that the dispersion contribution is negligible attending to the isolated 2D SiC model employed in this study, but its consideration is relevant when weak interactions are studied. Hence, when performing NCI topological analysis, it is recommended to include this correction to give an accurate description of the weak interactions in solid systems [37].

In order to predict the chemical bonding of the titled material, electronic density (ρ) has been calculated and then its scalar function analyzed by means of quantum theory of atoms in molecules (QTAIM) [38]. Here, QTAIM divides direct space into discrete atomic basins, which predicts self-consistent local properties such as charges and volumes, as a topological interatomic bond path motif, which is attributed to the molecular structure [38]. In this approach, the electron density is exhaustively partitioned to a set of electronic domains called basins (Ω). These basins are disjoint with a space filling regions [38]. Each of these basins contains a maximum or attractors formed by four types of critical points (CP) which emerge from the condition of zero flux of the gradient of the electron density: $\nabla\rho(\boldsymbol{r})\cdot\boldsymbol{n}(\boldsymbol{r}) = 0$ [38]. The integration of atomic properties inside the basins (Ω) can provides a detailed information about the chemical bonding of our structure. To analyze ionicity of our 2D material, we have compared each $\mathcal{Q}(\Omega)$ to its corresponding oxidation number ($OS(\Omega)$) by means of the *degree of ionicity* index, defined as $c = \frac{1}{N}\sum_{\Omega=1}^{N}\frac{\mathcal{Q}(\Omega)}{OS(\Omega)}$ [39].

Additional bonding analysis were also did with the electron localization function (ELF). This index was originally designed [38] to identify the localized electronic groups in atomic and molecular systems [38] in a Hartree-Fock framework. From this original definition, different interpretations were given, for example in the context of Markovian processes [40,41]. However, the most intuitive ones is that proposed by Savin et al. [42] in the DFT framework for which ELF can be understood as a local measure of the excess of local kinetic energy of electrons due to the Pauli principle [43], $t_p(\vec{r})$. This quantity is computed by subtracting the bosonic contribution, $|\nabla\rho(\vec{r})|^2/8$, from the kinetic energy density of the system, $t(\vec{r})$. Re-scaling it with respect to the homogeneous electrons gas like in the original definition provides the core of ELF, $\chi(\vec{r})$:

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