FERROELECTRIC JANUS MONOLAYER APPLICATION

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Abstract

We have performed an *ab initio* study of janus monolayers, a SiX state with as a direct wide bandgap semiconducting ferroelectric material, two-dimensional, 2D, silicon carbide has the potential to bring revolutionary advances into optoelectronic and electronic devices. It can overcome current limitations with silicon, bulk SiC, and gapless graphene. In addition to SiC, which is the most stable form of monolayer silicon carbide, other compositions, i.e., XC, are also predicted to be energetically favorable. Depending on the stoichiometry and bonding, monolayer SiC may behave as a semiconductor, semimetal or topological insulator. With different Si/C ratios, the emerging 2D silicon carbide materials could attain novel electronic, optical, magnetic, mechanical, and ferroelectric properties that go beyond those of graphene, silicene, and already discovered 2D semiconducting materials. This paper summarizes key findings in 2D SiX and provides insight into how changing the arrangement of silicon and carbon atoms in SiC will unlock incredible electronic, ferroelectric properties. It also highlights the significance of these properties for electronics, optoelectronics, and energy devices.

Keywords: Ferroelectric, Janus monolayer, quantum-mechanical, DFT

1. INTRODUCTION

One of the most intensively studied materials is Janus materials [1]. The Janus monolayer include two combinations of different chemical elements and some of them possess a suitable ferroelectric -structural transitions that are often accompanied by significant changes of their properties [2]. In particular, the off-stoichiometric SiX (X = C, Ge, Sn) compounds exhibit unusual ferroelectric and piezoelectric [3] The Stoichiometric SiX possess a long range in-plane ferroelectric arrangement of moments below the Curie temperature, then become a paraelectric compound above the Curie temperature [4].

Exceptionally high carrier mobility and zero band gap semi metallic [5] conductivity are only two of the peculiar optical and electrical characteristics of this 2D silicon material, which also contains a single Dirac point where the valence and conduction bands cross. It is one of the strongest materials known to man and incredibly mechanically flexible. Because it may be used in nanoscale energy harvesting, sensors, and actuators, piezoelectricity in 2D van der Waals materials has drawn a lot of attention. However, strain and electric polarization are restricted to the basal plane in every system examined so far, which restricts the functionality of piezoelectric devices. The freshly synthesized Janus MXY (M=Mo or W, X/Y=S, Se or Te) monolayer [6] and multilayer structures with large out-of-plane piezoelectric polarization materials are described in this study based on ab initio calculations.

2. COMPUTATIONAL METHODOLOGY

We used DFT implemented within the Quantum-ESPRESSO 6.8[5] ab initio software package. Depending on the material simulated, ion cores were treated using projector augmented-wave (PAW) pseudopotentials. Electron exchange and correlation effects were described using the generalized gradient- corrected Perdew-

Burke-Ernzerhof (PBE) approximation [6]. Periodic boundary conditions were employed in all three dimensions using an orthorhombic unit cell containing either two silicon atoms and two carbon atoms for SiC. Note the hexagonal primitive cell was not used in order to align the direction of polarization along one of the lattice vectors (i.e., the x-axis). A 20 Å cell height was used in the z-direction to prevent periodic images from interacting with each other.

The electronic wave function was expanded in a plane wave basis set with an energy cutoff of 60 Ry. The charge density was expanded in a basis set with a 240 Ry plane wave cutoff. Brillouin zone sampling was done using a Monkhorst- Pack mesh [7] of 12× 12× 1 k-points. All ionic relaxations and cell optimizations were performed using a threshold of of 10^{-4}Ry/Bohr for the force and 10^{-6} Ry for the unit cell energy.

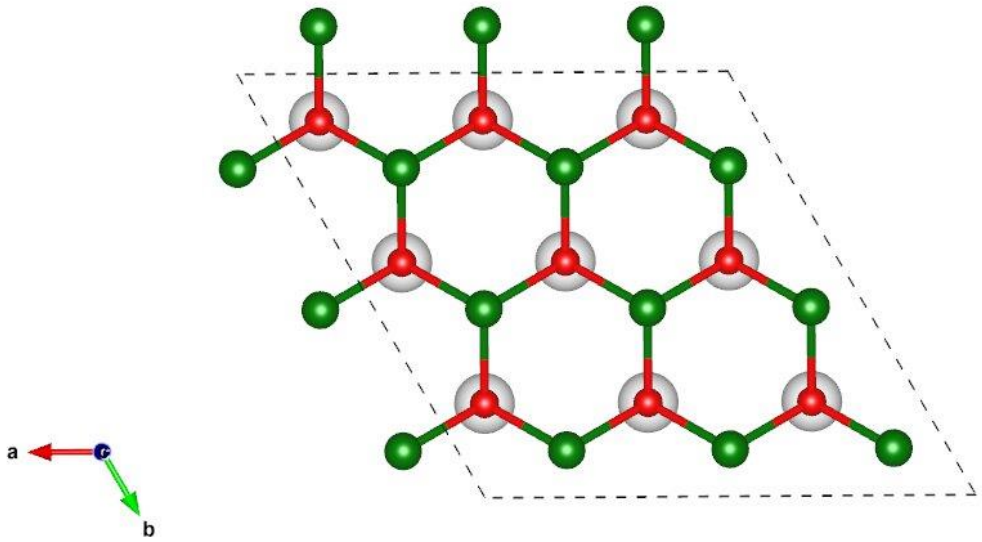

Figure 1 Schematic visualizations of 12-atom conventional supercell of Janus-structure

3. RESULTS

Figure 1 shows the 2D Janus SiX optimized crystal structures. In order to create the Janus SiX structures (X = C, Ge, Sn), the kind of atoms at one side must be swapped out for a different element. 2d materials that exhibit spontaneous electric polarization at Pmn_{21} phase (fig 01), we found the calculated strong in-plane polarization (x direction [1 0 0]) In **Figure 2**, we show that there is a linear relationship between uniaxial strain and polarization change in the x. The slope of the corresponding polarization shift with applied uniform strain along the x-direction of the rectangular cell may be used to calculate the piezoelectric coefficients e_{11}. Using the computed e_{11}, value, the corresponding clamped-ion coefficient d_{11} is produced. The polarizations along the axe is computed using the Berry phase method included in quantum espresso code. **Table 2** shows the clamped-ion findings for the e_{11}, d_{11}, coefficients.

Table1 Calculated and band gap Eg (eV), lattice constant (Å), and the spontaneous electric polarization (Ps) in pico-coulombs per metre (pC/m) of SiC, GeC, and SnC monolayers with Local-density approximation (LDA) and generalized gradient approximation (GGA).

material	Ps(pC/m) GGA	Ps(pC/m) LDA	Eg (eV)	Lattice constant (Å)
SiC	71.43	71.81	2.21	3.11
SiGe	54.24	53.87	1.85	3.46
SiSn	44.55	42.34	1.76	3.62

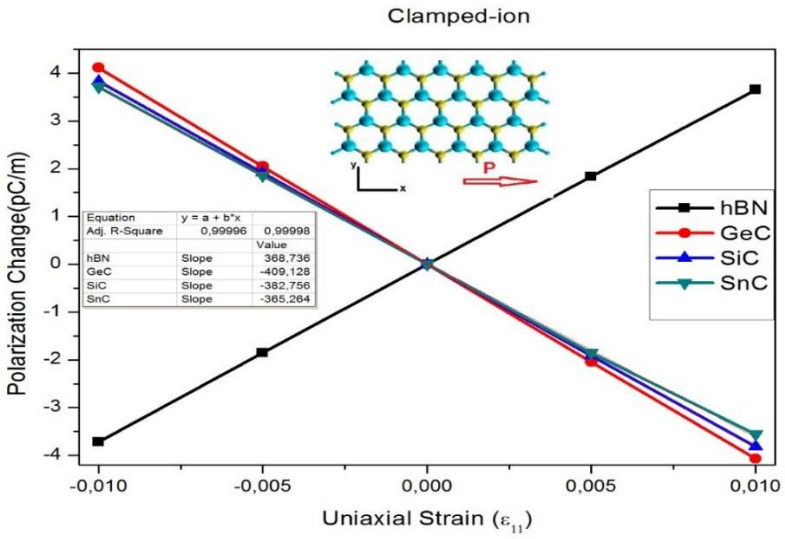

Figure 2 Applying an uniaxial in-plane strain to SiC induces a change in the polarization perpendicular to the sheet. At low strains, this relationship is linear where the slope gives the e_{11} piezoelectric coefficient.

Table 2 Calculated clamped-ion piezoelectric coefficients, e_{11} and d_{11}, of SiC, GeC, and SnC monolayers. The piezoelectric coefficient of h-BN and MoS_2 monolayers calculated by Duerloo et al. [8], are listed for comparison

Material	e_{11} (10^{-10} C·m^{-1})	d_{11} (pm·V^{-1})
SiC	-3.83	-2.46
GeC	-4.09	-2.90
SnC	-3.65	-3.2
h-BN	3.68	1.48
h-BN cal. [9]	3.71	1.50
MoS_2 cal. [9]	3.06	2.91

4. CONCLUSION

We have performed a density functional theory study of new ferroelectric Janus monolayer structures, our research focuses on SiX type monolayers with (X = C, Ge, Sn). We use First Principles method based on DFT, and our findings of optimization of the free parameters and lattice parameters of the three compounds are placed in the ranges of confusing results for the others in the same family, thus we have determined that the three SiX compounds are piezoelectric materials. The electronic characteristics were investigated, and the results revealed that they are semi-conductors. to ensure the state's mechanical stability. Fundamentally, we have a problem with these compounds being stable in the hexagonal phase at the price of the elastic constant. The obtained results encourage us to extend our work on this type of material and to study the optical and thermodynamic properties of these compounds.

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