Out-of-plane high-temperature ferromagnetic monolayer CrSCl with large vertical piezoelectric response

San-Dong Guo¹, Xiao-Shu Guo¹, Yu-Tong Zhu¹ and Yee-Sin Ang²
¹School of Electronic Engineering, Xi’an University of Posts and Telecommunications, Xi’an 710121, China and
²Science, Mathematics and Technology (SMT), Singapore University of Technology and Design (SUTD), 8 Somapah Road, Singapore 487372, Singapore

For two-dimensional (2D) material, piezoelectric ferromagnetism (PFM) with large out-of-plane piezoresponse is highly desirable for multifunctional ultrathin piezoelectric device application. Here, we predict that Janus monolayer CrSCI is an out-of-plane ferromagnetic (FM) semiconductor with large vertical piezoelectric response and high Curie temperature. The predicted out-of-plane piezoelectric strain coefficient $d_{31}$ is $-1.58$ pm/V, which is higher than ones of most 2D materials (compare absolute values of $d_{31}$). The large out-of-plane piezoelectricity is robust against electronic correlation and biaxial strain, confirming reliability of large $d_{31}$. Calculated results show that tensile strain is conducive to high Curie temperature, large magnetic anisotropy energy (MAE) and large $d_{31}$. Finally, by comparing $d_{31}$ of CrYX ($Y=S$; $X=Cl$, Br I) and CrYX ($Y=O$; $X=F$, Cl, Br), we conclude that the size of $d_{31}$ is positively related to electronegativity difference of $X$ and $Y$ atoms. Such findings can provide valuable guidelines for designing 2D piezoelectric materials with large vertical piezoelectric response.

Keywords: Ferromagnetism, Piezoelectronics, 2D materials
Email: sandongyuwang@163.com

INTRODUCTION

The multifunctional 2D piezoelectric materials can give rise to unprecedented opportunities for intriguing physics, and provide a potential platform for multifunctional electronic devices[1]. The coexistence of piezoelectricity, electronic topology and ferromagnetism, namely piezoelectric quantum anomalous Hall insulator (PQAHI), has been predicted in Janus monolayer Fe$_2$IX ($X=Cl$ and Br)[2], which provides possibility to use the piezoelectric effect to control quantum anomalous Hall (QAH) effects. The piezoelectric properties of ferrovalley (FV) materials have been investigated[3, 4], and the anomalous valley Hall effect induced by piezoelectric effect has been proposed in GdCl$_2$ monolayer[4]. Searching for PFMs has been a research hotspot[5–10]. An eminent 2D PFM with a typical triangle lattice structure should meet these conditions: (1) the strong FM coupling, which means high Curie temperature; (2) the out-of-plane magnetic anisotropy, which means a long-range phase, not a quasi-long-range phase; (3) the large out-of-plane piezoresponse, which is highly desirable for ultrathin piezoelectric device application. However, the reported PFMs satisfy some of these conditions. For example NiClI monolayer, the large out-of-plane piezoelectricity ($d_{31}=1.89$ pm/V) has been predicted, but it has very weak FM coupling and in-plane magnetic anisotropy[10]. For InCrTe$_3$ monolayer, it has large FM coupling and out-of-plane magnetic anisotropy, but the out-of-plane piezoelectricity is weak ($d_{31}=0.39$ pm/V)[9]. Therefore, searching for 2D PFMs with strong out-of-plane FM coupling and large vertical piezoelectric response is significant and challenging.

2D Janus materials have attracted increasing attention[11, 12], and the representative MoSSe monolayer has been successfully fabricated in experiment[13, 14]. Due to broken out-of-plane symmetry, the out-of-plane piezoelectricity can be observed in these Janus materials. Therefore, 2D Janus materials provide potential platform for searching good 2D PFMs. Recently, Janus monolayer Cr-based dichalcogenide halides CrYX ($Y=S$, Se, Te; $X=Cl$, Br, I) have been predicted by the first-principle calculations, and the CrSX ($X=Cl$, Br, I) are FM semiconductors[15]. The size of out-of-plane piezoelectric coefficient may have a positive relation with electronegativity difference of $X$ and $Y$ atoms for Janus MXY materials with M sandwiched between X and Y[16].

Due to large electronegativity difference of S and Cl atoms, in this work, we detailedly explore the magnetic, electronic and piezoelectric properties of CrSCl. It is found that CrSCl possesses an out-of-plane magnetization and high Curie temperature. The predicted $d_{31}$
is -1.58 pm/V, which is higher than ones (less than 1 pm/V) of most 2D materials (compare absolute values of \(d_{31}\)). More importantly, the large vertical piezoelectric response is robust against the electronic correlation and biaxial strain, which ensures high reliability of large \(d_{31}\). Moreover, tensile strain can enhance FM coupling, out-of-plane MAE and \(d_{31}\), which is in favour of eminent 2D PFM. Finally, we investigate \(d_{31}\) of CrYX (Y=S; X=Cl, Br I) and CrYX (Y=O; X=F, Cl, Br), and the calculated results show that the large electronegativity difference of X and Y atoms indeed can give rise to large \(d_{31}\).

**Computational detail**

Based on density functional theory (DFT)[17], the first-principle calculations are carried out by using the projector augmented wave (PAW) method as implemented in Vienna ab initio Simulation Package (VASP)[18–20]. The exchange-correlation functional is used by adopting generalized gradient approximation of Perdew, Burke and Ernzerhof (GGA-PBE)[21]. To consider on-site Coulomb correlation of Cr-3d electrons, we adopt \(U=2.1\) eV[15] by the rotationally invariant approach proposed by Dudarev et al[22], where only the effective \(U (U_{eff})\) based on the difference between the on-site Coulomb interaction parameter and exchange parameters is meaningful. The spin-orbital coupling (SOC) is included to calculate electronic structures and MAE of CrSCl. To attain reliable results, we set the energy cut-off of 500 eV, total energy convergence criterion of \(10^{-8}\) eV and force convergence criterion of less than 0.0001 eVÅ\(^{-1}\). We add a vacuum space of more than 16 Å between slabs along the z direction to eliminate the spurious interactions. The phonon spectrum with a 5×5×1 supercell is calculated by using the Phonopy code[23]. The Curie temperature is estimated by Monte Carlo (MC) simulations, as implemented in Mcsolver code[24]. A 40×40 supercell with periodic boundary conditions and 10\(^5\) loops are used to perform the MC simulation using Wolff algorithm. The elastic stiffness and piezoelectric stress tensors (\(C_{ij}\) and \(e_{ij}\)) are calculated by using strain-stress relationship (SSR) and density functional perturbation theory (DFPT) method[25], respectively. The first Brillouin zone (BZ) is sampled by a 21×21×1 k-point grid for electronic structures and \(C_{ij}\), and 12×21×1 for FM/antiferromagnetic (AFM) energies and \(e_{ij}\).

**Main calculated results**

For Janus CrSCl monolayer, as shown in Figure 1, Cr atoms are surrounded by six anions (three S and three Cl) to form a distorted octahedral structure, which exhibits a hexagonal lattice by Cl-Cr-S misalignment stacking with a space group of \(P\bar{3}m1\) (No.156). The difference in atomic size and electronegativity of S and Cl atoms will result in inequivalent Cr-S and Cr-Cl bonding lengths and charge distributions, which gives rise to intrinsic polar electric field and out-of-plane piezoelectric response. To confirm the magnetic ground state of CrSCl, we calculate the total energies of the FM and AFM configurations (see Figure 1). Calculated results show that the energy difference between AFM and FM orderings is 183 meV/rectangle supercell. So, the FM configuration is the ground state, which is related to the superexchange interaction. The optimized lattice constant \(a\) is 3.474 Å, and the Cr-Cl-Cr and Cr-S-Cr bonding angles are 87.85° and 94.56°. Based on the Goodenough-Kanamori-Anderson (GKA) rules, FM superexchange interaction with near 90° will dominate the interaction between Cr atoms, which gives rise to the FM coupling[26, 27].

To verify the dynamical stability of CrSCl, we calculate its phonon spectra, as shown in Figure 2 (a). No negative frequency phonons are observed in the whole BZ, which implies that CrSCl is dynamically stable. To further confirm its thermal stability, we perform ab-initio molecular dynamics (AIMD) simulations at 300 K for 7 ps using a 4×4×1 supercell and a time step of 1 fs. As shown in FIG.1 of electronic supplementary information...
(ESI), during the simulation period, little energy fluctuation is observed and the structures at the end of the AIMD simulations show no structural transitions, indicating that CrSCl is stable at a temperature of 300 K. To determine the mechanical stability of CrSCl, the linear elastic constants are calculated, and the 2D elastic tensor (Voigt notation) with space group P3m1 can be reduced into:

\[
C = \begin{pmatrix}
C_{11} & C_{12} & 0 \\
C_{12} & C_{11} & 0 \\
0 & 0 & (C_{11} - C_{12})/2
\end{pmatrix}
\]

(1)

Only two independent elastic constants \((C_{11}=62.82\text{ Nm}^{-1}\) and \(C_{12}=13.67\text{ Nm}^{-1}\) can be observed, which meet Born-Huang criteria of mechanical stability \((C_{11} > 0 \text{ and } C_{11} - C_{12} > 0)\) [28], thereby verifying mechanical stability of CrSCl.

For 2D hexagonal symmetric system with a typical triangle lattice structure, the magnetocrystalline direction determines type of magnetic phase transition. The in-plane one (an easy magnetization plane) means that there is no energetic barrier to the rotation of magnetization in the \(xy\) plane, which will produce a Berezinskii-Kosterlitz-Thouless magnetic transition to a quasi-long-range phase [29, 30]. However, the out-of-plane one can give rise to a long-range FM phase. It is difficult to simulate quasi-long-range phase with in-plane magnetic anisotropy by DFT calculations. In previous studies, the electronic structures are calculated by assuming magnetocrystalline direction along \(x\) axis, which should be different from ones of quasi-long-range phase. For most 2D systems, the magnetocrystalline direction has small effects on their electronic properties. However, some essential influences on electronic and topological properties have been observed in some 2D materials [31, 32]. Although the magnetocrystalline direction of 2D materials can be regulated by external magnetic field, the needed magnetic field may be very large (For example, the energetic barrier of 1 meV is equivalent to applying an external magnetic field of around 5-10 T.). Thus, it is very realistic to search for 2D out-of-plane magnetic materials with a typical triangle lattice structure. The intrinsic magnetic anisotropy of CrSCl can be determined by MAE. We define MAE as energy difference \((E_2 - E_1)\), where \(E_2/E_1\) is the energy per primitive cell when the magnetization is along the \(x/z\) direction. The positive/negative MAE means out-of-plane/in-plane direction. The calculated MAE is 36 \(\mu\text{eV}\), indicating that the intrinsic easy axis of CrSCl is out-of-plane. Thus, CrSCl is a 2D long-range FM material.

The spin-resolved electronic band structures calculated by using GGA and GGA+SOC are plotted in Figure 2(b) and (c). Around the Fermi level, the fully spin-polarized valence band and conduction band are in the same spin channels. The GGA results show that CrSCl is an indirect gap semiconductor (gap value of 1.98 eV) with both the valence band maximum (VBM) and conduction band minimum (CBM) lying between the K and \(\Gamma\) points. It is noted that the two extremums of top valence band are very close, and the energy difference is only 5.3 meV. With the inclusion of SOC, the gap is reduced to 1.87 eV. Moreover, sizable Zeeman-type valley splitting occurs at the \(\Gamma\) point for spin-down direction, and the splitting is 66.5 meV. According to the Cr-\(d\) band structure projection (FIG. 2 of ESI), the Cr atoms change from 4\(s^23d^5\) to 4\(s^03d^6\) in the electronic arrangement during the synthesis of CrSCl, which means that CrSCl would have a theoretical magnetic moment of 3 \(\mu_B\). Calculated results show a net magnetic moment of 3 \(\mu_B\) per CrSCl chemical formula.

To simply estimate Curie temperature \(T_C\), the spin Hamiltonian under the Heisenberg model can be expressed as:

\[
H = -J \sum_{i,j} S_i \cdot S_j - A \sum_i (S_i^z)^2
\]

(2)

where \(J, S\) and \(A\) are the nearest exchange parameter, spin quantum number and MAE, respectively. By comparing energies of AFM (\(E_{AFM}\)) and FM (\(E_{FM}\)) configurations of CrClBr with rectangle supercell, the \(J\) with normalized spin vector (\(|S|=1\)) is determined from these equations:

\[
E_{AFM} = E_0 + 2J - 2A \quad E_{FM} = E_0 - 6J - 2A
\]

(3)

\[
J = \frac{E_{AFM} - E_{FM}}{8}
\]

(4)

where \(E_0\) is the energy without magnetic coupling. The normalized magnetic moment and auto-correlation as a function of temperature with \(J=22.86\text{ meV}\) are plotted in Figure 2(d), and the predicted \(T_C\) is about 275 K.
TABLE I. For monolayer CrYX (Y=S and O; X=F, Cl, Br or I), the lattice constants \(a_0\) (Å), the energy difference between AFM and FM ordering \(\Delta E\) (meV), the magnetic anisotropy energy MAE (µeV), the elastic constants \(C_{ij}\) (Nm\(^{-1}\)), the piezoelectric coefficients \(e_{ij}\) (10\(^{-10}\) C/m ) and \(d_{ij}\) (pm/V).

| Name | \(a_0\) | \(\Delta E\) | MAE | \(C_{11}\) | \(C_{12}\) | \(e_{11}\) | \(e_{31}\) | \(d_{11}\) | \(d_{31}\) |
|------|--------|-------------|-----|---------|---------|--------|--------|--------|--------|
| CrSCl | 3.474  | 183 | 36 | 62.82 | 13.67 | -0.39 | -1.21 | -0.80 | -1.58 |
| CrSBr | 3.560  | 189 | 52 | 61.19 | 13.27 | -0.19 | -0.71 | -0.40 | -0.96 |
| CrSI  | 3.712  | 168 | 185 | 59.98 | 12.72 | 0.13 | -0.02 | 0.28 | -0.03 |
| CrOF  | 3.039  | 80  | 150 | 113.98 | 25.19 | -0.21 | -0.97 | -0.24 | -0.70 |
| CrOCl | 3.175  | 33  | 136 | 102.67 | 25.14 | 1.05 | 0.22 | 1.35 | 0.18 |
| CrOBr | 3.259  | 5   | 120 | 102.13 | 26.51 | 1.59 | 0.79 | 2.10 | 0.61 |

Due to unique Janus structure of CrSCl, both in-plane and out-of-plane piezoelectric response can be observed. By using Voigt notation, the 2D piezoelectric stress and strain tensors for \(P3m1\) symmetry can be reduced into[33, 34]:

\[
e = \begin{pmatrix} e_{11} & -e_{11} & 0 \\ 0 & 0 & -e_{11} \\ e_{31} & e_{31} & 0 \end{pmatrix}
\]

(5)

\[
d = \begin{pmatrix} d_{11} & -d_{11} & 0 \\ 0 & 0 & -2d_{11} \\ d_{31} & d_{31} & 0 \end{pmatrix}
\]

(6)

When an uniaxial in-plane strain is imposed, both in-plane and out-of-plane piezoelectric response can be induced \((e_{11}/d_{11} \neq 0\) and \(e_{31}/d_{31} \neq 0\)). However, by applying a biaxial in-plane strain, only out-of-plane piezoelectric response can exist \((e_{11}/d_{11}=0\), but \(e_{31}/d_{31} \neq 0\)). These mean that pure out-of-plane piezoelectric response can be achieved by imposed biaxial strain. Here, the two independent \(d_{11}\) and \(d_{31}\) can be derived by \(e_{ik} = d_{ij}C_{jk}\):

\[
d_{11} = \frac{e_{11}}{C_{11} - C_{12}} \text{ and } d_{31} = \frac{e_{31}}{C_{11} + C_{12}}
\]

(7)

We use the orthorhombic supercell (see Figure 1) to calculate the \(e_{11}/e_{31}\) of CrCIS. The calculated \(e_{11}/e_{31}\) is \(-0.39 \times 10^{-10}/-1.21 \times 10^{-10}\) C/m with ionic part \(0.29 \times 10^{-10}/0.18 \times 10^{-10}\) C/m and electronic part \(-0.68 \times 10^{-10}/-1.39 \times 10^{-10}\) C/m. For both \(e_{11}\) and \(e_{31}\), the electronic and ionic contributions have opposite signs, and the electronic part dominates the piezoelectricity. And then, the \(d_{11}/d_{31}\) of CrSCl can be obtained from Equation 7, and the corresponding value is \(-0.80/-1.58\) pm/V. For most 2D materials, their out-of-plane piezoelectric response is less than 1 pm/V, such as oxygen functionalized MXenes \((0.40-0.78\) pm/V)[35], Janus TMD monolayers \((0.03\) pm/V)[36], functionalized h-BN \((0.13\) pm/V)[36], kalium decorated graphene \((0.3\) pm/V)[36], Janus group-III materials \((0.46\) pm/V)[36], Janus BiTeI/TePtSe \((0.37-0.66\) pm/V)[39], \(\alpha\)-In\(_2\)S\(_3\) \((0.415\) pm/V)[40] and MoSO \((0.7\) pm/V)[41]. For the needs of practical application, a large out-of-plane piezoelectric response is highly desired to be compatible with the nowadays bottom/top gate technologies. Some progresses have been made for large out-of-plane piezoelectric response, such as NiClI \((1.89\) pm/V)[10], TePtS/TePtSe \((2.4-2.9\) pm/V)[42] and CrBrI\(_{1.5}\)I\(_{1.5}\) \((1.138\) pm/V)[8]. However, compared with these materials, the CrSCl possesses out-of-plane FM ordering with high Curie temperature, which is beneficial to practical application. So, CrSCl is a potential PFM with large out-of-plane piezoelectric response.

To confirm reliability of large \(d_{31}\), electronic correlation is considered to investigate piezoelectric properties of CrSCl. The lattice constants \(a\) at different \(U\) (0-4 eV) are optimized, and the change is about 0.066 Å with increasing \(U\). It is found that CrSCl is always a FM ground state (see Figure 3 (a)), and the \(J\) changes from 21.60 meV to 22.97 meV with increasing \(U\) (variation of 1.37 meV), indicating that high \(T_C\) is robust against \(U\). Moreover, the CrSCl has a steady out-of-plane magnetic anisotropy with increasing \(U\) (see Figure 3 (b)).
and the MAE decreases. The evolutions of energy band structures as a function of $U$ are calculated by using GGA+SOC, and the gap versus $U$ is plotted in FIG.3 of ESI. The CrSCl is always a semiconductor in considered $U$ range, and the gap increases with increasing $U$. The elastic constants ($C_{11}$, $C_{12}$, $C_{11}+C_{12}$) and piezoelectric stress coefficients ($e_{11}$ and $e_{31}$) along the ionic and electronic contributions as a function of $U$ are plotted in FIG.4 and FIG.5 of ESI. It is found that these elastic constants ($C_{11}+C_{12}$ and $C_{11}+C_{12}$) and piezoelectric stress coefficients ($e_{11}$ and $e_{31}$) have weak dependence on $U$. The piezoelectric strain coefficients ($d_{11}$ and $d_{31}$) versus $U$ are plotted in Figure 3 (c) and (d). It is observed that the $d_{31}$ (absolute value) is always larger than 1.51 pm/V within considered $U$ range. Thus, the large $d_{31}$ is robust against electronic correlation for CrSCl monolayer.

It is well known that the GGA may overestimate lattice constants of materials, and strain exists naturally in the process of synthesizing materials. So, the strain effects on piezoelectric properties of CrSCl are considered to confirm large $d_{31}$. The $a/a_0$ (0.96-1.04) is used to simulate biaxial strain, where $a/a_0$ denotes strained/unstrained lattice constant. Taking $U=2.1$ eV, we investigate the strain effects on physical properties of CrSCl. According to Figure 4 (a), all strained CrSCl are FM ground state in considered strain range. The tensile strain can enhance FM interaction, which makes for high Curie temperature. The normalized magnetic moment and auto-correlation as a function of temperature at $a/a_0=1.04$ are plotted in FIG.6 of ESI, and the predicted $T_C$ is improved to 303 K. Figure 4 (b) shows that tensile strain can enhance MAE, while compressive strain can reduce MAE. At about $a/a_0=0.96$, the easy axis of CrSCl changes from out-of-plane to in-plane. In considered strain range, CrSCl maintains semiconductor characteristics, and the gap as a function of $a/a_0$ is plotted in FIG.7 of ESI. It is found that the gap of CrSCl decreases with $a/a_0$ from 0.96 to 1.04. The elastic constants ($C_{11}$, $C_{12}$, $C_{11}+C_{12}$ and $C_{11}+C_{12}$) and piezoelectric stress coefficients ($e_{11}$ and $e_{31}$) along the ionic and electronic contributions as a function of $a/a_0$ are plotted in FIG.8 and FIG.9 of ESI. The $d_{11}/d_{31}$ versus $a/a_0$ is plotted in Figure 3 (c)/(d). It is found that increasing strain can improve $d_{31}$ (absolute value) due to decreased $C_{11}+C_{12}$ and enhanced $e_{11}$ (absolute). The $d_{31}$ (absolute value) is also enhanced with increasing strain, which is due to reduced $C_{11}+C_{12}$. In considered strain range, the $d_{31}$ (absolute value) is larger than 1.40 pm/V, indicating its robustness against strain. Calculated results show that tensile strain is beneficial to high Curie temperature, large MAE and large $d_{11}/d_{31}$ (absolute value).

**CONCLUSION**

In fact, Janus monolayer CrsX (X=Cl, Br I) and CrOX (X=F, Cl, Br) have all been predicted to be out-of-plane FM semiconductors[15, 43], and we investigate their piezoelectric properties. The optimized lattice constants, energy difference between AFM and FM ordering, MAE, elastic constants and piezoelectric coefficients $e_{ij}$ are summarized in Table I. They all are mechanically stable due to satisfying criteria of mechanical stability for calculated elastic constants. The piezoelectric stress coefficients ($e_{11}$ and $e_{31}$) along the ionic/electronic contribution are plotted in FIG.10 of ESI. It is found that, for both $e_{11}$ and $e_{31}$, the electronic and ionic contributions have opposite signs. The $d_{31}$ of CrSCl is the largest among CrsX (X=Cl, Br I), while the highest $d_{31}$ among CrOX (X=F, Cl, Br) is CrOF, which may be explained by different atomic electronegativities of upper and lower layers. The $d_{31}$ (absolute value) of CrsX (Y=S; X=Cl, Br I) and CrsX (Y=O; X=F, Cl, Br) along with the electronegativity difference of X and Y atoms are plotted in Figure 5. It is observed that the large electronegativity difference of X and Y atoms is related with large $d_{31}$. For CrsX (X=Cl, Br I), the $d_{31}$ decreases with X from Cl to Br to I, and the $d_{31}$ (absolute value) is only 0.03 pm/V due to very small electronegativity difference of S and I atoms. For CrOX (X=F, Cl, Br), the $d_{31}$ decreases, and then increases, when X changes from F to Cl to Br.

In conclusion, the electronic structures, magnetic and piezoelectric properties of CrSCl are systematically investigated by first-principles calculations. Calculated results show that CrSCl is an out-of-plane FM semiconductor with high Curie temperature. Most importantly, the findings reveal that CrSCl exhibits large out-of-plane piezoelectric coefficient $|d_{31} (>1.50$ pm/V), which is very larger than those of most known 2D materials. It is found that out-of-plane FM ground state and large out-of-plane piezoelectric response are robust against...
electronic correlation. The tensile strain can enhance FM interaction, MAE and \( |d_{31}| \), which provide the alternative solution for enhancing out-of-plane piezoelectric effect. These comparisons about \( d_{31} \) (absolute value) of CrYX (Y=S; X=Cl, Br I) and CrYX (Y=O; X=F, Cl, Br) provide a development guide for searching Janus 2D materials with large out-of-plane piezoelectric response.

**SUPPLEMENTARY MATERIAL**

See the supplementary material for AIMD results; elastic and piezoelectric properties of CrSCl as a function of \( U \) or \( a/a_0 \); \( e_{ij} \) of CrYX (Y=S; X=Cl, Br I) and CrYX (Y=O; X=F, Cl, Br).

**Conflicts of interest**

There are no conflicts to declare.

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