Sensitive electronic correlation effects on electronic properties in ferrovalley material
Janus FeClIF monolayer
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The electronic correlation may have essential influence on electronic structures in some materials with special structure and localized orbital distribution. In this work, taking Janus monolayer FeClIF as a concrete example, the correlation effects on its electronic structures are investigated by using generalized gradient approximation plus U (GGA+U) approach. For perpendicular magnetic anisotropy (PMA), the increasing electron correlation effect can induce the ferrovalley (FV) to half-valley-metal (HVM) to quantum anomalous Hall (QAH) to HVM to FV transitions. For QAH state, there are a unit Chern number and a chiral edge state connecting the conduction and valence bands. The HVM state is at the boundary of the QAH phase, whose carriers are intrinsically 100% valley polarized. With the in-plane magnetic anisotropy, no special QAH states and prominent valley polarization are observed. However, for both out-of-plane and in-plane magnetic anisotropy, sign-reversible Berry curvature can be observed with increasing $U$. It is found that these phenomena are related with the change of $d_{xy}/d_{x^2−y^2}$ and $d_2$ orbital distributions and different magnetocrystalline directions. It is also found that the magnetic anisotropy energy (MAE) and Curie temperature strongly depend on the $U$. With PMA, taking typical $U=2.5$ eV, the electron valley polarization can be observed with valley splitting of 109 meV, which can be switched by reversing the magnetization direction. The analysis and results can be readily extended to other nine members of monolayer FeXY (X/Y=F, Cl, Br and I) due to sharing the same Fe-dominated low-energy states and electronic correlations with FeClIF monolayer. Our works emphasize the importance of electronic correlation to determine the electronic state of some materials, and the electronic correlation can induce exceptional phase transition.

Keywords: Electronic correlation, Valleytronics, Magnetic anisotropy
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I. INTRODUCTION

In recent years, the valley as a new degree of freedom of electrons for two-dimensional (2D) graphene-related materials has attracted intensive attention\textsuperscript{1−7}. The local energy extremes in the conduction band or valence band are referred to as valleys, and they provide a new effective degree of freedom, in addition to conventional charge and spin. With the broken centrosymmetry, the two inequivalent sublattices give rise to a degenerate but inequivalent pair of valleys, which are well separated in the 2D hexagonal Brillouin zone\textsuperscript{1}. To achieve valley application, the external conditions, such as the optical pumping, magnetic field, magnetic substrates and magnetic doping\textsuperscript{8−11}, have been used to trigger polarization. The FV materials may be the best choice for valleytronics due to spontaneous valley polarization\textsuperscript{12}, and many FV materials have been predicted by the first-principle calculations\textsuperscript{13−20}.

The FV materials possess magnetism, and generally contain transition metal elements with localized d electrons, where the electronic correlations may have important effects on the magnetic, topological, and valley properties of these materials. Recently, the some of monolayer FeXY (X/Y=F, Cl, Br and I) family, such as FeX\textsubscript{2} (X=Cl, Br and I) and FeClBr\textsuperscript{21−24}, are predicted to be FV materials. Some differences can be found for their valley properties\textsuperscript{21,22,24}, which is because different exchange-correlation functional is adopted. For example, for FeCl\textsubscript{2}, the valley polarization appears at the valence bands by using GGA\textsuperscript{21,24}, but that exists at the conduction bands with HSE06 and GGA+U (>1.9 eV)\textsuperscript{22,24}. Within GGA, it is found that the valley polarization can be observed at the valence bands for FeX\textsubscript{2} (X=Cl, Br and I) and FeClBr\textsuperscript{21,21,24}. These mean that the electronic correlations have important effects on physical properties of monolayer FeXY family. In fact, the different correlation strengths can make FeCl\textsubscript{2} monolayer into different ground states, like HVM and QAH states, with the assumption of PMA\textsuperscript{24}. However, the correlation strength of a given material is fixed. So, it is very necessary for calculating electronic properties of FeXY family to consider different strength of electronic correlation.

In light of these factors about monolayer FeXY family mentioned above, we take Janus monolayer FeClIF as a concrete example to investigate the correlation effects on its electronic structures by GGA+U approach. Unlike previous studies\textsuperscript{24} (The lattice constants are optimized with GGA, and the electronic structures are studied by GGA+U), the lattice constants are optimized with varied $U$, and the corresponding electronic structures and magnetic properties are investigated. It is found that different correlation strengths ($U$) along with different magnetic anisotropy (out-of-plane and in-plane) can drive the system into different electronic states. For PMA, the increasing $U$ can induce the FV to HVM to QAH to HVM to FV transitions. For in-plane situation, there
FIG. 1. (Color online) The (a) top view and (b) side view of crystal structure of Janus monolayer FeClF, and the rhombus primitive cell is marked by the black frame. (c) The Brillouin zone with high-symmetry points labeled.

FIG. 2. (Color online) For Janus monolayer FeClF, the lattice constants and energy differences (rectangle supercell) between FM and AFM ordering as a function of $U$.

are no special QAH states and prominent valley polarization. These can be explained by considering the different Fe-$d$ orbital contributions, when including spin-orbital coupling (SOC). However, calculated results show sign-reversible Berry curvature with increasing $U$ for both out-of-plane and in-plane magnetic anisotropy. Finally, it is proved that correlation strengths have very important effects on Curie temperature $T_C$ of FeClF. The $T_C$ (311 K) with $U = 1.5$ eV is five time that (63 K) with $U = 2.5$ eV. Our works highlight the role of correlation effects in the 2D FeXY family materials.

The rest of the paper is organized as follows. In the next section, we shall give our computational details and methods. In the next few sections, we shall present structure and stability, electronic structure and valley properties of Janus monolayer FeClF. Finally, we shall give our discussion and conclusion.

II. COMPUTATIONAL DETAIL

The spin-polarized first-principles calculations are performed employing the projected augmented wave (PAW) method within density functional theory (DFT), as implemented in VASP code, as the exchange-correlation effect is treated by the GGA of Perdew-Burke-Ernzerhof (PBE-GGA). The energy cut-off of 500 eV and total energy convergence criterion of $10^{-8}$ eV are used in the static calculations. The force convergence criteria is set to be less than 0.0001 eV/Å on each atom. The on-site Coulomb correlation of Fe atoms is considered within the GGA+$U$ scheme by the rotationally invariant approach proposed by Dudarev et al, in which only the effective $U$ ($U_{eff}$) based on the difference between the on-site Coulomb interaction parameter and exchange parameters is meaningful. The SOC effect is explicitly included in the calculations to investigate MAE and electronic structures of FeClF monolayer. A vacuum space of more than 18 Å is used to avoid the interactions between the neighboring slabs. The k-mesh of $24 \times 24 \times 1$ is used to sample the Brillouin zone for calculating electronic structures and elastic properties, and $12 \times 24 \times 1$ Monkhorst-Pack k-point mesh for the energies of ferromagnetic (FM) and antiferromagnetic (AFM) states with rectangle supercell, as shown in FIG.1 of electronic supplementary information (ESI).

The elastic stiffness tensor $C_{ij}$ are calculated by using strain-stress relationship (SSR) method, where 2D elastic coefficients $C_{ij}^{2D}$ have been renormalized by $C_{ij}^{2D} = L_z C_{ij}^{3D}$ with the $L_z$ being the length of unit cell along z direction. The phonon dispersion spectrum is calculated with the $5 \times 5 \times 1$ supercell by using finite displacement method, as implemented in the Phonopy code. The $40 \times 40$ supercell and $10^7$ loops are used to perform the Monte Carlo (MC) simulations, as implemented in Mesolver code. The mostly localized Wannier functions including the $d$-
orbital of Fe atom and the p-orbitals of Cl and F atoms are constructed on a k-mesh of $24 \times 24 \times 1$ by the Wannier90 package\cite{Wannier90}. The edge states are calculated with the software package Wanniertools by the renormalized effective tight binding Hamiltonian\cite{Ren TB}. The Berry curvatures of FeClF monolayer are calculated directly from the calculated wave functions based on Fukui’s method\cite{Fukui method}. implemented in the VASP\cite{VASP}.

III. STRUCTURE AND STABILITY

The crystal structures of the Janus FeClF monolayer are plotted in Figure 1, along with Brillouin zone with high-symmetry points. It is clearly seen that the FeClF monolayer consists of Cl-Fe-F sandwich layer, which can be built by replacing one of two Cl layers with F atoms in FeCl$_2$ monolayer. In experiment, Janus monolayer MoSSe can be achieved from MoS$_2$ by replacing one of two S layers with Se atoms\cite{MoSSe}. Due to broken vertical mirror symmetry, the space group of FeClF monolayer is $P3m1$ (No.156), which is lower than $P6m2$ of FeCl$_2$ monolayer (No.187). The FeClF (FeCl$_2$) has the same symmetry with MoSSe (MoS$_2$). The lattice constants $a$ is optimized with different $U$ (0-3 eV), which is plotted in Figure 2. It is found that the $a$ increases with increasing $U$, and ranges from 3.165 Å to 3.276 Å. To determine magnetic ground state, the energy differences between AFM and FM ordering as a function of $U$ are also plotted in Figure 2. In considered $U$ range, the FM order is the most stable magnetic state. It is found that the FM interaction decreases with increasing $U$, which can produce important effects on Curie temperature of FeClF monolayer.

To demonstrate the stability of Janus FeClF monolayer, the phonon spectra and elastic constants are calculated by using GGA method. The phonon band dispersions of FeClF monolayer calculated along the high-symmetry directions of the Brillouin zone without imaginary frequency modes are plotted in FIG.1 of ESI, suggesting its dynamical stability. To check the mechanical stability of monolayer FeClF, the elastic properties are investigated. Due to $P3m1$ space group, using Voigt notation, the elastic tensor can be reduced into:

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

The independent $C_{11}$ and $C_{12}$ of FeClF monolayer are 68.88 Nm\textsuperscript{-1} and 22.21 Nm\textsuperscript{-1}. These elastic constants satisfy the Born criteria of mechanical stability\cite{Born criteria}: $C_{11}>0$ and $C_{11} - C_{12}>0$, confirming its mechanical stability. The Youngs moduli $C^{2D}$, shear modulus $G^{2D}$ and Poisson’s ratios $\nu^{2D}$ of FeClF monolayer are mechanically isotropic due to hexagonal symmetry, and the corresponding values are 61.72 Nm\textsuperscript{-1}, 23.34 Nm\textsuperscript{-1} and 0.32.

IV. OUT-OF-PLANE MAGNETIC ANISOTROPY

Firstly, we consider that the magnetocrystalline direction of FeClF monolayer is along the out-of-plane. The out-of-plane FM maintains the horizontal mirror symmetry, and breaks all possible vertical mirrors, which allows a nonvanishing Chern number of the 2D system\cite{Chern number}. The evolutions of electronic band structures with $U$ are investigated by GGA+SOC. The energy band gaps as a function of $U$ are plotted in Figure 3. The representative energy band structures at different $U$ values are shown in Figure 4. When $U < 1.4$ eV, the gap decreases with increasing $U$. However, with increasing $U$, the gap increases for $U > 1.5$ eV. Between $U=1.4$ eV and 1.5 eV, very little gap can be observed, which may show nontrivial topological properties.

For $U < 1.4$ eV, a remarkable valley polarization can be observed in the valence bands at the -K and K points, and the -K point is polarized. However, for $U > 1.5$ eV, the noteworthy valley polarization occurs in the conduction bands, and the K point is polarized. In these two regions, the monolayer FeClF is a FV material. Around the $U=1.40$ eV, the band gap of -K point gets closed, and a narrow band gap still holds at K point, signifying
FIG. 4. (Color online) For out-of-plane magnetic anisotropy, the energy band structures of Janus monolayer FeClF with $U$ being 0.00 eV, 1.00 eV, 1.40 eV, 1.45 eV, 1.50 eV and 2.50 eV.

FIG. 5. (Color online) For out-of-plane magnetic anisotropy, topological edge states of Janus monolayer FeClF calculated along the (100) direction with $U$ being 1.45 eV, including left (a) and right (b) edges.

the HVM, whose conduction electrons are intrinsically 100% valley polarized\textsuperscript{24}. The HVM can also be observed around the $U=1.5$ eV, but the band gap at K point disappears, and a narrow band gap exists at -K point. The gap closes, reopens, and then closes, which suggests a possible topological phase transition. Between the two HVM states, a QAH insulator phase may exist, which can be characterized by chiral edge states. The edge states are calculated along (100) direction with $U=1.45$ eV, which is plotted in Figure 5. It is clearly seen that there does exist a chiral edge state connecting the conduction bands (-K/K valley) and valence bands (K/-K valley) for left/right edge. A single gapless chiral edge band means that the Chern number is equal to one ($C=1$), which is consistent with integration over the Berry curvatures (See Figure 6), giving a nonzero Chern number ($C=1$). It is found that the QAH phase coexists with a valley structure for both conduction and valence bands. When shifting the Fermi level into conduction/valence bands, the K/-K valley is polarized. In a word, the FeClF monolayer undergoes the FV, HVM, QAH, HVM and FV states with increasing $U$ (see Figure 3).

Berry curvature is a powerful tool to investigate the valley physics. The Berry curvature is calculated with
1.45 eV and 2.50 eV are plotted in FIG.2 of ESI. For all Fe-
tronic correlation and SOC on the band structure, the
conduction bands. To explain the peculiar effect of elec-
tion bands for
lence bands, but the valley polarization is in the conduc-
tion bands for $U < 1.5$ eV. For $U$ between 1.4 eV and 1.5
eV, the valley polarization can exit in both valence and
conduction bands. To explain the peculiar effect of electron
ic correlation and SOC on the band structure, the
Fe-$d$-orbital characters of energy bands for $U =$1.00 eV,
1.45 eV and 2.50 eV are plotted in FIG.2 of ESI. For all

considered $U$, the -K and K valleys in both valence and
conduction bands are dominated by $d_{z^2}$ or $d_{x^2-y^2}/d_{xy}$
orbitals. For $U < 1.4$ eV, the -K and K valleys in val-
ence bands are dominated by $d_{x^2-y^2}$ and $d_{xy}$ orbitals,
and those in the conduction bands are mainly from the
$d_{z^2}$ orbitals. For $U > 1.5$ eV, the opposite situation can
be observed. When $U$ is between 1.4 eV and 1.5 eV, the
-K valley in the conduction bands and K valley in the
valence band are dominated by $d_{x^2-y^2}$ and $d_{xy}$ orbitals,
and the -K valley in the valence bands and K valley in
the conduction band are dominated by $d_{z^2}$ orbitals.

The valley polarization induced by SOC is due to the
intra-atomic interaction:

$$\hat{H}^{0}_{SOC} = \lambda \hat{L} \cdot \hat{S} = \hat{H}^0_{SOC} + \hat{H}^1_{SOC}$$

in which $\lambda$ is the coupling strength, and $\hat{L}$ and $\hat{S}$ are
the orbital angular moment and spin angular moment,
respectively. The magnetic exchange interaction results
in that $\hat{H}^1_{SOC}$ (the interaction of opposite spin states)
can be ignored. So, the $\hat{H}^{0}_{SOC}$ (the interaction between
the same spin states) dominates the $\lambda \hat{L} \cdot \hat{S}$. The $\hat{H}^{0}_{SOC}$
can be written as$^{12,22,23}$,

$$\hat{H}^0_{SOC} = \lambda \hat{S}_z (\hat{L}_z \cos \theta + \frac{1}{2} \hat{L}_x \cos \theta + \frac{1}{2} \hat{L}_y \cos \theta)$$

(3)

where $\theta$ and $\phi$ are the polar angles of spin orientation.
For out-of-plane magnetization ($\theta = 0^\circ$), $\hat{H}^0_{SOC}$
can be reduced to:

$$\hat{H}^0_{SOC} = \alpha \hat{L}_z$$

(4)

At -K and K valleys, the group symmetry is $C_{3h}$. Hence,
the orbital basis for -K and K valleys can be expressed as$^{12,22,23}$:

$$|\phi^\tau > = \frac{1}{\sqrt{2}} (\hat{d}_{x^2-y^2} > +i\tau \hat{d}_{xy} > )$$

or

$$|\phi^\tau > = \hat{d}_{z^2} >$$

(5)

where the subscript $\tau$ represent valley index ($\tau = \pm 1$).
The resulting energy at K and -K valleys can be expressed as:

$$E^\tau = <\phi^\tau |\hat{H}^0_{SOC}|\phi^\tau >$$

(6)
FIG. 8. (Color online) For in-plane magnetic anisotropy, the energy band structures of Janus monolayer FeClF with $U$ being 1.00 eV, 1.45 eV and 2.50 eV.

FIG. 9. (Color online) The MAE of Janus monolayer FeClF as a function of $U$ (0-3 eV).

If the -K and K valleys are dominated by $d_{x^2-y^2}$ and $d_{xy}$ orbitals, the valley energy difference $|\Delta E|$ at -K and K points (valley splitting) can be expressed as:

$$|\Delta E| = E^K - E^\mathrm{-K} = 4\alpha$$

(7)

If the -K and K valleys are mainly from the $d_z^2$ orbitals, the valley splitting $|\Delta E|$ is given by:

$$|\Delta E| = E^K - E^\mathrm{-K} = 0$$

(8)

So, these different orbital components of -K and K valleys with varied $U$ determine the valley polarization distribution.

V. IN-PLANE MAGNETIC ANISOTROPY

Next, we consider that the magnetocrystalline direction of FeClF monolayer is along the in-plane. The electronic band structures with different $U$ are calculated by GGA+SOC. The energy band gaps vs $U$ are shown in Figure 7, and the representative energy band structures are plotted in Figure 8. It is found that the energy band gap firstly decreases, and then increases, when the $U$ increases. The critical $U$ value is about 1.45 eV. Compared to out-of-plane magnetocrystalline direction, no special intermediate region exists. Figure 8 shows no observable valley polarization in both the valence and conduction bands, which can be explained by $\Delta E = 4\alpha \cos\theta$. When the magnetocrystalline direction of FeClF monolayer is along in-plane direction ($\theta=90^\circ$), the valley splitting will vanish ($\Delta E=0$). The Fe-$d$-orbital characters of energy bands for $U =$1.00 eV, 1.45 eV and 2.50 eV are plotted in FIG.3 of ESI. It is found that the distributions of Fe-$d$-orbital characters are akin to the cases of out-of-plane. According to FIG.4 of ESI, the sign-reversible Berry curvature can be observed, when the $U$ value strides over the critical point (about $U =1.45$ eV). Calculated results show that the hot spots in the Berry curvature are around two valleys with opposite signs and almost the same magnitudes. To explore the topological properties of FeClF monolayer at different $U$, we calculate the dispersion of the edge state. The edge states with representative $U$ are plotted in FIG.5 of ESI (only left edge), which show that no chiral edge states traverse the bulk band gap. This mean that, for in-plane magnetocrystalline direction, no QAH states appear. So, the magnetocrystalline direction is very important to investigate electronic properties of FeClF monolayer.

VI. MAGNETIC ANISOTROPY ENERGY AND ANOMALOUS VALLEY HALL EFFECT

The magnetocrystalline direction of FeClF monolayer can be regulated by external magnetic field. However, we use MAE to determine intrinsic magnetic anisotropy of FeClF monolayer at different $U$ value. Within GGA+SOC+$U$, the MAE can be calculated by $E_{\mathrm{MAE}} = E_{(100)} - E_{(001)}$, which is plotted in Figure 9. The positive value means that the easy axis is perpendicular to the plane, while the negative value suggests the in-plane di-
For $U < 1.15$ eV, the FeClF monolayer possesses out-of-plane magnetic anisotropy. For $U > 1.15$ eV, the direction of the easy axis of FeClF monolayer is in plane. We investigate the valley properties of FeClF monolayer with representative $U (2.5 \text{ eV})^{40,41}$, and its magnetocrystalline direction can be switched to out-of-plane by external magnetic field. The spin-polarized band structures of monolayer FeClF without and with SOC are shown in Figure 10. According to Figure 10 (a), a distinct spin splitting can be observed in the band structures because of the exchange interaction, and the FeClF monolayer is a direct band gap semiconductor with VBM and CBM provided by the same spin-down. The valleys of -K and K are degenerate in energy for both conduction and valence bands. Figure 10 (b) shows that the SOC effect can induce valley polarization in the conduction bands. The valley splitting $|\Delta E|$ is 109 meV, and the energy of K valley is lower than one of -K valley. Moreover, the valley polarization can be switched by reversing the magnetization direction with magnetic moment of Fe along the negative z direction, which is confirmed by Figure 10 (c). Because the low-energy bands at -K and K belong to the same spin minority channel, the spin polarization of the carriers is simultaneously switched.

It is also known that Berry curvature $\Omega(k)$ is associated with anomalous velocity $v$ of Bloch electrons under an in-plane longitudinal electric field $E$: $v \sim E \times \Omega(k)^{10}$. According to Figure 6, Berry curvature $\Omega(k)$ is characterized with unequal values and opposite signs for the -K and K valleys. With the reversed opposite magnetic moment, the valley polarization will also be reversed. The corresponding values of the Berry curvatures at the K and -K valleys will be exchanged, but their sign remains unchanged. Under such condition, the anomalous valley Hall effect can be observed in monolayer FeClF. When shifting the Fermi level between the K and -K valleys, the spin-down electrons at K valley will accumulate on one side of the sample[Figure 11 (a)]. By reversing the magnetization direction, the spin-up electrons at -K valley will gain opposite transverse velocities, moving towards another side [Figure 11 (b)] of the sample due to its opposite Berry curvature.

**VII. CURIE TEMPERATURE**

We also estimate the Curie temperature $T_C$ of monolayer FeClF at representative U values by MC simulations with the Wolf algorithm based on the Heisenberg model. The effective classical spin model can be written as:

$$H = -J \sum_{i,j} S_i \cdot S_j - A \sum_i (S_i^z)^2$$  \hspace{1cm} (9)

where $S_i/S_j$, $S_i^z$, $J$ and $A$ are the spin vectors of each Fe atom, the spin component parallel to the z direction,
the nearest neighbor exchange parameter and MAE, respectively. To extract $J$, we compare energies of the FM ($E_{FM}$) and AFM ($E_{AFM}$) configurations of monolayer FeClF with rectangle supercell. The spin vector is normalized ($|S|=1$), and the corresponding energies are given by:

$$E_{FM} = E_0 - 6J - 2A$$  \hspace{1cm} (10)$$

$$E_{AFM} = E_0 + 2J - 2A$$ \hspace{1cm} (11)$$

where $E_0$ is the energy without magnetic coupling. According to these equations, the $J$ can be attained as:

$$J = \frac{E_{AFM} - E_{FM}}{8}$$ \hspace{1cm} (12)$$

The calculated normalized $J$ at $U=1.5$ eV and 2.5 eV are 25.30 meV and 4.40 meV. The normalized magnetic moment and auto-correlation of monolayer FeClF vs temperature are shown in Figure 12, and the predicted $T_C$ is about 311 K and 63 K. These mean that electron correlation can produce important effects on Curie temperature, which is also can be understood by energy differences between FM and AFM ordering vs $U$ (see Figure 2). The Curie temperature of FeClBr is predicted to be very high (651 K), which is due to adopt GGA method ($U=0$ eV).

**VIII. DISCUSSION AND CONCLUSION**

The importance of electron correlations on the electronic properties of monolayer FeClF has been demonstrated by the first-principles calculations. The different correlation strength can give rise to different electronic states, like FV, HVM and QAH states. Although the monolayer FeClF as a concrete example is investigated, the analysis and results in the work can be readily extended to other members of monolayer FeXY (X/Y=F, Cl, Br and I), including ten monolayers. This is because the low-energy states and the electronic correlations are dominated by Fe atoms, and the rich correlation-driven physics should be common among the FeXY family. Similar phase diagram of monolayer FeClF with varied $U$ has been investigated, where the out-of-plane magnetocrystalline direction is always assumed. The spontaneous valley polarization of monolayer FeClBr has also been studied by using GGA, and the MAE is 14 $\mu$eV/Fe with out-of-plane direction, which is lower than one (132 $\mu$eV/Fe) of FeClF within GGA. The predicted Curie temperature of FeClBr monolayer is very high (651 K), which should be reduced with increasing $U$ according to our calculated results. The correlation-driven topological and valley states in septuple atomic monolayer VSi$_2$P$_4$ have been revealed, whose intermediate three layers (VP$_2$) share the similar structure with FeXY family. For a given material, the correlation strength should be constant, which should be determined from experiment. However, the rich electronic states can be realized by tuning correlation effect, which can be achieved by applied strain. The electronic correlation depends on the competition between kinetic and interaction energies, and the strain can modify the bandwidth, adjust correlation effect. The rich phase diagram in septuple atomic monolayer VSi$_2$N$_4$ has been achieved by strain, and sign-reversible valley-dependent Berry phase effects and QAH states have been investigated.

In summary, we have demonstrated the significance of electron correlation in Janus monolayer FeClF, as a representative of the 2D FeXY material family. It is found that different correlation strength (varied $U$) can result in different electronic state due to interplay between magnetic, correlation and SOC. The multiple transitions are observed, including the magnetic anisotropy, valley structure, electroconductibility and electronic topology. For...
PMA, there exists a QAH phase, whose boundary corresponds to the HVM state with fully valley polarized carriers. For FV phases, the polarization can exist for both electrons (conduction bands) and holes (valence bands), which depends the correlation strengths. The polarization at -K and K valleys can be switched by reversing which depends the correlation strengths. The polarization related with Curie temperature can be distinctly influenced by correlation strength. Our works provide a comprehensive understanding of the correlation effects in the 2D FeXY family, which can be spread to other 2D FV materials.

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