Coexistence of intrinsic piezoelectricity, ferromagnetism and nontrivial band topology in Li-decorated Janus monolayer Fe$_2$SSe with high Curie temperature

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Recently, the quantum anomalous Hall (QAH) insulators are predicted in Lithium-decorated iron-based superconductor monolayer materials (LiFeX (X=S, Se and Te)) with very high Curie temperature (PRL 125, 086401 (2020)), which combines the topological and ferromagnetic (FM) orders. It is interesting and useful to achieve coexistence of intrinsic piezoelectricity, ferromagnetism and nontrivial band topology in single two-dimensional (2D) material, namely 2D piezoelectric quantum anomalous Hall insulator (PQAHI). In this work, 2D Janus monolayer Li$_2$Fe$_2$SSe is predict to be a room-temperature PQAHI, which possesses dynamic, mechanical and thermal stabilities. It is predicted to be a half Dirac semimetal without spin-orbit coupling (SOC). It is found that the inclusion of SOC opens up a large nontrivial gap, which means the nontrivial bulk topology (QAH insulator), confirmed by the calculation of Berry curvature and the presence of two chiral edge states (Chern number C=2). Calculated results show that monolayer Li$_2$Fe$_2$SSe possesses robust QAH states against biaxial strain and electronic correlations. Compared to LiFeX, the glide mirror $G_2$ of Li$_2$Fe$_2$SSe disappears, which will induce only out-of-plane piezoelectric response. The calculated out-of-plane $\varepsilon_{33}$ of monolayer Li$_2$Fe$_2$SSe is -0.238 pm/V comparable with ones of other 2D known materials. Moreover, very high Curie temperature (about 1000 K) is predicted by using Monte Carlo (MC) simulations, which means that the QAH effect can be achieved at room temperature in Janus monolayer Li$_2$Fe$_2$SSe. Similar to monolayer Li$_2$Fe$_2$Se, the PQAHI can also be realized in the Janus monolayer Li$_2$Fe$_2$SeTe. Our works open a new avenue in searching for PQAHI with high temperature and high Chern numbers, which provide a potential platform for multi-functional spintronic applications.

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I. INTRODUCTION

The quantum Hall (QH) effect can be achieved in a 2D electron gas by a strong perpendicular external magnetic field$^7$, while the occurrence of the QAH effect aries from SOC and time-reversal (TR) symmetry broken in the presence of magnetic order$^2$. The QAH effect is generally confirmed by a nonzero Chern number in accordance with the number of edge states, and only one spin species are allowed to flow unidirectionally, resulting in a quantized Hall conductance$^{3,5}$. The discovery of TR invariant topological insulators promotes the experimental realization of QAH effect$^{6,7}$. Following the theoretical work$^8$, the QAH effect is achieved experimentally in thin films of Cr doped (Bi,Sb)$_2$Te below 30 mK, with quantized Hall conductance being observed$^9$. The QAH effect achieves the coexistence of magnetism and topological electronic band structure in a single compound. It’s a natural idea to combine more properties in a material, like the coexistence of QAH effect and piezoelectricity.

The piezoelectricity of 2D materials has been widely investigated in recent years$^{10}$. The piezoelectricity of 2D materials has been observed experimentally$^{11-14}$, and the density functional theory (DFT) calculations have also predicted the piezoelectric properties of many 2D materials$^{15-24}$, which lack centrosymmetry. Recently, some 2D multifunctional piezoelectric materials have been predicted by the first-principle calculations. In the 2D vanadium dichalcogenides, VSi$_2$P$_4$, CrBr$_{1.5}$I$_{1.5}$ and InCrTe$_3$,$^{25-28}$, the piezoelectric ferromagnetism (PFM) has been predicted, which combines piezoelectricity and ferromagnetism. The combination of piezoelectricity with topological insulating phase, namely piezoelectric quantum spin Hall insulator (PQSHI), has also been realized in monolayer InXO (X=Se and Te)$^{29}$ and Janus monolayer SrAlGaSe$_4$.$^{30}$ These discoveries provide possibility for using piezoelectric effect to control the quantum or spin transport process, which may induce novel device applications or scientific breakthroughs.

In fact, in our recent work, the PQAHI has also been achieved in Janus monolayer Fe$_2$IX (X=Cl and Br)$^{31}$, based on QAH insulator Fe$_2$I$_2$.$^{32}$ Recently, the lithium decoration of layered iron-based superconductor materials FeX (X=S, Se and Te), namely LiFeX, are predicted as room-temperature QAH insulators with high Chern number (C=2)$^{33}$, and the guidances on experimental realization have also been discussed. The LiFeX (X=S, Se and Te) have similar crystal structure with Fe$_2$I$_2$, and no piezoelectricity can be observed due to inversion symmetry. A natural idea is to achieve PQAHI from LiFeX (X=S, Se and Te) monolayer by removing inversion symmetry. As an example, the monolayer FeSe has particular sandwiched structure (Se-Fe-Se), and Janus structure can be built by replacing the top Se atomic layer with S
atoms (Fe$_2$SSe), and then apply the gating techniques to inject a large amount of Li ions into monolayer Fe$_2$SSe (Li$_2$Fe$_2$SSe). The related experimental techniques have been widely used$^{34-38}$. 

In this work, it is found that, by first-principles calculations, Janus monolayer Li$_2$Fe$_2$SSe is a 2D ferromagnetic semiconductor with out-of-plane magnetization, which can achieve the QAH effect at quite high temperature. Janus monolayer Li$_2$Fe$_2$SSe is proved to be dynamically, mechanically and thermally stable. According to the results of Berry curvature and Chiral edge states, a high Chern number C=2 is obtained for Li$_2$Fe$_2$SSe. It is found that QAH effect of Li$_2$Fe$_2$SSe is robust against biaxial strain and electronic correlations. A very high Curie temperature of about 1000 K is estimated by MC simulations using Heisenberg model. A particular symmetry leads to only out-of-plane piezoelectric response, and the predicted out-of-plane $d_{33}$ is -0.238 pm/V, which is comparable with ones of other 2D known materials. These results indicate that 2D Janus Li$_2$Fe$_2$SSe may be promising candidate for realizing the room-temperature PQAHI in experiments, which is very useful for developing 2D piezoelectric spin topological devices.

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 crystal structure, structural stabilities, topological properties, strain and correlation effects on topological properties, Curie temperature and piezoelectric properties of 2D Janus Li$_2$Fe$_2$SSe. Finally, we shall give our discussion and conclusions.

II. COMPUTATIONAL DETAIL

All the calculations on the elastic, electronic, topological and piezoelectric properties are based on DFT$^{39}$, as implemented in the VASP code$^{40-42}$. The projector-augmented-wave (PAW) potential and the plane-wave basis with a kinetic energy cutoff of 500 eV are employed for Janus monolayer Li$_2$Fe$_2$SSe. We use popular generalized gradient approximation (GGA) of Perdew, Burke and Ernzerhof$^{43}$ as the exchange-correlation functional, and the SOC is included by a second variational procedure on a fully self-consistent basis. The total energy convergence criterion is set for $10^{-8}$ eV with the Gaussian smearing method. The force convergence criterion is set for less than 0.0001 eV Å$^{-1}$ for optimizing the lattice constants and atomic coordinates by the conjugate gradient (CG) scheme. To avoid artificial interactions caused by the periodic boundary condition, the vacuum layer is

![FIG. 1. (Color online)The (a) top view and (b) side view of crystal structure of Janus monolayer Li$_2$Fe$_2$SSe. The black frame represents the primitive cell. (c):The FM and AFM energy of Janus monolayer Li$_2$Fe$_2$SSe as a function of $a/a_0$. (d):The phonon band dispersions of Janus monolayer Li$_2$Fe$_2$SSe with FM order.]
set to more than 15 Å. The Fe-3d orbitals generally have important correlation effects, and the DFT+U method is employed for the treatment of the strongly correlated 3d electrons with $U_{eff} = 2.5$ eV\cite{32,45}.

With FM ground state, the interatomic force constants (IFCs) with the $5 \times 5 \times 1$ supercell are calculated through the direct supercell method. Based on harmonic IFCs, the phonon dispersions are attained by using Phonopy code\cite{46}. An effective tight-binding Hamiltonian constructed from the maximally localized Wannier function (MLWF) is used to calculate the surface states and Berry curvature with the iterative Green function method, as implemented in the package WannierTools\cite{47,48}. The Curie temperature is determined by MC simulations, as implemented by Msolver code\cite{49}.

The elastic stiffness tensor $C_{ij}$ and piezoelectric stress tensor $e_{ij}$ are carried out by using strain-stress relationship (SSR) with GGA and density functional perturbation theory (DFPT) method\cite{50} using GGA+SOC. The Brillouin zone (BZ) integration is sampled by using a $18 \times 18 \times 1$ Monkhorst-Pack grid for the self-consistent calculations and elastic coefficients $C_{ij}$. A very dense mesh of $26 \times 26 \times 1$ k-points in the BZ is adopted to attain the accurate $e_{ij}$. The 2D elastic coefficients $C_{ij}^{2D}$ and piezoelectric stress coefficients $e_{ij}^{2D}$ have been renormalized by $C_{ij}^{2D}=L_zC_{ij}^{3D}$ and $e_{ij}^{2D}=L_ze_{ij}^{3D}$, where the $L_z$ is the length of unit cell along $z$ direction.

III. CRYSTAL STRUCTURE

The FeSe monolayer has Se-Fe-Se trilayers with a tetragonal lattice in the $P4/nmm$ space group, the unit cell of which contains four atoms with two co-planar Fe atoms. It is proved that the room-temperature QAH insulator can be achieved by Li decoration of FeSe monolayer\cite{33}. In fact, the Fe$_2$I$_2$ monolayer, having the same crystal structure with FeSe, is predicted to be a QAH insulator\cite{32}. The I element has one more valence electron than Se element, and the Li atom with an ultralow electronegativity easily loses one valence. So, the Li decoration of FeSe monolayer can become a QAH insulator. It is well known that Janus monolayer MoSSe (S-Mo-Se) can be constructed from MoSe$_2$ with three atomic sublayers (Se-Mo-Se)\cite{34}. In our previous work, the Janus monolayer Fe$_2$I$_2$X (X=Cl and Br) is predicted to be PQAHI\cite{31}, which is built by replacing one of two I layers with X (X=Cl and Br) atoms in monolayer Fe$_2$I$_2$. It is a natural idea to construct Janus Fe$_2$SSe monolayer (S-Fe-Se) by replacing one of two Se layers with S atoms in monolayer FeSe, and then to obtain PQAHI by Li decoration of Janus monolayer Fe$_2$SSe (Li$_2$Fe$_2$SSe). Compared with FeSe monolayer, the Li$_2$Fe$_2$SSe monolayer with $P4mm$ space group (No.99) lacks centrosymmetry, giving rise to piezoelectricity. The top and side views of schematic crystal structure of Janus monolayer Li$_2$Fe$_2$SSe are shown in Figure 1.

The ground state of Janus monolayer Li$_2$Fe$_2$SSe can be determined by comparing the energy difference between antiferromagnetic (AFM) and FM states. The magnetic ground state of Li$_2$Fe$_2$SSe monolayer is FM, which can be seen from the (c) in Figure 1. The optimized lattice constants $a_0$ is 3.636 Å with FM order, which is between ones of LiFeS (3.542 Å) and LiFeSe (3.655 Å)\cite{31}. The thermal stability of magnetic ordering can be described by the magnetic anisotropy energy (MAE), stemming from the SOC effect. The (100) and (001) directions are used to obtain relative stabilities by using GGA+SOC. The energy difference of the magnetic moments constrained in the (100) and (001) direction is 172 μeV/Fe, indicating that the out-of-plane (001) direction is the easy one for magnetization in monolayer Li$_2$Fe$_2$SSe. A built-in electric field can be produced by the the inequivalent bond lengths and bond angles (see Table I) due to different atomic sizes and electronegativities of S and Se atoms. For LiFeSe monolayer, the key space-group symmetry operations contain space inversion $P$, $C_4$ rotation, $M_x$ and $M_y$ mirrors and glide mirror $G_z = \{M_z \frac{1}{2}, \frac{1}{2}, 0\}$\cite{32}. For Li$_2$Fe$_2$SSe monolayer, besides the missing $P$, the glide mirror $G_z$ is also removed.

![Figure 1](image1.png)

**FIG. 1.** (Color online) The energy band structures of Janus monolayer Li$_2$Fe$_2$SSe without and with SOC at the FM order. The blue (red) lines represent the spin-up (spin-down) bands without SOC.

![Figure 2](image2.png)

**FIG. 2.** (Color online) Band structure of Janus monolayer Li$_2$Fe$_2$SSe without the SOC for spin up (left) and spin down (right). The contribution of Fe, S, Se and Li atoms to the Bloch states are denoted by red, green, blue and yellow dots.
FIG. 5. (Color online) At the absence of SOC, the band structure of Janus monolayer Li$_2$Fe$_2$SSe for spin down with the contribution of $d_{xy}$, $d_{yz}$, $d_{z^2}$, $d_{xz}$ and $d_{x^2-y^2}$ orbitals to the Bloch states.

FIG. 6. (Color online) (a): The distribution of Berry curvature of Janus monolayer Li$_2$Fe$_2$SSe contributed by occupied valence bands in the momentum space. (b): The topological edge states of Li$_2$Fe$_2$SSe calculated along the (100) direction.

TABLE I. For Janus monolayer Li$_2$Fe$_2$SSe, the lattice constants $a_0$ (Å); Fe-Se ($d_1$), Fe-S ($d_2$), Li-Se ($d_3$), Li-S ($d_4$) bond lengths (Å); Se-Fe-Se ($\theta_1$) and S-Fe-S ($\theta_2$) angles; the thickness layer height $t$ (Å); the elastic constants $C_{ij}$ in Nm$^{-1}$.

| $a_0$   | $d_1$ | $d_2$ | $d_3$ | $d_4$ | $\theta_1$ |
|--------|-------|-------|-------|-------|------------|
| 3.636  | 2.587 | 2.467 | 2.599 | 2.612 | 89.26       |

| $\theta_2$ | $t$  | $C_{11}$ | $C_{12}$ | $C_{66}$ |
|------------|-----|----------|----------|----------|
| 94.94      | 4.347 | 91.26    | 32.15    | 43.00    |

IV. STRUCTURAL STABILITY

The phonon calculation of Li$_2$Fe$_2$SSe (see (d) in Figure 1) reveals that there are no imaginary frequency modes, confirming its dynamic stability, which means that Li$_2$Fe$_2$SSe monolayer can exist as free-standing 2D crystal. A total of 18 branches due to 6 atoms per unit cell can be observed, including 15 optical and 3 acoustical phonon branches. The out-of-plane acoustic (ZA) branch (out-of-plane vibrations) deviates from linearity, in accord with the conclusion that the ZA phonon branch should have quadratic dispersion for the unstrained monolayer$^{51,52}$. The thermal stability of Li$_2$Fe$_2$SSe monolayer is further assessed by performing ab initio molecular dynamics (AIMD) simulations using NVT ensemble with a 4x4x1 supercell at 300 K. For Li$_2$Fe$_2$SSe monolayer, the temperature and total energy fluctuations as a function of the simulation time are shown in Figure 2. It is found that the total energy and temperature fluctuate smoothly with small amplitudes after the preheating process, which means a favorable thermal stability for Li$_2$Fe$_2$SSe monolayer at room temperature.

The mechanical stability of monolayer Li$_2$Fe$_2$SSe can be checked by Born criteria of mechanical stability:

$$C_{11} > 0, \quad C_{66} > 0, \quad C_{11} - C_{12} > 0$$

(1)

where the $C_{11}, C_{12}$ and $C_{66}$ are three independent elastic constants. By using Voigt notation, the elastic tensor with 4mm point-group symmetry can be reduced into:

$$C = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{66} \end{pmatrix}$$

(2)

The calculated $C_{11}, C_{12}$ and $C_{66}$ are 91.26 Nm$^{-1}$, 32.15 Nm$^{-1}$ and 43.00 Nm$^{-1}$, which satisfy the above Born criteria of mechanical stability, indicating mechanical stability of monolayer Li$_2$Fe$_2$SSe.

Due to $C_4$ rotation symmetry, the mechanical properties of monolayer Li$_2$Fe$_2$SSe have $C_4$ symmetry, and the direction-dependent in-plane Young’s moduli $C_{2D}(\theta)$ and Poisson’s ratios $\nu_{2D}(\theta)$ can be attained by$^{53,54}$:

$$C_{2D}(\theta) = \frac{C_{11}C_{22} - C_{12}^2}{C_{11}m^4 + C_{22}n^4 + (B - 2C_{12})m^2n^2}$$

(3)
It is clearly seen that the bulk states are connected by two chiral edge states, which indicates the topologically nontrivial edge states inside the bulk gap of a semiinfinite system. The local density of states vs momentum and energy at the edge can be obtained from the imaginary part of the surface Green’s function:

\[ A(k, \omega) = -\frac{1}{\pi \eta \rightarrow 0^+} \text{ImTr} G_s(k, \omega + i\eta) \]  

The topological edge states along the (100) direction are dominated by the Fe-d orbitals for spin down, which are plotted in Figure 6. As can be observed, the nonzero Berry curvature is mainly distributed around four Dirac cones, and they have the same position of Dirac cone, giving rise to a Chern number of 1.

\[ C = \frac{1}{2\pi} \int_{BZ} d^2k \Omega_z(k) \] 

in which the \( \mu_{n,k} \) is the lattice periodic part of the Bloch wave functions. The distributions of Berry curvature of monolayer Li\(_2\)Fe\(_2\)SSe are shown in Figure 6. As can be observed, the nonzero Berry curvature is mainly distributed around four Dirac cones, and they have the same sign because of \( C_4 \) symmetry. Two Berry curvature peaks contribute to the nonzero Chern number 1, and the total Chern number from the 4 Berry curvature peaks equals 2. In other words, a quantized Berry phase of \( \pi \) can be attained for each gapped Dirac cone, and the total Berry phase of \( 4\pi \) is attained (four Dirac cones), giving rise to a Chern number C=2.

Based on the bulk-edge correspondence, the non-zero Chern number can be further confirmed by the number of nontrivial chiral edge states inside the bulk gap of a semiinfinite system. The local density of states vs momentum and energy at the edge can be obtained from the imaginary part of the surface Green’s function:

\[ A(k, \omega) = -\frac{1}{\pi \eta \rightarrow 0^+} \text{ImTr} G_s(k, \omega + i\eta) \] 

The topological edge states along the (100) direction are shown in Figure 6. It is clearly seen that the bulk states are connected by two chiral edge states, which indicates that Chern number equals to 2. These results show that monolayer Li\(_2\)Fe\(_2\)SSe is a QAH insulator.
VI. STRAIN AND CORRELATION EFFECTS ON TOPOLOGICAL PROPERTIES

The strain generally can tune the SOC-induced bulk gap, MAE and magnetic order. It is important to investigate robustness of QAH properties of monolayer Li$_2$Fe$_2$SSe against biaxial strain. Here, we use $a/a_0$ (0.96-1.04) to describe the biaxial strain, where $a$ ($a_0$) is the strained (equilibrium) lattice constants. The energy difference between FM and AFM orders and MAE as a function of $a/a_0$ are plotted in Figure 7. It is found that all strained monolayers are FM ground state in considered strain range, and the energy difference between FM and AFM order decreases with $a/a_0$ from 0.96 to 1.04. However, the MAE shows nonmonotonicity, which firstly increases, and then decreases. In considered strain range, the out-of-plane (001) direction is always the easy one. The energy band structures of some representative strained monolayer Li$_2$Fe$_2$SSe using GGA+SOC are plotted in Figure 8, and the gap as a function of strain is shown in Figure 9. It is found that the gap increases almost linearly with increasing strain in considered strain range, and the gap changes from 49.7 meV to 135.8 meV. The topological edge states of strained monolayer Li$_2$Fe$_2$SSe are calculated, and they all are QAH insulators with Chern number $C=2$. We show topological edge states at representative 1.04 strain in Figure 10, which shows clearly two chiral topologically protected gapless edge states. These results show that the QAH topological properties of monolayer Li$_2$Fe$_2$SSe are robust against strain.

To check the Coulomb interaction $U$ effects on QAH properties, we calculate the energy difference between FM and AFM orders, MAE, energy bands and topological edge states with different values of $U$ (0-4 eV). The energy difference between FM and AFM order and MAE as a function of $U$ are plotted in Figure 7. It is found that the ground state always is FM order with different $U$. It is found that the MAE increases with increasing $U$. When the $U$ value is larger than 0 eV, the out-of-plane (001) direction is always the easy one in considered $U$ range. For $U=0$ eV, the MAE only is -0.5 $\mu$eV/Fe, and the spin orientation in the energy band calculations is chosen in the out-of-plane direction. The energy band structures of monolayer Li$_2$Fe$_2$SSe with some representative $U$ value using GGA+SOC are plotted in Figure 8, and the gap as a function of $U$ is shown in Figure 9. With increasing $U$, it is clearly seen that the gap increases from -4.1 meV to 257.6 meV. For $U=0$ eV, the monolayer Li$_2$Fe$_2$SSe becomes metal. In considered $U$ range except $U=0$ eV, the topological edge states of monolayer Li$_2$Fe$_2$SSe are calculated, and they all are QAH insulators with Chern number $C=2$. The topological edge states at representative $U=4$ eV are shown in Figure 10, and two chiral topologically protected gapless edge states are present in the bulk gap. These results indicate the
FIG. 10. (Color online) Topological edge states of Janus monolayer Li$_2$Fe$_2$SSe calculated along the (100) direction with $a/a_0=1.04$ (a) and $U=4$ eV (b).

FIG. 11. (Color online) The normalized magnetic moment ($S$) and auto-correlation of Janus monolayer Li$_2$Fe$_2$SSe as a function of temperature.

robustness of nontrivial topology against the correlation effect in the 3$d$ electrons of Fe atoms.

VII. CURIE TEMPERATURE

One of the important properties of ferromagnets for the practical application is the Curie temperatures ($T_C$). Using MC simulations based on the Heisenberg model, we have calculated the Curie temperature of monolayer Li$_2$Fe$_2$SSe. For simplicity, only the nearest neighbor (NN) exchange interaction is considered, and the spin Heisenberg Hamiltonian is defined as:

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

where $J$, $S$ and $A$ are the exchange parameter, the spin vector of each atom and MAE, respectively. Based on the energy difference between AFM and FM, the magnetic coupling parameter is calculated as $J=(E_{AFM}-E_{FM})/8$ with normalized $S$ ($|S|=1$). The calculated $J$ value is 137.6 meV, and the $A$ is 172 $\mu$eV/Fe.

A 50×50 supercell with periodic boundary conditions is employed, and $10^7$ loops are adopted to perform the MC simulation. We show the normalized magnetic moment and auto-correlation of monolayer Li$_2$Fe$_2$SSe as a function of temperature in Figure 11. It is found that $T_C$ is as high as 996 K for monolayer Li$_2$Fe$_2$SSe, which is smaller than ones of Li-decorated monolayer FeX (X= S, Se and Te)\cite{31}. However, the $T_C$ of monolayer Li$_2$Fe$_2$SSe is significantly higher than that of previously reported many 2D FM semiconductors, like CrI$_3$ monolayer (about 45 K)\cite{56}, CrOCl monolayer (about 160 K)\cite{57}, Janus Fe$_2$IX (X=Cl and Br) monolayer (about 400 K)\cite{31}, Fe$_2$I$_2$ monolayer (about 400 K)\cite{32} and Cr$_2$Ge$_2$Te$_6$ monolayer (about 20 K)\cite{58}.

VIII. PIEZOELECTRIC PROPERTIES

The piezoelectric effects of a material can be described by third-rank piezoelectric stress tensor $e_{ijk}$ and strain tensor $d_{ijk}$. The $e_{ijk}$ and $d_{ijk}$ can be expressed as:

$$e_{ijk} = \frac{\partial P_i}{\partial \varepsilon_{jk}} = e_{elc}^{ijk} + e_{ion}^{ijk}$$

and

$$d_{ijk} = \frac{\partial P_i}{\partial \sigma_{jk}} = d_{elc}^{ijk} + d_{ion}^{ijk}$$

They can be related by elastic tensor $C_{mnjk}$:

$$e_{ijk} = \frac{\partial P_i}{\partial \varepsilon_{jk}} = \frac{\partial P_i}{\partial \sigma_{mn}} \frac{\partial \sigma_{mn}}{\partial \varepsilon_{jk}} = d_{ijm} C_{mnjk}$$

in which $P_i$, $\varepsilon_{jk}$ and $\sigma_{jk}$ are polarization vector, strain and stress, respectively. The $e_{elc}^{ijk}/d_{elc}^{ijk}$ is clamped-ion piezoelectric coefficients (only electronic contributions). The $e_{ion}^{ijk}/d_{ion}^{ijk}$ is relax-ion piezoelectric coefficients as a realistic result (the sum of ionic and electronic contributions).

The Li-decorated monolayer FeX (X= S, Se and Te) are centrosymmetric, which means that they have no
FIG. 12. (Color online) For Janus monolayer Li$_2$Fe$_2$SSe, the elastic constants $C_{ij}$, the piezoelectric stress coefficients ($e_{31}$) and the piezoelectric strain coefficients ($d_{31}$) as a function of $U$.

piezoelectricity. However, the monolayer Li$_2$Fe$_2$SSe lacks glide mirror $G_z$ symmetry, but has $M_x$ and $M_y$ mirrors symmetry, which gives only out-of-plane piezoelectricity, and the in-plane piezoelectricity will disappear. By using Voigt notation, the piezoelectric stress and strain tensors of monolayer Li$_2$Fe$_2$SSe can be expressed as:

$$
e = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ e_{31} & e_{31} & 0 \end{pmatrix}$$

Equation 12

FIG. 13. (Color online) For Janus monolayer Li$_2$Fe$_2$SeTe, the phonon spectra (Left) and the energy band structure with GGA+SOC (Right).

The $e_{31}$ can be directly calculated by VASP code, and the $d_{31}$ can be derived by Equation 11, Equation 12 and Equation 13.

$$d = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ d_{31} & d_{31} & 0 \end{pmatrix}$$

Equation 13

$$d_{31} = \frac{e_{31}}{C_{11} + C_{12}}$$

Equation 14

Next, we use the primitive cell to calculate the $e_{31}$ of Janus monolayer Li$_2$Fe$_2$SSe. Calculated results show that the $e_{31}$ is $-0.294 \times 10^{-10}$ C/m with the ionic contribution $0.133 \times 10^{-10}$ C/m and electronic one $-0.427 \times 10^{-10}$ C/m. It is found that the electronic and ionic parts have the opposite contributions, and the electronic contribution dominates the $e_{31}$. Based on Equation 14, the calculated $d_{31}$ is $-0.238$ pm/V. The $d_{31}$ of Janus monolayer Li$_2$Fe$_2$SSe is higher than or comparable with ones of many 2D materials. The Coulomb interaction $U$ effects on piezoelectric properties of monolayer Li$_2$Fe$_2$SSe are also considered. The elastic constants $C_{ij}$, the piezoelectric stress coefficients ($e_{31}$) and the piezoelectric strain coefficients ($d_{31}$) as a function of $U$ are plotted in Figure 12. A complex $U$ dependence for $e_{31}$ is observed, which leads to complicated $U$ effects on $d_{31}$. It is found that the smallest $d_{31}$ is $-0.100$ pm/V with $U=3$ eV.

IX. DISCUSSION AND CONCLUSION

In fact, Janus monolayer Li$_2$Fe$_2$SeTe is also a QAH insulator. The energy difference between AFM and FM orders is 0.875 eV per unitcell, and the out-of-plane (001) direction is the easy one with MAE of 45 $\mu$eV/Fe. The calculated $C_{11}$, $C_{12}$ and $C_{66}$ are 79.13 Nm$^{-1}$, 19.06 Nm$^{-1}$ and 31.36 Nm$^{-1}$, which satisfy Born criteria of mechanical stability, indicating mechanical stability of monolayer Li$_2$Fe$_2$SeTe. The phonon spectra of Li$_2$Fe$_2$SeTe
is plotted in Figure 13 with no imaginary frequency modes, confirming its dynamic stability. The AIMD simulations also confirm the thermal stability of monolayer LiFe$_2$SeTe at room temperature. The energy band structures and topological edge states of monolayer Li$_2$Fe$_2$SeTe are shown in Figure 13 and Figure 14, respectively. The energy band gap is 161 meV, and the bulk states are connected by two chiral edge states, indicating Chern number C=2. The calculated $d_{31}$ is 0.1 pm/V with $e_{31}$ of 0.099 x 10$^{-10}$ C/m.

In summary, using DFT+$U$ calculations, we have performed a systematic investigation of the electronic, magnetic, topological and piezoelectric properties in Janus monolayer Li$_2$Fe$_2$SeTe, which is predicted as an intriguing 2D PQAHI. It is proved that monolayer Li$_2$Fe$_2$SeTe is mechanically, dynamically and thermally stable. Also, the nontrivial properties are confirmed by a nonzero Chern number (C=2) and two gapless chiral edge states. Moreover, the monolayer Li$_2$Fe$_2$SeTe possesses out-of-plane magnetic anisotropy and very high Curie temperature (about 1000 K). The emergence of QAH effect in monolayer Li$_2$Fe$_2$SeTe is robust against strain and Hubbard $U$ electronic correlation. The predicted $d_{31}$ is comparable with ones of other 2D known materials. The predicted PQAHI in monolayer Li$_2$Fe$_2$SeTe is expected to work safely above room temperature, and provides a more promising platform for realizing low-dissipation topotronics devices, and provides possibility to use the piezotronic effect to control QAH effects.

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