Quantum Spin Hall Effect in 2D Transition Metal Dichalcogenide Haeckelites

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Abstract

By using first-principles calculation, we have found that a family of 2D transition metal dichalcogenide haeckelites with square-octagonal lattice $MX_2$-4-8 ($M=$Mo, W and $X=$S, Se and Te) can host quantum spin hall effect. The phonon spectra indicate that they are dynamically stable and the largest band gap is predicted to be around 54 meV, higher than room temperature. These will pave the way to potential applications of topological insulators. We have also established a simple tight-binding model on a square-like lattice to achieve topological nontrivial quantum states, which extends the study from honeycomb lattice to square-like lattice and broads the potential topological material system greatly.
I. INTRODUCTION

Inspired by the impressed progress in theory and applications, numerous researchers turn their attentions to two-dimensional (2D) systems especially miraculous graphene. Recently, another 2D system, transition metal dichalcogenides (TMDs) MX$_2$ with M=Mo, W, Ti, etc. and X=S, Se, Te, has been widely explored due to wide range of electronic properties and easy fabrication. Bulk TMDs are composed of 2D X-M-X layers stacked on top of each other. The bonding within those trilayer sheets is covalent while the coupling between adjacent sheets is weak van der Waals (vdW) interaction. 2D TMD layers can be manufactured not only by mechanical and chemical exfoliation of their layered bulk counterparts, but also by chemical vapor deposition (CVD) or two-step thermolysis. However, defect will be inevitably produced during the manufacture, and it will modify the electronic structure significantly in low dimensional system.

Graphene with 5-7 defects, which is often called Haeckelites in honor of the German biologist and naturalist Ernst Haeckel, has been theoretically proposed about twenty years ago. In contrast to comprehensive understanding of the defect in graphene, defect in 2D TMDs may just launch on. There are still so many issues need to be tackled. W. Li et al. and H. Terrones et al. proposed that a new planar sheet could be generated from original hexagonal TMDs when introducing 4-8 defects. This new planar sheet is TMD Haeckelites with square-octagonal lattice. The periodic 4-8 defects have been observed in the grain boundaries of MoS$_2$ and most probably will exist in other TMDs too. High-resolution transmission electron microscopy (HR-TEM) is a powerful instrument to selectively suppress or enhance bond rotations and produce defects in sample due to the ballistic procedure between high energetic electrons and sample atoms. Using aberration corrected HR-TEM device, a disordered graphene Haeckelite has been produced in situ. Combing first-principles calculations and HR-TEM experiments, H. Komsa demonstrated that it is possible to observe defect formation under exposure to an 80 keV electron beam in MoS$_2$ system.

Recently, Qian et al. predicted that some 2D TMDs with 1T' structure can be large-gap 2D topological insulators (TIs) though most of them are in 1H structure and are not TIs. It is natural to ask whether TI state can exist in the defected 2D TMDs based on 1H structure. 2D TI, also known as quantum spin hall (QSH) insulator, was firstly proposed in graphene,
where spin-orbit coupling (SOC) opens a band gap at the Dirac point. On account of weak SOC strength, the band gap is so small (order of $10^{-3}$ meV)\textsuperscript{23} that this proposal is hardly to be verified by experiments. So far, QSH effect has only been observed in HgTe/CdTe\textsuperscript{25} and InAs/GaSb\textsuperscript{26} quantum wells. Both of them require precisely controlled MBE growth and ultralow temperature. The study of 2D TI has been seriously hampered due to lack of proper materials with large band gap, stable structure and easy fabrication.\textsuperscript{27} In this work, based on first-principles calculations, we find monolayer of WX$_2$ and MoX$_2$ Haeckelite are 2D TIs and the largest band gap is around 54 meV. Distinguished from other predicted QSH materials\textsuperscript{28–32} based on honeycomb lattice, these MX$_2$-4-8 Haeckelites have square-like lattice and a simple tight-binding model with one orbital per site and four sites per unit cell has been established to achieve topologically nontrivial QSH state. Such extension from honeycomb lattice to square-like lattice have largely broad the potential candidates for topological materials.\textsuperscript{33,34}

The paper is arranged as follows. In section II we will introduce the details of first-principles calculations. In section III, the calculation results are presented and TB analysis is performed. Finally, section IV contains a conclusion of this work.

II. CALCULATION METHOD AND CRYSTAL STRUCTURE

First-principles calculations were carried out using the projector augmented wave method\textsuperscript{35,36} implemented in Vienna \textit{ab initio} simulation package (VASP)\textsuperscript{37,38}. Exchange and correlation potential was treated within the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof type\textsuperscript{39}. SOC was taken into account by the second variation method self-consistently. The cut-off energy for plane wave expansion was 500 eV. The k-points sampling grid in the self-consistent process was $9 \times 9 \times 3$. The crystal structures have been fully relaxed until the residual forces on each atom were less than 0.001 eV/Å. The crystal parameters for all TMD Haeckelites are shown in Table I. A vacuum of 20 Å between layers was considered in order to minimize image interactions from the periodic boundary condition. PHONOPY has been employed to calculate the phonon dispersion\textsuperscript{40}. To explore the edge states of TMD Haeckelites, maximally localized wannier functions (MLWFs) for the $d$ orbitals of W and $p$ orbitals of S have been constructed and used to get \textit{ab initio} tight-binding (TB) hamiltonian\textsuperscript{41–43}. Atomic SOC is added to the TB hamiltonian by fitting the
FIG. 1: (color online). Top view (a) and side view (b) of relaxed WS$_2$-4-8. Gray ball is W and yellow ball is S. The primitive cell is shown in light blue rectangle. (c) 2D and projected edge first BZ with high symmetry point (red dots). (d) Phonon dispersion of WS$_2$-4-8.

All TMD Haeckelites have the same non-symmorphic space group Pbam ($D_{2h}^9$). Except the difference of lattice constants, all other TMD Haeckelites have nearly the same properties as WS$_2$. So we choose WS$_2$-4-8 later as an example and the results of other TMD Haeckelites can be found in the Appendix. The relaxed crystal structure and Brillouin zone (BZ) for WS$_2$-4-8 are shown in Fig. 1. It is noted that bond length between W 1 and 3 is reduced compared to that in honeycomb lattice. As we will see later, this bond is vital to topological phase transition. The dynamic stability of WS$_2$-4-8 has been investigated by calculating its phonon spectrum. Imaginary frequencies can not be found in the phonon dispersion of WS$_2$-4-8, which indicates the structure is stable (Fig. 1(d)).
TABLE I: Lattice parameters and band gaps for some TMD Haeckelites MX$_2$-4-8.

| Structure | a(Å) | b(Å) | Gap(meV) |
|-----------|------|------|----------|
| WS$_2$    | 6.34 | 6.41 | 53.82    |
| WSe$_2$   | 6.40 | 6.86 | 30.03    |
| WTe$_2$   | 6.65 | 7.38 | 14.743   |
| MoS$_2$   | 6.36 | 6.33 | 13.38    |
| MoSe$_2$  | 6.65 | 6.59 | 26.80    |

FIG. 2: (color online). GGA (a) and GGA+SOC (b) band structures of WS$_2$-4-8. The calculated edge states for X (c) and Y (d) edge, respectively.

III. RESULTS

Both GGA and GGA+SOC band structures of WS$_2$-4-8 are shown in Fig. 2. Along Γ-X direction, there is a band crossing in GGA band structure. The little group of k point located on this direction is $C_{2v}$. The two crossing bands belong to different irreducible
representations and such band crossing is protected by \{C_{2x}\frac{1}{2}\} operation. When SOC is included, as we can see in Fig. 2 (b), WS\_2-4\_8 is a well defined insulator with indirect band gap around 53.8 meV. Gaps for other TMD Haeckelites are listed in the Table 1. For system possesses both time reversal (TR) and space inversion symmetry, the parity criterion proposed by Fu and Kane is a convenient method to judge its band topology \(Z_2\) number.\[^{46}\] Since the space group of it is non-symmorphic, similar as that in single layer ZrTe\_5 and HfTe\_5\[^{33}\], all the bands at the three time reversal invariant momenta X, S, Y having degeneracy of even and odd states. Only the band inversion at \(\Gamma\) can leads to nontrivial band topology. It is true that the total parity of occupied states at \(\Gamma\) is -1 and the other three are +1. Therefore, the topological index \(Z_2\) equals to 1, which means WS\_2-4\_8 is a QSH insulator. Considering the possible underestimation of band gap of GGA, non-local Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional\[^{47}\] is further supplemented to check the topological property. The band topology does not change.

Since the existence of nontrivial edge states is the hallmark of QSH effect, we have calculated the edge states of WS\_2-4\_8. As shown in Fig. 2 (c, d), there is edge Dirac cone dispersion connecting the bulk occupied and unoccupied states with Dirac point at \(\bar{\Gamma}\) for both X and Y edges.

In order to understand the band inversion process at \(\Gamma\) point explicitly, a Slater-Koster TB has been constructed. Obviously, the main physics comes from the isolated group of four bands around the Fermi level. The band character and projected density of states (PDOS) analyses indicate that the low energy bands near the Fermi level are mainly contributed by the \(d_{z^2}\) and \(d_{x^2-y^2}\) orbitals of W. The \(d_{x^2-y^2}\) can mix with \(d_{z^2}\) due to the distortion of 4-8 defects. For simplicity, only \(d_{z^2}\) is taken into account for each W and one primitive cell contains four W atoms. Therefore, it is possible and reasonable to construct a \(4 \times 4\) TB hamiltonian for non-SOC case. The non-SOC TB hamiltonian with four localized \(d_{z^2}\) bases \(|\omega_i\rangle\) (i=1, 2, 3, 4) can be written as follows in momentum space

\[
H_0(k) = \begin{pmatrix}
0 & 2t_1 \cos(\frac{1}{2}k_x) & t_2 e^{\frac{i}{2}(-k_x+k_y)} & 2t_3 \cos(\frac{1}{2}k_y) \\
2t_1 \cos(\frac{1}{2}k_x) & 0 & 2t_3 \cos(\frac{1}{2}k_y) & t_2 e^{\frac{i}{2}(-k_x-k_y)} \\
t_2 e^{\frac{i}{2}(k_x-k_y)} & 2t_3 \cos(\frac{1}{2}k_y) & 0 & 2t_1 \cos(\frac{1}{2}k_x) \\
2t_3 \cos(\frac{1}{2}k_y) & t_2 e^{\frac{i}{2}(k_x+k_y)} & 2t_1 \cos(\frac{1}{2}k_x) & 0
\end{pmatrix}
\]  

(1)
where the hopping parameters are defined as

\[ t_1 = \langle w_1 | H_0 | w_2 \rangle \]  
\[ t_2 = \langle w_1 | H_0 | w_3 \rangle \]  
\[ t_3 = \langle w_1 | H_0 | w_4 \rangle \]  

|\omega_i\rangle means the orbital \( d_{z^2} \) on \( i \)-th W atom labelled in Fig. (a). However, one should note that periodic boundary condition is sacrificed here in order to get a concise form of Eq. (1). When the calculated properties concern global phase such as berry phase, we need to transform \( H_0(k) \) into another form which satisfies periodic boundary condition.

Similar to graphene, SOC is a second order effect for WS\(_2\)-4-8. The intrinsic atomic SOC for W is of the order of 200 meV while it is about 4 meV for graphene. Compare to the extremely small gap for graphene, a large band gap (53.8 meV) is obtained for WS\(_2\)-4-8 at last. The hybridization between |\omega_i \uparrow\rangle and |\omega_j \downarrow\rangle is zero due to \( m_z \) symmetry. If TR symmetry is preserved, we will have \( H_\uparrow\uparrow_{so}(k) = H_\uparrow\downarrow_{so}(k)^T \). Therefore, even the hamiltonian size will be doubled when SOC is taken into account, we can still focus on spin up (spin down) subspace only. Spin down (spin up) subspace can be obtained using above restricted conditions. Considering all the symmetries, we obtain a generic matrix form for \( H_\uparrow\uparrow_{so}(k) \).

\[
H_{so}^{\uparrow\uparrow}(k) = \begin{pmatrix}
0 & 2\lambda_1 \cos(\frac{1}{2}k_x) & 0 & 2\lambda_3 \cos(\frac{1}{2}k_y) \\
2\lambda_1^* \cos(\frac{1}{2}k_x) & 0 & 2\lambda_3^* \cos(\frac{1}{2}k_y) & 0 \\
0 & 2\lambda_3 \cos(\frac{1}{2}k_y) & 0 & 2\lambda_1 \cos(\frac{1}{2}k_x) \\
2\lambda_3^* \cos(\frac{1}{2}k_y) & 0 & 2\lambda_1^* \cos(\frac{1}{2}k_x) & 0
\end{pmatrix}
\]  

where \( \lambda_1 \) and \( \lambda_3 \) (pure imaginary numbers) are defined as

\[ \lambda_1 = \langle w_1 \uparrow | H_{so} | w_2 \uparrow \rangle \]  
\[ \lambda_3 = \langle w_1 \uparrow | H_{so} | w_4 \uparrow \rangle \]  

Only the total sign(\( t_1t_2t_3 \)) makes sense. Sign(\( t_1t_2t_3 \)) < 0 can be inferred by inverting the whole bands of sign(\( t_1t_2t_3 \)) > 0. So we take \( t_1 > 0, t_2 > 0 \) and \( t_3 > 0 \). As discussed above, only the band inversion at \( \Gamma \) point can change the band topology. The four eigen states and their parities can be obtained explicitly as following:
FIG. 3: (color online). Non-SOC (black lines) and SOC (red lines) band structure evolution calculated with different $t_2$ in TB model. The parameters are $\lambda_1 = -\lambda_3 = 0.08i$, $t_1 = 1$, $t_3 = 0.6$, $t_2 = 2.2$ (a), $t_2 = 2.0$ (b), $t_2 = 1.8$ (c), $t_2 = 1.2$ (d) and $t_2 = 1.0$ (e). (f) $t_1 = 0.6$, $t_3 = 1$ and $t_2 = 1.8$. Parity information at $\Gamma$ has been given.

\[ E_1 = 2t_1 + t_2 + 2t_3 \quad \text{parity} + \quad (8) \]
\[ E_2 = -2t_1 + t_2 - 2t_3 \quad \text{parity} + \quad (9) \]
\[ E_3 = 2t_1 - t_2 - 2t_3 \quad \text{parity} - \quad (10) \]
\[ E_4 = -2t_1 - t_2 + 2t_3 \quad \text{parity} - \quad (11) \]

Obviously, the $E_1$ has the highest energy. The band inversion happens between $E_2$ and $E_3$ or $E_2$ and $E_4$ can lead to QSH state. That means the band inversion will exist as long as $|t_2| < \max(|2t_1|, |2t_3|)$. Fig. 3 show the band structure calculated with the TB model with different sets of parameters. When $|t_2| > 2|t_1| > 2|t_3|$ (Fig. 3 (a)), the bonding and anti-bonding states are far away from each other. This is a trivial insulator. There will be a
band touching at Γ point if $|t_2| = 2|t_1| \ (\text{Fig. 3(b)})$. When $2|t_1| > |t_2| > 2|t_3|$, band inversion will happen (Fig. 3(c)) and the system enters into QSH state. The two valence bands ($E_2$ and $E_4$) with opposite parity will be degenerate at Γ if $|t_2| = 2|t_3| \ (\text{Fig. 3(d)})$. When $2|t_1| > 2|t_3| > |t_2|$, they will separate each other (Fig. 3(e)). Topological phase transition will not take place in this parametric region from Fig. 3(c) to (e), since the band inversion process occurs between two occupied valence bands. Another interesting thing is that $t_1$ and $t_3$ control the position of band crossing in non-SOC band structure. If $t_1 > t_3$, the crossing will be situated at Γ – X direction (Fig. 3(c)) and it will move to Γ – Y direction (Mo case in Appendix) for $t_1 < t_3 \ (\text{Fig. 3(f)})$.

Uniaxial strain effect has also been investigated with first-principles calculations, which can be used to tune the relative strength of these hopping parameters and control the topological quantum state transition. If we fix crystal constant $a$ and decrease $b$, $t_3$ will increase faster than $t_1$ and $t_2$. This means the band crossing in non-SOC band structure will move from Γ – X to Γ – Y and uniaxial strain is always beneficial for band inversion. Similar results can be get for uniaxial strain along b-axis. Therefore the topology in WS$_2$-4-8 is robust against uniaxial strain.

IV. CONCLUSION

In summary, we have performed first-principles calculations for the electronic properties of TMD Haeckelites MX$_2$-4-8 and found that they are 2D TIs. A simple TB model with one orbital per site and four sites per unit cell has been established to understand the band inversion mechanism. The nearest hopping parameter $t_2$ is vital to trigger the topological phase transition and can be tuned through lattice strain effect. Such simple square-like lattice model to achieve various topological quantum states is very stimulating. It will lead further study based on square lattice instead of honeycomb lattice and largely extend the searching range for topological materials.

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V. APPENDIX: OTHER TMD HAECKELITES MX\textsubscript{2}-4-8

![Diagram of crystal structures](image)

FIG. 4: (color online). Top views of crystal structure of WSe\textsubscript{2}-4-8 (a), WTe\textsubscript{2}-4-8 (a), MoS\textsubscript{2}-4-8 (c) and MoSe\textsubscript{2}-4-8 (d).
FIG. 5: (color online). Band structures of WSe$_2$-4-8 (a, b), WTe$_2$-4-8 (c, d), MoS$_2$-4-8 (e, f) and MoSe$_2$-4-8 (g, h). Left panel for non-SOC case and right panel for SOC case.
FIG. 6: (color online). Phonon dispersions of WSe$_2$-4-8 (a), WTe$_2$-4-8 (b), MoS$_2$-4-8 (c) and MoSe$_2$-4-8 (d).
FIG. 7: (color online). Edge states for WSe$_2$-4-8 (a, b), WTe$_2$-4-8 (c, d), MoS$_2$-4-8 (e, f) and MoSe$_2$-4-8 (g, h). Left panel for X edge and right panel for Y edge.