Tight-binding modeling of altermagnet candidate MnTe

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My CV

Applying PhD

Introduction

Altermagnet is a type of antiferromagnets (AFMs), which breaks time-reversal symmetry. Thus, the energy bands show the spin-splitting. As a consequence, altermagnets expect to show a large spontaneous anomalous Hall effect. The DFT calculation suggests that the Néel vector is either in the x-direction (110) or in the y-direction (-110) in the figure below.

Bravais primitive vectors (Mn sites)

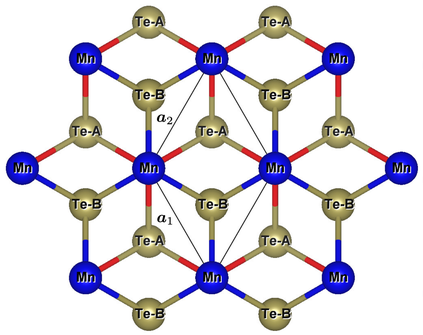
$$\boldsymbol{a}_1 = \frac{1}{2}a\hat{\boldsymbol{x}} - \frac{\sqrt{3}}{2}a\hat{\boldsymbol{y}}, \quad \boldsymbol{a}_2 = \frac{1}{2}a\hat{\boldsymbol{x}} + \frac{\sqrt{3}}{2}a\hat{\boldsymbol{y}}, \quad \boldsymbol{a}_3 = d\hat{\boldsymbol{z}}$$

Basis vectors in a unit cell

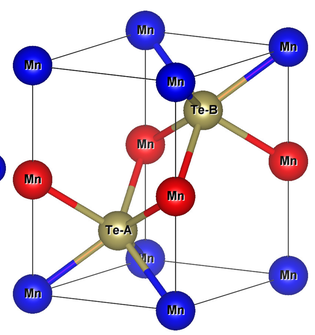
$$\mathrm{Te}_A = \frac{a}{2}\hat{\boldsymbol{x}} + \frac{\sqrt{3}}{6}a\hat{\boldsymbol{y}} - \frac{d}{4}\hat{\boldsymbol{z}} \qquad \mathrm{Mn}_A = -\frac{d}{2}\hat{\boldsymbol{z}}$$

$$\mathrm{Te}_B = \frac{a}{2}\hat{\boldsymbol{x}} - \frac{\sqrt{3}}{6}a\hat{\boldsymbol{y}} + \frac{d}{4}\hat{\boldsymbol{z}} \qquad \mathrm{Mn}_B = \boldsymbol{0}$$

Top view



Unit cell



Mn layers are antiferromagnetic, where red and blue layers have opposite spins. Two non-magnetic Te sites break the time-reversal symmetry.

Tight-binding model; Slater-Koster LCAO method

In our work, we construct the analytical tight-binding Hamiltonian of an altermagnetic semi-conductor candidate MnTe, using the Slater-Koster (SK) Linear Combination of Atomic Orbitals (LCAO) method. We obtain all the numerical values for 20 introduced parameters, including spin-orbit coupling, by fitting the DFT results.

Atomic orbitals of Te A & B $\{|x^A_\uparrow\rangle, |y^A_\uparrow\rangle, |z^A_\uparrow\rangle, |x^B_\uparrow\rangle, |y^B_\uparrow\rangle, |z^B_\uparrow\rangle, |x^A_\downarrow\rangle, |y^A_\downarrow\rangle, |z^A_\downarrow\rangle, |x^B_\downarrow\rangle, |y^B_\downarrow\rangle, |z^B_\downarrow\rangle\}$

Te-Te direct hoppings

σ spin; n, n', m orbitals; i, j Bravais lattice points; τ, τ' Te basis A or B

$$\mathcal{H}_{\mathrm{Te-Te}} = \sum_\sigma \sum_{i,\tau} \sum_n \epsilon_n\, p^\dagger_{ni\tau\sigma} p_{ni\tau\sigma} + \sum_\sigma \sum_{n,n'} \sum_{<i,j>} \sum_{\tau\neq\tau'}{}' t_1\, p^\dagger_{ni\tau\sigma} p_{n'j\tau'\sigma}$$

On-site $\mathrm{Te_A}$, $\mathrm{Te_B}$

1st n.n. hopping $\mathrm{Te_A} \leftrightarrow \mathrm{Te_B}$

$$+ \sum_\sigma \sum_{n,n'} \sum_{\ll i,j \gg} \sum_\tau t_2\, p^\dagger_{ni\tau\sigma} p_{n'j\tau\sigma} + \sum_\sigma \sum_{n,n'} \sum_{\lll i,j \ggg} \sum_{\tau\neq\tau'}{}' t_3^\sigma\, p^\dagger_{ni\tau\sigma} p_{n'j\tau'\sigma} + H.c.$$

2nd n.n. hopping $\mathrm{Te_A} \leftrightarrow \mathrm{Te_A}$, $\mathrm{Te_B} \leftrightarrow \mathrm{Te_B}$

3rd n.n. hopping $\mathrm{Te_A} \leftrightarrow \mathrm{Te_B}$

SK parametrization for hopping matrix elements

Mn (5d) orbitals mixed with to Te (5p) orbitals

$$\mathcal{H}_{\mathrm{Te-Mn}} = \sum_\sigma \sum_{n,m} \sum_{<i,j>} \sum_{\tau\neq\tau'}{}' t^\sigma_{pd}\, p^\dagger_{ni\tau\sigma} d_{mj\tau'\sigma} + H.c.$$

p-d hopping A↔Mn, B↔Mn

Schrieffer-Wolff transformation

(2nd-order perturbative correction) p-d-p hopping A↔Mn ↔B

$$\mathcal{H}_o = \begin{pmatrix} \mathcal{H}_{\mathrm{Te-Te}} & \lambda\mathcal{H}_{\mathrm{Mn-Te}} \\ \lambda\mathcal{H}^\dagger_{\mathrm{Mn-Te}} & \mathcal{H}_{\mathrm{Mn-Mn}} \end{pmatrix}$$

$$\Delta\mathcal{H}^{(2)}_{\mathrm{Te-Mn}} = \frac{\mathcal{H}^\dagger_{\mathrm{Te-Mn}} \mathcal{P}_{\mathrm{Te}} \mathcal{H}_{\mathrm{Te-Mn}}}{\epsilon_p - \epsilon_d}$$

$$\mathcal{H}'_o = e^{-S}\mathcal{H}_o e^S = \begin{pmatrix} \mathcal{H}_{\mathrm{Te-Te}} + \Delta\mathcal{H}^{(2)}_{\mathrm{Mn-Te}} & 0 \\ 0 & \mathcal{H}_{\mathrm{Mn-Mn}} + \Delta\mathcal{H}'^{(2)}_{\mathrm{Mn-Te}} \end{pmatrix} + \mathcal{O}(\lambda^3)$$

Results

Analytical tight-binding (TB) Hamiltonian for (5p) Te bands

$$\mathcal{H}_h = \mathcal{H}_{\mathrm{Te-Te}} + \Delta\mathcal{H}^{(2)}_{\mathrm{Te-Mn}} = \sum_{n_1,n_2,n_3} e^{i\boldsymbol{k}\cdot\boldsymbol{R}(n_1,n_2,n_3)} \begin{pmatrix} t^{AA}_{R(n_1,n_2,n_3)} & t^{AB}_{R(n_1,n_2,n_3)} \\ t^{BA}_{R(n_1,n_2,n_3)} & t^{BB}_{R(n_1,n_2,n_3)} \end{pmatrix}$$

Lattice & SK parameters

$\{a, d, \epsilon_p, \epsilon_d, V^\pm_{pd\sigma}, V^\pm_{pd\pi}, V_{1pp\sigma}, V_{1pp\pi}, V_{2pp\sigma}, V_{2pp\pi}, V^\pm_{3pp\sigma}, V^\pm_{3pp\pi}\}$

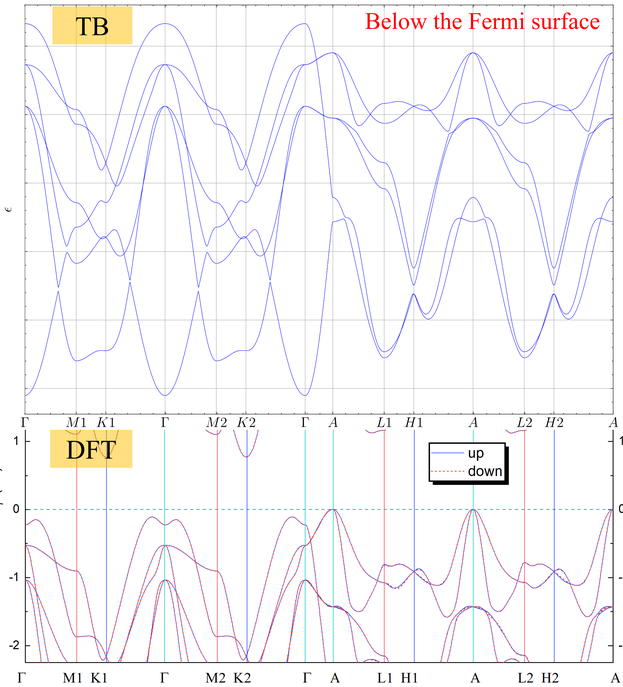
Conversions

$\{a, d, \epsilon_p, \lambda_\pm, c^\pm_1, c^\pm_2, V_{1pp\sigma}, V_{1pp\pi}, V_{2pp\sigma}, V_{2pp\pi}, V^\pm_{3pp\sigma}, V^\pm_{3pp\pi}\}$

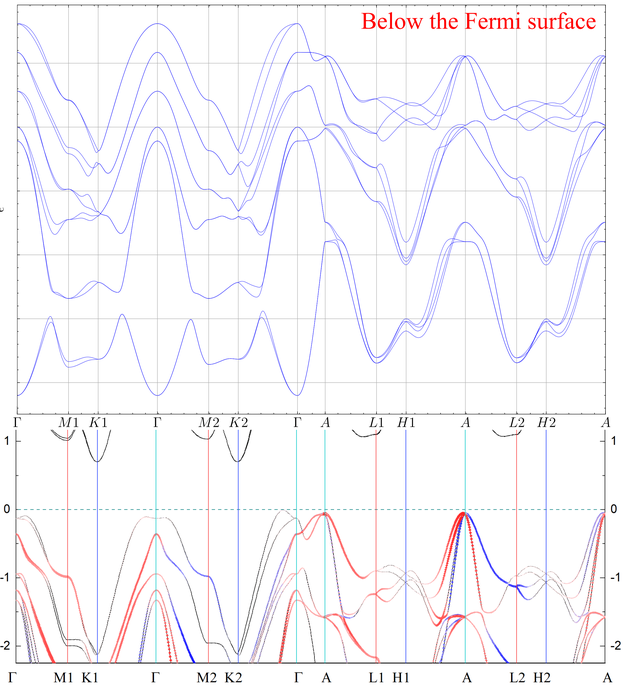
$V_{1pp\sigma} = 0.535$, $V_{1pp\pi} = -0.019$, $V_{2pp\sigma} = 0.438$, $V_{2pp\pi} = 0.026$
$V^+_{3pp\sigma} = 0.109$, $V^+_{3pp\pi} = 0.027$, $V^-_{3pp\sigma} = -0.286$, $V^-_{3pp\pi} = -0.012$
$c^+_1 = -0.028$, $c^+_2 = 1.175$, $c^-_1 = -0.059$, $c^-_2 = 1.353$
$\lambda_+ = -0.052$, $\lambda_- = -0.192$, $\epsilon_x = 2.90$, $\epsilon_y = 2.90$, $\epsilon_z = 2.99$
$\lambda_{SO} = 0.44$, $a = 4.171$, $d = 6.686$

Fitting the hopping matrices to DFT

Non-SOC



SOC (110)



Conclusion

- We calculate the energy bands below the Fermi-surface of altermagnet candidate MnTe, whose Mn layers are colinear A-type AFM.
- Our minimum TB model precisely captures the electronic band structure of MnTe.
- Our method effectively accounts for the A-type AFM in Mn layers and can be applied to various altermagnetic materials.

Since DFT includes the higher hopping matrices, there are discrepancies in the numerical values, but the symmetry of the band mixing is consistent through all the paths within the Brillouin zone.

References

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This work is supported by the Department of Energy, Basic Energy Science under Grant No. DE-SC0020221.