GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

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SPIN HALL CONDUCTIVITY OF FERROMEGNETIC Fe_3GeTe_2 MONOLAYER

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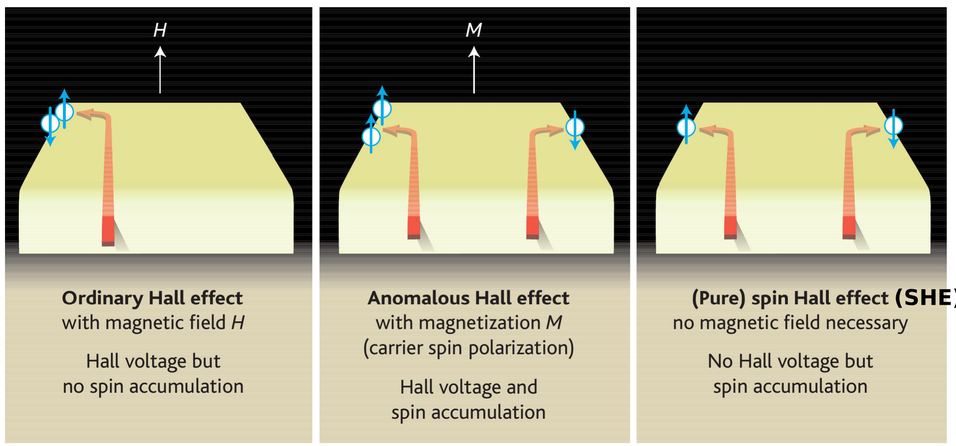
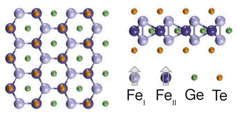
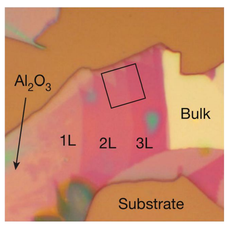
BACKGROUND

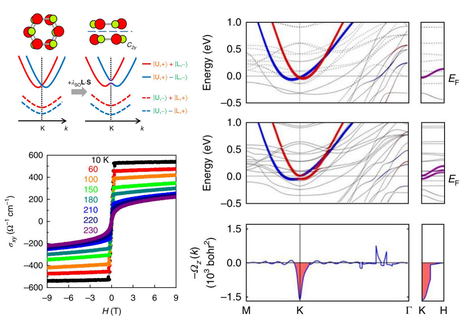


Three types of Hall effects



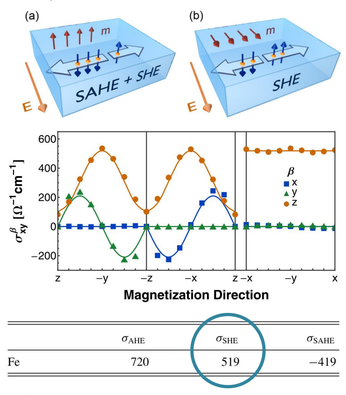


Ferromagnetism in Fe_3GeTe_2 (FGT)



Anomalous Hall effect in FGT

Spin anomalous Hall effect (SAHE)



	σ_{AHE}	σ_{SHE}	σ_{SAHE}
Fe	720	519	−419

SHE: Independent to magnetization

Spin Hall effect in FGT

METHOD

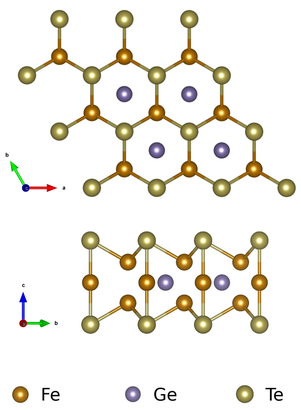
The intrinsic spin Hall conductivity (SHC) is given by Kubo formula:

$$\sigma_{xy}^{\mathrm{spinz}}(\omega) = \hbar \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} \sum_n f_{n\boldsymbol{k}} \times \sum_{m\neq n} \frac{2\,\mathrm{Im}[\langle n\boldsymbol{k}|\hat{j}_x^{\mathrm{spinz}}|m\boldsymbol{k}\rangle\langle m\boldsymbol{k}|-e\hat{v}_y|n\boldsymbol{k}\rangle]}{(\epsilon_{n\boldsymbol{k}}-\epsilon_{m\boldsymbol{k}})^2-(\hbar\omega+i\eta)^2}, \quad \hat{j}_x = \tfrac{1}{2}\{\hat{s}_z, \hat{v}_x\} \tag{1}$$

The spin Berry curvature term is separated from Eq. (1):

$$\Omega_{n,xy}^{\mathrm{spinz}}(\boldsymbol{k}) = \hbar^2 \sum_{m\neq n} \frac{-2\,\mathrm{Im}[\langle n\boldsymbol{k}|\frac{1}{2}\{\hat{\sigma}_z, \hat{v}_x\}|m\boldsymbol{k}\rangle\langle m\boldsymbol{k}|\hat{v}_y|n\boldsymbol{k}\rangle]}{(\epsilon_{n\boldsymbol{k}}-\epsilon_{m\boldsymbol{k}})^2-(\hbar\omega+i\eta)^2} \tag{2}$$

SHC is the integral of spin Berry curvature.



Atomic structure of FGT monolayer

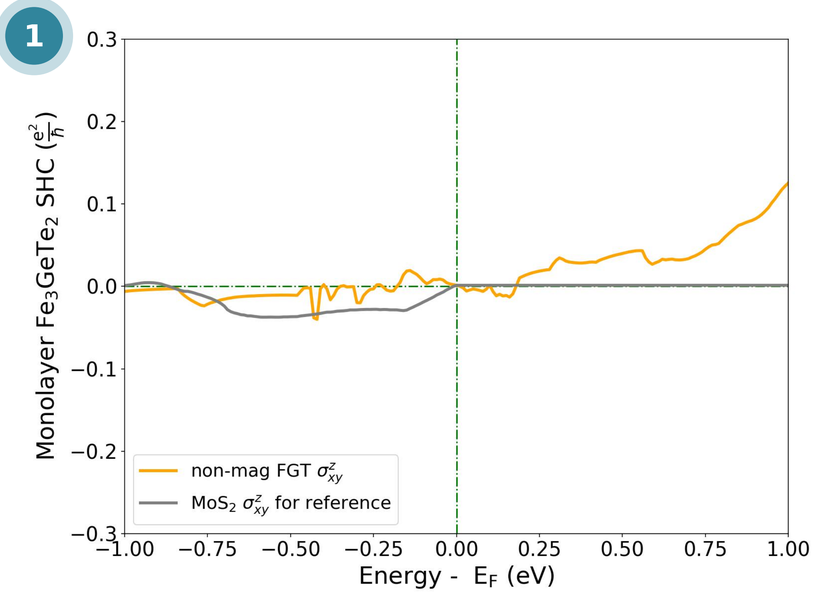
QUANTUM ESPRESSO + WANNIER90

DFT
Density functional theory

MLWF
Maximally localized Wannier function

RESULTS

1



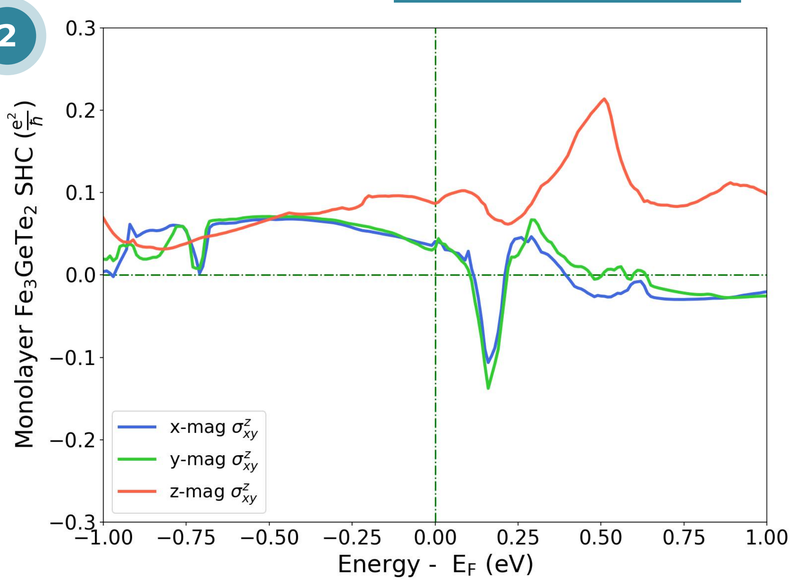
- SHC of nonmagnetic FGT *versus* SHC of MoS_2: Comparable
- SHC of FGT is ~zero at Fermi energy (E_F)
- SHC of FGT increases with right-shifting E_F

The SHC of FGT monolayer is weak at E_F at the nonmagnetic state.

FGT monolayer exhibits nonmagnetism at room temperature.

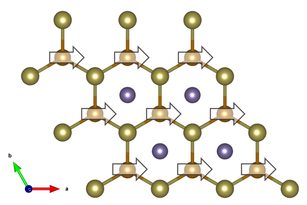
RESULTS

2

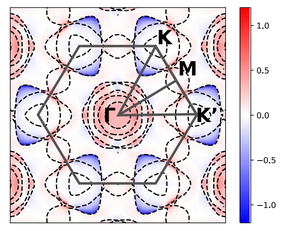


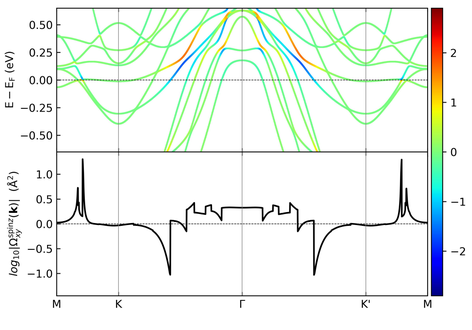
- SHE of ferromagnetic FGT monolayer with x/y/z magnetization
- The x-mag SHC and y-mag SHC differ: Magnetization dependence due to crystalline anisotropy
- The SHC of z-mag is enhanced thanks to the contribution of SAHE.

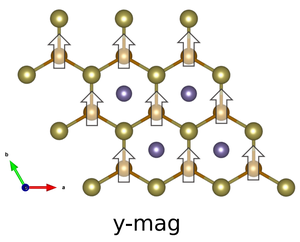
SHC of z-mag FGT > SHC of x/y-mag FGT > SHC of non-mag FGT.



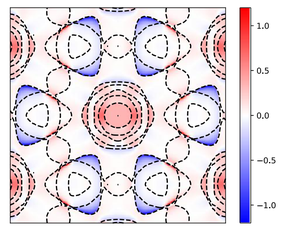
x-mag

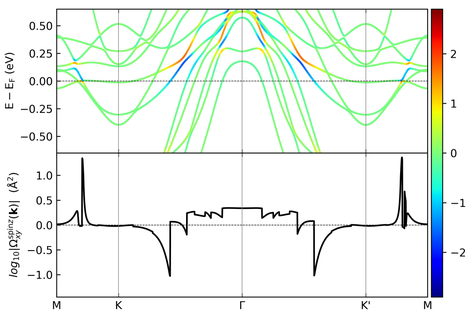


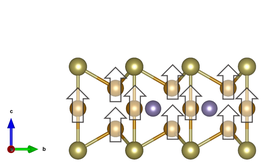




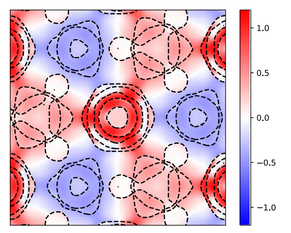
y-mag

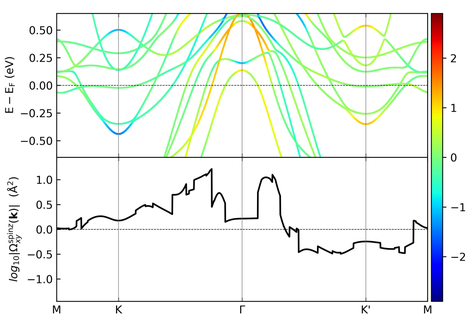






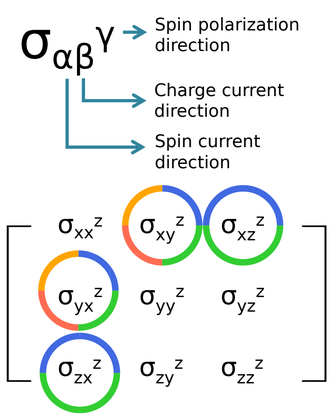
z-mag



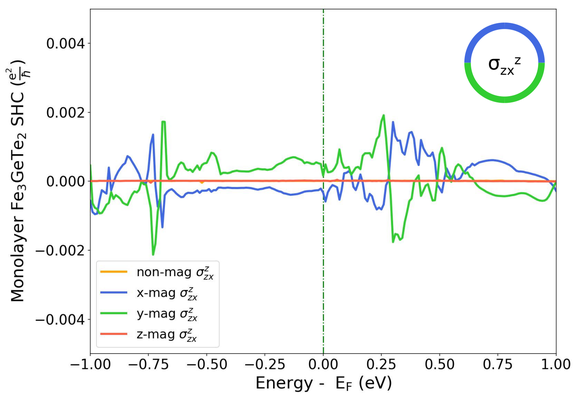


The spin Berry curvatures in two-dimensional Brillouin zone / along the path of high-symmetry points

3



Non-zero tensors for magnetizations



Magnetization-dependent SHE tensors.

CONCLUSIONS

1. SHE is greatly affected by magnetization.
2. Spin conductivity of Fe_3GeTe_2 monolayer is enhanced by SAHE.
3. Magnetizations can induce diverse SHE tensors by breaking symmetry.

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