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Supplementary Materials for

Large anomalous Hall effect driven by a nonvanishing Berry curvature in the noncolinear antiferromagnet Mn_3Ge

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This PDF file includes:

Our ab-initio DFT calculations were performed by the Vienna Ab-initio Simulation Package (VASP) with projected augmented wave (PAW) potential (*27*). The exchange and correlation energy was considered in the generalized gradient approximation (GGA) level (*28*). The experimental lattice structure was used in the calculations. We projected the Bloch wave functions into Wannier functions as s, p and d atomic-like orbitals (*29*) and derived the tight-binding Hamiltonian for Mn_3Ge. The intrinsic transverse Hall conductivity can be understood as the integral of the Berry curvature for the occupied states in the reciprocal space (*1*). Hence, we have calculated the Berry curvature from the ab-initio tight binding model, to interpret the measured anomalous Hall effect.

The intrinsic anomalous Hall conductivity (AHC) tensor, $\sigma^{\gamma}_{\alpha\beta}$, is calculated as the sum of the Berry curvature for a given electronic state, n, that is defined by the quantity, $\Omega^{n,\gamma}_{\alpha\beta}(\vec{k})$, over all the occupied electronic states, as described by the equation

$$\sigma^{\gamma}_{\alpha\beta} = ie^2\hbar\, \Sigma_n \int_{\vec{k}} \frac{d\vec{k}}{(2\pi)^3} f(E_{n,\vec{k}})\, \Omega^{n,\gamma}_{\alpha\beta}(\vec{k}) \tag{1}$$

where α, β, γ can be any of x,y,z, $f(E_{n,\vec{k}})$ is the Fermi-Dirac distribution, and $\Omega^{n,\gamma}_{\alpha\beta}(\vec{k})$, a is given by

$$\Omega^{n,\gamma}_{\alpha\beta}(\vec{k}) = Im\ \sum_{n'\neq n} \frac{<u(n,\vec{k})|\hat{v}_\alpha|u(n',\vec{k})><u(n',\vec{k})|\hat{v}_\beta|u(n,\vec{k})>-(\alpha\leftrightarrow\beta)}{\left(E_{n,\vec{k}}-E_{n',\vec{k}}\right)^2} \tag{2}$$

where, $E_{n,\vec{k}}$ is the eigenvalue for the *n-th* eigen state $|u(n,\vec{k})>$ at the $\vec{k}$ point, and $\hat{v}_\alpha = \frac{1}{\hbar}\frac{\partial H(\vec{k})}{\partial k_\alpha}$ is the velocity operator. A *k*-grid of $101 \times 101 \times 101$ was used in the integral over the Brillouin zone.

We have calculated the intrinsic spin Hall conductivity σ_{xy}^{z} with field along *y*, spin current along *x*, and spin polarization in *z* direction. The spin Hall conductivity was calculated by using the Kubo formula approach (*30*)

$$\sigma_{xy}^{z} = \frac{e\hbar}{V}\sum_{\vec{k}}\sum_{n} f_{\vec{k},n}\left(-2\,\mathrm{Im}\sum_{n'\neq n}\frac{<u_{n\vec{k}}\,|\,\hat{J}_{x}^{z}\,|\,u_{n'\vec{k}}><u_{n'\vec{k}}\,|\,\hat{v}_{y}\,|\,u_{n\vec{k}}>}{\left(E_{n\vec{k}}-E_{n'\vec{k}}\right)^{2}}\right)$$

where the spin current operator $\hat{J}_{x}^{z} = \frac{1}{2}\{\hat{v}_{x} \quad \hat{s}_{z}\}$, the spin operator $\vec{s}_{z}$.

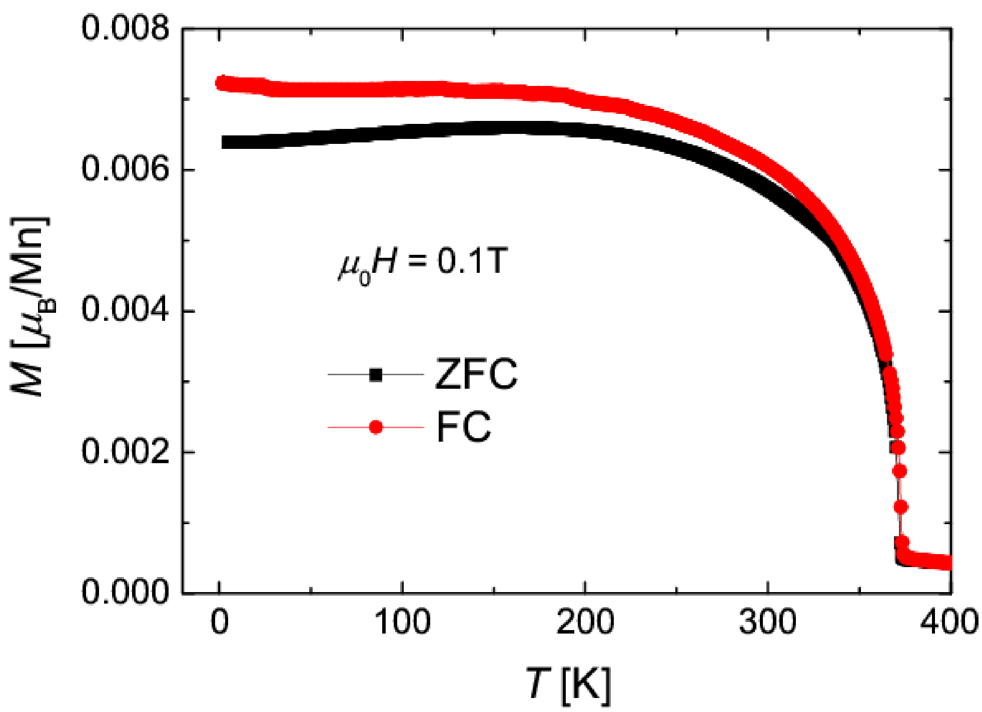

fig. S1. Temperature dependence of magnetization. *M* (*T*) measured with field parallel to a-b plane.

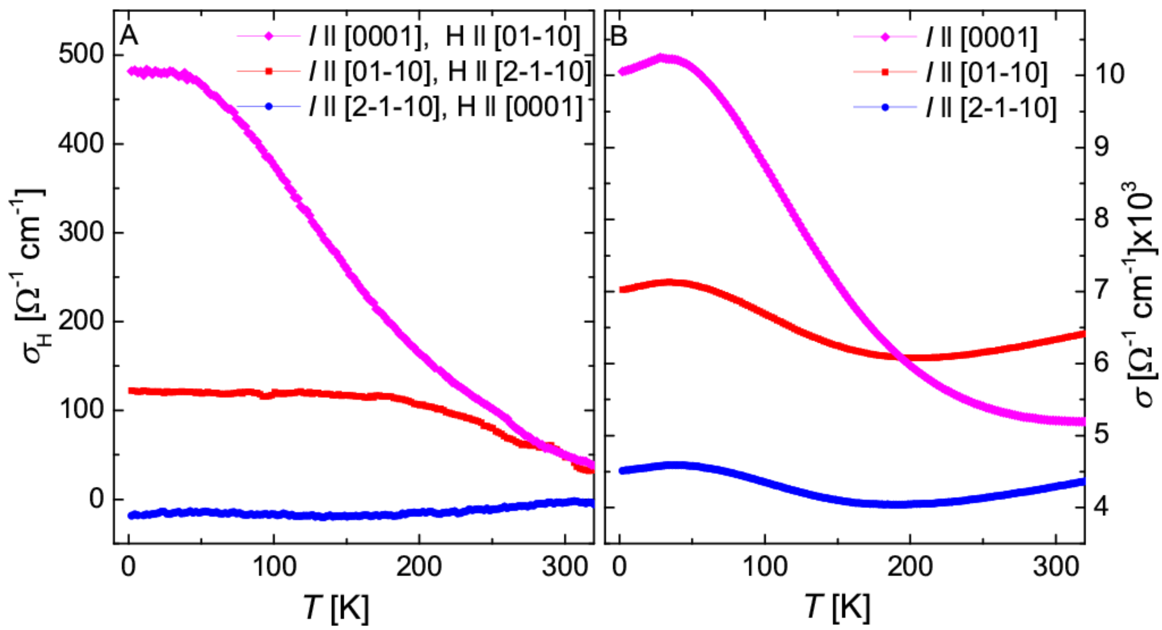

fig. S2. Conductivity with temperature. **A**, Temperature dependence of Hall conductivity measured with the current along three different crystallographic directions. The magnetic field was kept at 0.1 T for all measurements. **B**, Temperature dependence of the normal conductivity measured in zero magnetic field for the same current configurations.

The temperature variation of the anomalous Hall conductivity measured in different current directions is shown in fig. S2A. Since Mn_3Ge exhibits extremely low coercivity, all measurements have been performed in the presence of a small field of 0.1 T. The Hall conductivity measured with *I* along [0001] and *H* along [01-10] exhibits a maximum value of 480 $(\Omega cm)^{-1}$ at 2 K and remains constant up to 40 K. Above 40 K, it decreases almost linearly with temperature leading to a value of approximately 40 $(\Omega cm)^{-1}$ at room temperature. By contrast, the temperature dependence of the low field Hall conductivity for *I* along [01-10] and *H* along [2-1-10] virtually remains constant with temperature, showing only a small decrease above 200 K. Similarly, Hall conductivity measured with *I* along [2-1-10] and H along [0001], which exhibits a negative value, remains nearly unchanged with temperature. To elucidate the relationship between hall conductivity and normal conductivity in Mn_3Ge, we have plotted the temperature dependence of the normal conductivity measured for different current profiles in fig. S2B. Indeed, we found that for same current direction the normal conductivity follows a similar temperature dependent behavior as that of Hall conductivity.