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Beyond germanides: anomalous Hall effect in the silicide $LaMn_2Si_2$

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By combining symmetry analysis and direct density functional calculations including the spin-orbit coupling, we demonstrate that anomalous Hall effect can be observed in not only germanides with general formula RMn_2Ge_2, where R is a rare-earth ion or Y. Our calculations predict a large anomalous Hall conductivity in $LaMn_2Si_2$, with a non-zero $\sigma_{xy}^{\mathrm{AH}}$ component of -360 S/cm, accompanied by a pronounced magneto-optical response. Remarkably, electron doping of $LaMn_2Si_2$ is expected to substantially enhance the Hall conductivity, with values reaching up to -650 S/cm. These results suggest that silicides with general formula RM_2Si_2 can be an interesting platform for studying anomalous Hall effect.

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Introduction. Layered intermetallic compounds of the RMn_2Si_2 family, where R denotes a rare-earth element or yttrium, crystallize in the $ThCr_2Si_2$-type structure and have attracted considerable interest due to their complex magnetic ordering and relatively high magnetic transition temperatures [1, 2]. In this structure, Mn atoms form two-dimensional square lattices that stack along the crystallographic c-axis, separated by Si and R layers. The magnetism in these compounds is primarily governed by the Mn sublattice and can be finely tuned through chemical substitution or external pressure, yielding a diverse landscape of exchange-driven magnetic transitions [3–6]. $LaMn_2Si_2$, which is the focus of this study, adopts a noncollinear magnetic structure, where Mn moments are ferromagnetically aligned along the c-axis while remaining antiferromagnetically coupled within the ab plane [4, 7]. This canted spin arrangement breaks the inversion while preserving certain crystallographic symmetries.

Calculation results. The non-collinear GGA calculation correctly reproduces the magnetic ground state of $LaMn_2Si_2$ refined in [4]. The spin moments on Mn are $\mathbf{m_s} = (\pm 2.55, 0, 1.55)\mu_B$, but they compensate each other in the x- direction in the spin space (such that the x-component of the total moment vanishes), while m_s^z orders ferromagnetically. We note, that strictly speaking real and spin spaces are, of course, decoupled unless the spin-orbit coupling (SOC) is introduced.

Including SOC has almost no effect on the spin moments, but producing tiny orbital moments, $\mathbf{m_l} = (\pm 0.02, 0, 0.01)\mu_B$, but it changes the electronic structure resulting in formation of band anti-crossings.

Symmetry analysis and anomalous Hall effect. As it has been mentioned in the introduction the magnetic structure is characterized by the $Im'm2'$ magnetic space group. This magnetic order breaks the inversion center connecting two magnetic sublattices, the C_4 rotation axes, which make all Mn ions in the ab plane equivalent, and one of the mirror planes present in the $I4/mmm$ space group. Finally, the magnetic point group turns out to be $m'm2'$. Here and below, we follow the conventional practice of considering magnetic symmetry using the same settings as for the parent paramagnetic structure.

For the $m'm2'$ point group, PT (parity $\times$ time-reversal) symmetry gets broken, and therefore one might expect various non-trivial physical phenomena. Formally, according to the classification of Cheong and Huang [8] this group belongs to the M-type of altermagnetism. However, its non-collinear antiferromagnetic structure may originate from exchange interaction rather than SOC. Therefore, classifying it as an altermagnet is premature. Nevertheless, the symmetry analysis performed using MTENSOR toolkit [9] demonstrates that $LaMn_2Si_2$ should exhibit the anomalous Hall effect. In particular, the xy component of conductivity is allowed to be non-zero, while all remaining off-diagonal elements must vanish. In order to verify this prediction we performed direct calculation of conductivity tensor $\sigma_{\alpha\beta}^{\mathrm{AH}}$ by Wannier90 package [10], where it is estimated via the Kubo formula [11].

We used Mn $3d$ and Si $3p$ states and a fine mesh in k-space for Wannier function projection. Integration

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was performed over the $100 \times 100 \times 40$ mesh and yielded $\sigma_{xy}^{\mathrm{AH}} = -365\,\mathrm{S/cm}$, while both $\sigma_{xz}^{\mathrm{AH}}$ and $\sigma_{yz}^{\mathrm{AH}}$ are of order of few S/cm, which perfectly agrees with symmetry consideration presented above.

Anomalous Hall conductivity in $LaMn_2Si_2$ is much higher (by absolute value) than large σ^{AH} observed for non-collinear antiferromagnet Mn_3Sn (experimentally $\sigma_{\mathrm{exp}}^{\mathrm{AH}} = 100\,\mathrm{S/cm}$ [12]), but it is still smaller when in germanide counterpart, $LaMn_2Ge_2$, with $\sigma_{\mathrm{exp}}^{\mathrm{AH}} = 928\,\mathrm{S/cm}$ [13].

Surprisingly, when treating $LaMn_2Si_2$ as a quasi-2D material containing a single unit cell (with the experimental $c = 10.56325\,\text{Å}$ [14]), the calculated anomalous Hall conductivity is $\sigma_{xy}^{\mathrm{AH}} = 0.996\,e^2/h$. This value is extremely close to the quantum conductance, which is rather unexpected for a metal and could potentially indicate the importance of topological features in the electronic structure. Our calculations resulted to no gap or pronounced pseudogap at the Fermi level. In Figure 1, we plot the Hall conductance as a function of the Fermi energy. This analysis is useful both for studying doping effects and for demonstrating the absence of plateaus in the conductivity, suggesting that the observed $\sigma_{xy}^{\mathrm{AH}} \approx e^2/h$ may be accidental.

We also note that a variation of δE_{F} comparable with that presented in Fig. 1 does not alter the magnetic ground state. The self-consistent GGA + SOC calculations show that even for $\delta E_{\mathrm{F}} = 0.2$ (near the maximum of $\sigma_{xy}^{\mathrm{AH}}$), the primary effect is only a slight decrease in the Mn moment canting to approximately 1.4°.

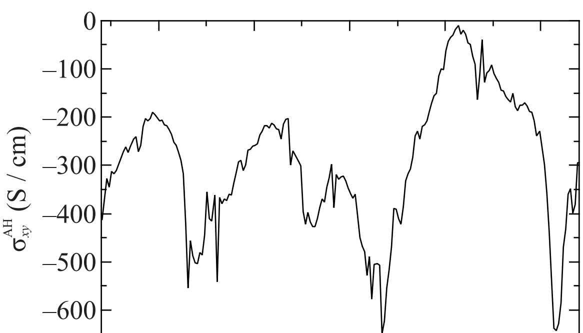

Fig. 1. Intrinsic anomalous Hall conductivity $\sigma_{xy}^{\mathrm{AH}}$ as function of the Fermi energy variation. Zero δE_{F} corresponds to the actual Fermi level in $LaMn_2Si_2$

Discussions and conclusions. Similar to anomalous Hall conductivity, one might expect spontaneous Nernst effect, which results in transverse electric field $E_i = \beta_{ij} \nabla_j T$ due to temperature gradient. For $N_{ij} = (\beta_{ij} - \pi_{ji})/2$ (where π_{ji} matrix relates the heat flux $q_i = \pi_{ij} J_j$ with current density, J_j), symmetry dictates that only $N_{xy} = N_{yx}$ can be finite.

To the best of our knowledge, neither the transverse piezomagnetic effect nor the anomalous Hall effect has been observed in RMn_2Si_2 materials so far. However, Hall conductivity measurements have been reported for their Ge counterparts such as $CeMn_2(Ge_xSi_{1-x})_2$ with $x = 1$ and $x = 0.2$ [15], $LaMn_2Ge_2$ [13], $CeMn_2Ge_2$ [16].

In the present paper, we show that not only germanides but also silicides with the $ThCr_2Si_2$ crystal structure can exhibit these phenomena. Moreover, as seen in Fig. 1, the absolute value of the Hall conductivity can be substantially increased by electron doping. Specifically, adding ~ 0.4 electrons per formula unit is expected to nearly double $\sigma_{xy}^{\mathrm{AH}}$, provided the doping does not alter the magnetic structure – a scenario supported by the simplest GGA + SOC calculations.

Furthermore, a detailed symmetry analysis of various magnetic structures suggests that the anomalous Hall effect, and the transverse piezomagnetic effect may occur not only in $LaMn_2Si_2$ but also in many other $ThCr_2Si_2$-type materials where such phenomena have not yet been observed [17]. It would be highly compelling to investigate these effects in future experiments.

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Conflict of interest. The authors of this work declare that they have no conflicts of interest.

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