

Altermagnetism and anomalous Hall effect in LaMn_2Si_2

Sergey V. Streltsov^{1,*} and Dmitry M. Korotin¹

¹*M. N. Mikheev Institute of Metal Physics, Ural Branch of Russian Academy of Sciences, 620137 Yekaterinburg, Russia*
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By combining symmetry analysis and direct density functional calculations including the spin-orbit coupling, we demonstrate that LaMn_2Si_2 is an M-type altermagnet. Our results predict a large anomalous Hall effect, with a non-zero σ_{xy}^{AH} component of -360 S/cm, accompanied by a pronounced magneto-optical response. Remarkably, electron doping of LaMn_2Si_2 is predicted to substantially enhance the Hall conductivity, with values reaching up to -650 S/cm. These results suggest that silicates with general formula RM_2Si_2 can be an interesting platform for studying both altermagnetism and anomalous Hall effect.

I. 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 [1–6] ($T_c \sim 310\text{K}$ for LaMn_2Si_2 and $T_c \sim 510\text{K}$ for YMn_2Si_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 [7–10].

The compound 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 [8, 11] (Fig. 1). This canted spin arrangement breaks the inversion while preserving certain crystallographic symmetries, a combination that can be evidence of altermagnetism in this system.

Recent studies on the isostructural compound LaMn_2Ge_2 have revealed topological and anomalous Hall effects [12, 13] near room temperature, motivating the investigation of these phenomena in LaMn_2Si_2 . The noncollinear magnetic order in LaMn_2Si_2 , characterized by the $Im'm2'$ magnetic space group. Our first-principles calculations with spin-orbit coupling demonstrate that this magnetic symmetry gives rise to M-type altermagnetism in LaMn_2Si_2 , manifested in momentum-dependent spin polarization of electronic bands and a substantial intrinsic anomalous Hall conductivity of σ_{xy}^{AH} . These results establish LaMn_2Si_2 as a prototype material for exploring transport in noncollinear ferromagnets, with implications for spintronic applications.

II. METHODS

We used Vienna Ab initio Simulation Package (VASP) to calculate electronic and magnetic properties of LaMn_2Si_2 . The generalized gradient approximation (GGA) in the form of Perdew-Burke-Ernzerhof exchange-correlation potential [14] and projected augmented wave (PAW) [15] method were utilized [14].

The crystal structure was taken from Ref. [7]. The energy cutoff for the plane-wave basis was chosen to be 337 eV. We took into account the nonspherical contributions due to the gradient correction inside the PAW spheres. In course of self-consistency we used $8 \times 8 \times 8$ k -mesh in the reciprocal space and applied the tetrahedron method for all summations. In contrast, for the Wannier function projection [17] a finer mesh of $12 \times 12 \times 7$ was performed. To calculate the intrinsic contribution to the anomalous Hall conductivity tensor, we systematically increased the k -point mesh density until convergence was achieved. The final results, presented for a mesh size of $100 \times 100 \times 40$, demonstrate satisfactory saturation of the

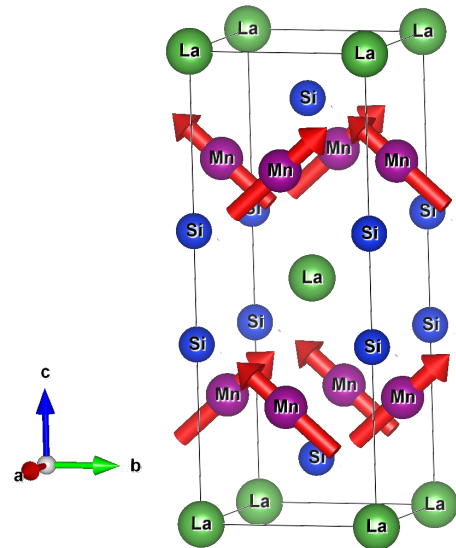


FIG. 1. Crystal and magnetic structure of LaMn_2Si_2 . Figure was plotted using VESTA [16].

* streltsov@imp.uran.ru

conductivity values.

III. CALCULATION RESULTS

A. Electronic and magnetic structure

The non-collinear GGA calculation correctly reproduces the magnetic ground state of LaMn_2Si_2 refined in Ref. [8] and shown in Fig. 1. 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 (such that the x -component of the total moment vanishes), while m_s^z orders ferromagnetically. The resulting band structure is presented in Fig. 2(a). Interestingly, there are regions in the Brillouin zone where bands exhibit moderate dispersion — for example, near the N point — along with several band crossings close to the Fermi level.

Including spin-orbit coupling (SOC) has almost no effect on the spin moments, producing only 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, as one can see from Fig. 2(a).

Analysis of band structure shows that the largest contribution to canting of the magnetic moment resulting in substantial m_x component of the spin moment comes from the G and M points, as can be seen from Fig. 3.

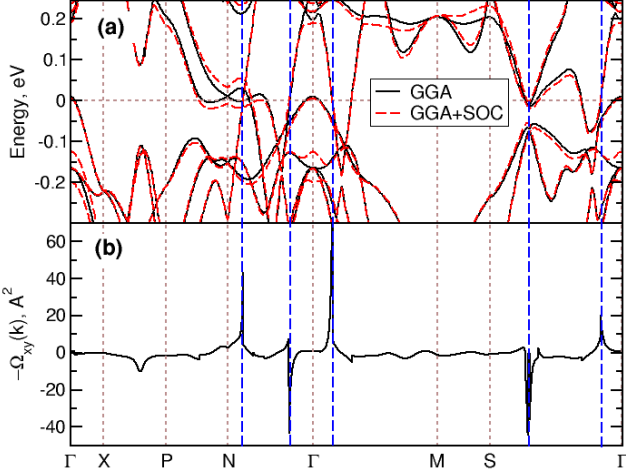


FIG. 2. Band structure as obtained in GGA and GGA+SOC calculations (a). Berry curvature Ω_{xy} along high-symmetry directions (b). The Fermi energy is at zero. Blue dashed lines show points along chosen path contributing the most to $\Omega_{xy}(\mathbf{k})$.

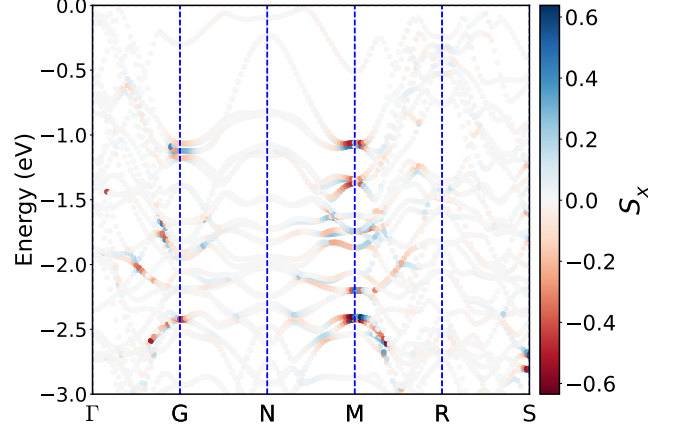


FIG. 3. GGA+SOC electronic band structure of LaMn_2Si_2 with x projection of spin shown by color. The Fermi energy is set to zero.

B. 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 paving road to altermagnetism. Additionally it breaks the C_4 rotation axes, which make all Mn ions in the ab plane equivalent, and one type of the mirror planes. 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. Therefore, we adopt non-standard settings (transformation to a standard for magnetic space group settings: $x \rightarrow x^s$, $y \rightarrow -z^s$, $z \rightarrow y^s$).

According to [18] $m'm2'$ magnetic point group can result in altermagnetism of M-type. In Fig. 3 we show top of the valence band, where one can observe some S_x -split bands, while net S_x in the unit cell vanishes.

M-type altermagnets must exhibit the anomalous Hall effect [18]. 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 $\sigma_{\alpha\beta}^{AH}$ by Wannier90 package[17], where it is estimated via the Kubo-Greenwood formula

$$\sigma_{\alpha\beta}^{AH} = \frac{e^2}{\hbar} \frac{1}{N_k V_c} \sum_{\mathbf{k}} (-1) \Omega_{\alpha\beta}(\mathbf{k}). \quad (1)$$

Here α and β numerate Cartesian coordinates, V_c is the cell volume, N_k is the number of k -points, $\Omega_{\alpha\beta}(\mathbf{k}) = \sum_n f_{n\mathbf{k}} \Omega_{n,\alpha\beta}(\mathbf{k})$ is total Berry curvature, n, m are the band indexes, and $f_{n\mathbf{k}}$ is the Fermi-Dirac distribution. $\Omega_{n,\alpha\beta}(\mathbf{k})$ can be evaluated as [19]

$$\Omega_{n,\alpha\beta}(\mathbf{k}) = -2\hbar^2 \text{Im} \sum_{m \neq n} \frac{v_{nm,\alpha}(\mathbf{k}) v_{mn,\beta}(\mathbf{k})}{(\varepsilon_m(\mathbf{k}) - \varepsilon_n(\mathbf{k}))^2}, \quad (2)$$

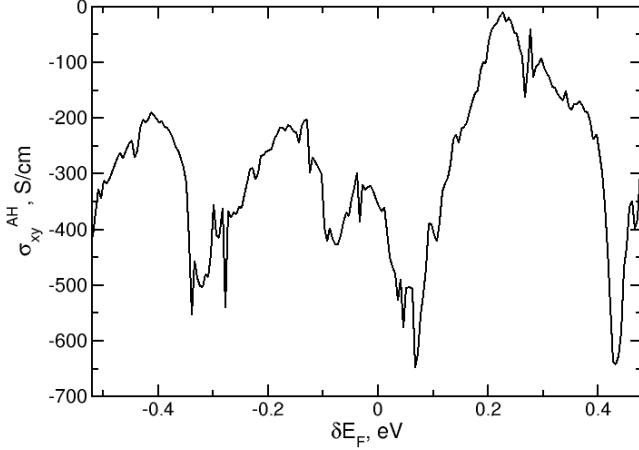


FIG. 4. Anomalous Hall conductivity σ_{xy}^{AH} as function of the Fermi energy variation. Zero δE_F corresponds to the actual Fermi level in LaMn_2Si_2 .

with band dispersion $\varepsilon_m(\mathbf{k})$ and velocities $v_{nm,\alpha}(\mathbf{k})$ obtained by wannierization.

We used Mn 3d and Si 3p states and a fine mesh in k -space for Wannier function projection. Integration in (2) was performed over the $100 \times 100 \times 40$ mesh and yielded $\sigma_{xy}^{AH} = -365 \text{ S/cm}$, while both σ_{xz}^{AH} and σ_{yz}^{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_{xy}^{AH} observed for non-collinear AFM Mn_3Sn (experimentally $\sigma_{xy}^{AH} = 100 \text{ S/cm}$ [20], while theoretical estimate is $\sigma_{DFT}^{AH} = 129 \text{ S/cm}$ [21]).

Surprisingly, if one considers LaMn_2Si_2 as a quasi-2D material with a lattice constant $c = 10.56325 \text{ \AA}$ [5], the anomalous Hall conductivity is found to be $\sigma_{xy}^{AH} = 0.996 e^2/h$. 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. In Fig. 4, 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 $\sigma_{xy}^{AH} \approx e^2/h$ may be accidental.

In Fig. 5 we also present frequency dependence of diagonal and off-diagonal elements of optical conductivity calculated by Kubo formula. One might notice a low frequency feature of the xy component, which not only saturates at static value corresponding to σ_{xy}^{AH} , but has a substantial contribution at optical frequencies.

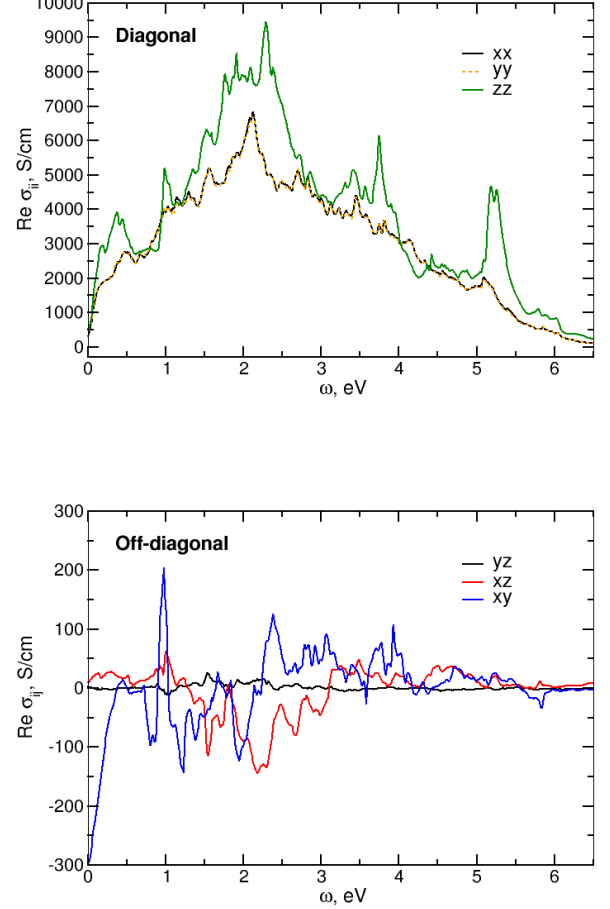


FIG. 5. Diagonal (top panel) and off-diagonal (lower panel) components of optical conductivity $\sigma_{\alpha\beta}$. One can see that the symmetry makes $\sigma_{yy}(\omega) = \sigma_{zz}(\omega)$. Off diagonal σ_{xz} and σ_{yz} vanish at zero frequency.

IV. 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.

Additional symmetry analysis demonstrates that there must be the direct and inverse piezomagnetic effects. The direct effect is dependence of magnetization M_i on the strain tensor σ_{jk} :

$$M_i = \Lambda_{ijk} \sigma_{jk}, \quad (3)$$

where the piezomagnetic tensor $\Lambda_{ijk} \rightarrow \Lambda_{\alpha\beta}$ can be written using Voigt notations $xx \rightarrow 1$, $yy \rightarrow 2$, $zz \rightarrow 3$, $yz, zy \rightarrow 4$, $xz, zx \rightarrow 5$, $xy, yx \rightarrow 6$. In case of

LaMn₂Si₂

$$\Lambda_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & \Lambda_{15} & 0 \\ 0 & 0 & 0 & \Lambda_{24} & 0 & 0 \\ \Lambda_{31} & \Lambda_{32} & \Lambda_{33} & 0 & 0 & 0 \end{pmatrix}, \quad (4)$$

which results in the transverse piezomagnetic effect, when strain along x or y leads to magnetization in the z direction, M_z .

To the best of our knowledge, neither the transverse piezomagnetic effect nor the anomalous Hall effect has been observed in RMn₂Si₂ materials so far. However, Hall conductivity measurements have been reported for their Ge counterparts such as CeMn₂(Ge_xSi_{1-x})₂ with $x = 1$ and $x = 0.2$ [22], LaMn₂Ge₂ [12, 13], CeMn₂Ge₂ [23, 24], PrMn₂Ge₂ [25, 26], NdMn₂Ge₂ [27, 28], SmAg₂Ge₂ [29], and SmMn₂Ge₂ [30, 31].

In the present paper, we show that not only germanates but also silicates with the ThCr₂Si₂ crystal structure can exhibit these phenomena. Moreover, as

seen in Fig. 4, 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 σ_{xy}^{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 altermagnetism, the anomalous Hall effect, and the transverse piezomagnetic effect may occur not only in LaMn₂Si₂ but also in many other ThCr₂Si₂-type materials where such phenomena have not yet been observed [32]. It would be highly compelling to investigate these effects in future experiments.

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