

Chirality induced spin and orbital Edelstein response in nonmagnetic B20 bulk crystals: The role of geometry, spin-orbit coupling, and finite temperature

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Chiral crystals have a noncentrosymmetric unit cell and can manifest spin-orbit coupling (SOC)-induced band splitting, even in the absence of an atomic magnetic moment. We examine the particular case of *Strukturbericht* B20 compounds, with AlPt as representative material, by means of first-principles electronic structure calculations. We show how nonzero, but punctually compensated $\mathbf{k}$ textures for both the spin and the orbital magnetic moment, emerge as a function of the lattice geometry, SOC, and in dependence on finite temperature. An applied electric field perturbation is shown to set up a bulk Edelstein effect in terms of both spin and orbital magnetic moment.

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I. INTRODUCTION

Electronic states for crystals with reduced symmetry exhibit a variety of peculiar effects. These have long been in the spotlight of theoretical and experimental research, with further impulse also toward possible technological applications, particularly in combination with magnetism and within the general context of spintronics [1].

When the unit cell is not centrosymmetric, even materials with zero atomic magnetic moments, i.e., with zero exchange splitting can exhibit nondegenerate electronic bands with a nonzero spin polarization, due to spin-orbit coupling [2] (SOC). Its $\mathbf{k}$ dependence leads to different types of spin textures in reciprocal space [3].

An externally applied electric field perturbation can then produce a corresponding spin current [spin Hall effect (SHE)] or spin polarization [spin Edelstein effect (SEE)]. Similarly, the associated $\mathbf{k}$ dependence for orbital polarization of the electronic states also leads to the orbital Hall and to the orbital Edelstein effects.

A subset of noncentrosymmetric systems has a chiral unit cell [4], and may or may not contain atoms carrying a finite, local magnetic moment. In its absence, the SOC-induced band splitting originates from the relative atomic positions through an effective term $H_{\text{SOC}} = \lambda_{\text{SOC}} \boldsymbol{\sigma} \cdot [\nabla V(\mathbf{r}) \times \mathbf{p}]$, with $\mathbf{p}$ and $\boldsymbol{\sigma}$

denoting, respectively, the linear momentum and the vector of Pauli matrices, and λ_{SOC} a possible scaling factor.

Effects resulting from chirality induced spin selectivity (CISS) have been already studied, for both finite systems such as in the case of double helix DNA chains [5–8], and for three-dimensional (3D) periodic lattices [4,9,10]. From the latter context, we examine here the example of *Strukturbericht* B20, i.e., of standard space group number 198 crystals, for which a variety of compositions in 1:1 AB stoichiometry have been experimentally synthesized [11–23]. We focus our attention mainly on AlPt, and we adopt fully relativistic, *ab initio* calculations based on density functional theory (DFT) to examine the above features of its electronic band structure, their dependence on λ_{SOC} and on the lattice geometry, the possible manifestation in terms of spin and orbital Edelstein response and its robustness with respect to finite-temperature effects.

As a first step, we confirm how the chosen first-principles framework provides qualitative agreement with e.g. ARPES measurements, which suggest split bands with a $\mathbf{k}$ -locked, approximately radial spin texture around the Γ point [24]. In order to pinpoint the role of unit cell geometry, this outcome is contrasted with the artificial test cases of same chemical elements arranged into a noncentrosymmetric but not chiral B3 (zincblende) lattice, or into a centrosymmetric B1 (rock-salt) lattice. Conversely, we then examine the degree of spin and of orbital polarization as a function of artificially scaled SOC strength. We also examine the possible impact of finite-temperature effects on the above band splitting, and on the associated spin and orbital $\mathbf{k}$ textures.

We then perform a simplified estimate of the resulting total Edelstein response, comparing AlPt also with other experimentally reported examples of nonmagnetic B20 compounds. The calculated trend for Edelstein response across B20 materials is interpreted as a consequence of the specific

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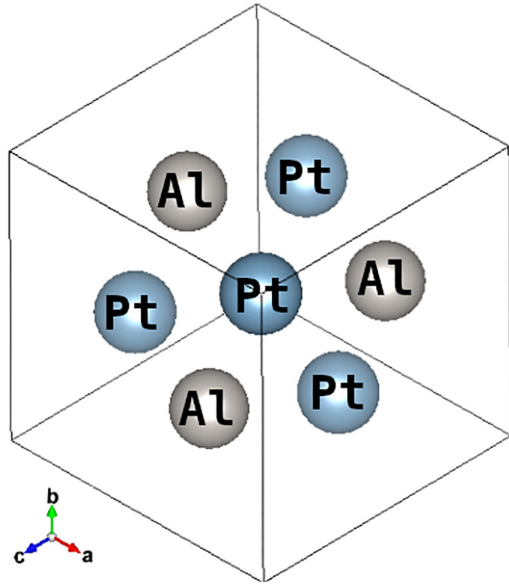


FIG. 1. Unit cell of AlPt in *Strukturbericht* B20, depicted along the $[111]$ chiral axis.

geometrical feature of two interpenetrating and antiparallel arrangements of A and of B sublattices.

Returning in more detail to AlPt, we finally validate the above conclusions and predictions for possible transport experiments by means of more comprehensive Kubo linear response theory, combined with finite-temperature effects treated at the level of a Debye model for positional disorder [25].

This paper is structured as follows. We first recall the relevant geometrical aspects, which are shared across various examples of group number 198 chiral materials (Sec. II). We then outline the theoretical scheme adopted for their *ab initio* study (Sec. III). Results from these electronic structure calculations follow in Sec. IV. We discuss these findings in Sec. V, and offer our conclusions in Sec. VI.

II. GEOMETRY AND COMPOSITION

The prototype geometry of iron silicide (FeSi), with group number 198 (i.e., Sohncke space group $P2_13$ or *Strukturbericht* B20), is realized by AB binary compounds in 1:1 stoichiometry ratio. The cubic unit cell hosts the A and B atoms at the two (x, x, x) and (x', x', x') Wyckoff positions 4a (Fig. 1). Unless otherwise noted, all calculations have been performed using experimental values for lattice parameter A_{lat} and for Wyckoff positions of A and B elements within the unit cell. For simplicity, we select in this work only AB materials with zero atomic magnetic moment. This excludes from present study compounds with elements such as Fe, Co, or Mn. To better explore the role of SOC effects, we take into consideration examples that span both small and large atomic numbers. These criteria lead to the list of compounds given in Table I.

These crystals have a chiral axes along the cubic body diagonal [4]. Atoms of the two chemical species lie in either alternating straight rows or in antiparallel windings along this direction. The unit cell is given by two interpenetrating group

TABLE I. Experimental lattice parameters for the materials examined in this study.

AB composition:	A_{lat} (Å):	Wyckoff A:	Wyckoff B:
RhSn [11]	5.134	$x = +0.142$	$x' = -0.159$
RhSi [12]	4.676	$x = +0.147$	$x' = -0.155$
RhGe [13]	4.862	$x = +0.135$	$x' = -0.160$
PtMg [14]	4.863	$x = +0.136$	$x' = -0.156$
HfSb [16]	5.590	$x = +0.134$	$x' = -0.155$
HfSn [17]	5.594	$x = +0.155$	$x' = -0.155$
PtGa [18]	4.910	$x = +0.135$	$x' = -0.155$
AuBe [20]	4.668	$x = +0.150$	$x' = -0.156$
PdAl [21]	4.859	$x = +0.143$	$x' = -0.153$
AlPt [22]	4.866	$x = +0.145$	$x' = -0.155$
PdGa [23]	4.897	$x = +0.157$	$x' = -0.142$

number 198 lattices, each containing only B or only A atoms. An enantiomorphic construction is achieved, upon inverting the sign of all coordinates for both Wyckoff positions. For comparison, the higher spatial symmetry of a noncentrosymmetric but not chiral zincblende (*Strukturbericht* B3), or of a centrosymmetric rocksalt geometry (*Strukturbericht* B1), could be artificially recovered for specific values of their Wyckoff positions 4a, while leaving the cubic unit cell volume unchanged (Table II).

These alternative scenarios are examined by means of *ab initio* calculations of the electronic band structure and linear response transport, as detailed below.

III. THEORETICAL SCHEME

We resort to density functional theory (DFT), in its local spin density approximation of exchange correlation (LDA), for all the following results. The ground state and all observables of interest have been computed by solving the Dirac Kohn-Sham problem within the Korringa, Kohn, Rostoker (KKR) Green's function method, as implemented in the SPRKKR electronic structure package [26].

A. Spin and orbital magnetic moment-projected electronic Bloch's spectral function

In the Green's function representation, the expectation value of any observable $\hat{O}$ can be estimated through evaluation

TABLE II. Correspondence between *Strukturbericht* B20 lattice geometry (group number 198) and higher-symmetry B1 (group number 225) or B3 (group number 216) crystals structures, for particular values of the two Wyckoff positions 4a.

Atomic types and Wyckoff positions	Equivalent group nr. and Wyckoff positions:	Example (<i>Strukturbericht</i>):
A at 4a: (0, 0, 0)	A at 4a: (0, 0, 0)	rocksalt (B1)
B at 4a: (.5, .5, .5) in group nr. 198	B at 4b: (.5, .5, .5) in group nr. 225	
A at 4a: (0, 0, 0)	A at 4a: (0, 0, 0)	zincblende (B3)
B at 4a: (.25, .25, .25) in group nr. 198	B at 4c: (.25, .25, .25) in group nr. 216	

of the relevant matrix elements. We consider here in particular the $\mathbf{k}$ -point and energy-resolved spin s , or orbital angular momentum ℓ , or relativistic current density $\mathbf{j}$ vectors, with $v = x, y, z$ components given by

$$A_v^{(O)}(\mathbf{k}, E) = -\frac{1}{\pi} \text{Im}(\text{Tr}(\underline{O}_v \underline{G}(\mathbf{k}, E))_c), \quad (1)$$

upon taking the limit $\eta \rightarrow 0^+$ for the complex energy argument $z = E + i\eta$. In case of disorder, angular brackets denote averaging over an ensemble of alternative configurations c . When necessary, this averaging is here performed through the effective medium construction given by coherent potential approximation (CPA). The technique is used in particular to simulate finite-temperature effects through the alloy analogy model of Ref. [25].

In Eq. (1), an underline denotes explicit matrix representation of the fully relativistic Green's function solution to the Kohn-Sham Dirac's Hamiltonian [27,28], indexed by the angular momentum quantum numbers $\Lambda = (\kappa, \mu)$. In this basis, the simplest case of matrix elements associated with the Dirac β matrix alone gives, for instance, the (total) Bloch's spectral function (BSF). This scalar quantity corresponds to the total charge density, with peaks, which follow the electronic dispersion $\varepsilon(\mathbf{k})$, i.e., the band structure, as: $A(\mathbf{k}, E) = \eta / [(E - \varepsilon(\mathbf{k}))^2 + \eta^2]$. On the other hand, in the presence of disorder, the CPA further includes within the Green's function a complex-valued self-energy term $\Sigma(\mathbf{k}, E) = \Delta(\mathbf{k}, E) + i\Gamma(\mathbf{k}, E)$, which accounts for deviations from long-range periodicity [29], with both shifts $\Delta(\mathbf{k}, E)$ of the electronic bands position and variation of their sharpness (i.e., broadening) $\propto \Gamma^2(\mathbf{k}, E)$ beyond the constant relaxation time approximation associated with a fixed η alone. We study in similar fashion the case of spin and of orbital magnetic moment (evaluated in terms of the atomic centered approximation [30]), and the relativistic current density [31].

In the following, Eq. (1) is first evaluated as a function of energy and of $\mathbf{k}$ point, to obtain bands structure plots. We then sample the Fermi level alone, i.e., $z = E_F$, either as a $k_z = 0$ Brillouin zone slice to visualize Fermi surface sections, or as a whole Brillouin zone average to examine the magnitude of spin and orbital magnetic moment contributions,

$$O^{\text{avg.}}(E_F) = \int_{\Omega_{\text{BZ}}} ||A^{(O)}(\mathbf{k}, E_F)|| d\mathbf{k}, \quad (2)$$

for $\hat{O} = s$ or ℓ . Integration over both the whole Brillouin zone and all occupied energies of, e.g., the spin vector $s = (s_x, s_y, s_z)$ would give in fact the corresponding spin magnetic moment per unit cell. However, we consider here cases where both the spin and orbital magnetic moment vectors have net zero moment due to mutual cancellation of nonzero contributions across opposite $\mathbf{k}$ points with respect to Γ (Sec. IV A),

preferring therefore to examine the average magnitude of these vector quantities. Similarly, we focus on generalized transport effects, which are dominated by electronic structure features at the Fermi level, and therefore we omit inside Eq. (2) an integration over valence bands. The same procedure is also applied to examine the robustness of such spin and orbital $\mathbf{k}$ textures as a function of simulated finite temperature. Adopting the alloy analogy model (AAM), thermal excitations are modeled as incoherent, random atomic displacements from their $T = 0$ K equilibrium positions. These take place slowly with respect to the electronic hopping time scale, and follow a root mean-square statistics given by the Debye model [25]. Since the materials under consideration have zero exchange splitting, i.e., no atomic magnetic moment, there is no need to also deploy the disordered local moment (DLM) approach [32,33], which would similarly sample relatively slow, random fluctuations in the direction of the exchange field also due to finite temperature.

We employ the CPA, both when calculating charge density to reobtain DFT self-consistency and when calculating spin and orbital contributions by means of Eq. (1), and when using Kubo linear response theory for generalized transport properties, as outlined in the next section below.

B. Simplified estimate of Edelstein response across different materials

An externally applied electric field perturbation modifies the electronic structure proportionally to the current density $A^{(j)}(\mathbf{k}, E)$. The charge conductivity, for instance, will generally depend mainly on the electronic structure at the Fermi level (Fermi surface term), although contributions from deeper valence bands (Fermi sea term) can also become important, especially for other transport properties [34]. We will return to this latter aspect in Sec. IV C below.

Focusing on the Edelstein effect [35], an intuitive description can be based on a simplified Boltzmann-like treatment. The Brillouin zone integral of contributions to spin ($\hat{O} = \hat{s}$) or to orbital ($\hat{O} = \hat{\ell}$) magnetic moment, projected along the current density $\hat{O} = \hat{j}$

$$C_{\mu\nu}^{(O)} \propto \int_{\Omega_{\text{BZ}}} A(\mathbf{k}, E_F) (A_{\mu}^{(O)}(\mathbf{k}, E_F) A_{\nu}^{(j)}(\mathbf{k}, E_F)) d\mathbf{k} \quad (3)$$

provides a simple estimate of how the applied electric field perturbation (with direction indexed by $\nu = x, y, z$) can produce a nonzero moment (in the direction indexed by $\mu = x, y, z$).

C. Temperature-dependent Edelstein response

A more comprehensive expression for the Edelstein response is given by the Kubo-Bastin approximation

$$\begin{aligned} C_{\mu\nu}^{(O)} = & \frac{-1}{4\pi V} \int_{-\infty}^{\infty} dE \frac{d f_T(E)}{dE} \text{Tr} \int_{\Omega_{\text{BZ}}} d\mathbf{k} (\underline{O}_{\mu} (\underline{G}(\mathbf{k}, z) - \underline{G}^{\dagger}(\mathbf{k}, z)) \underline{j}_{\nu} \underline{G}^{\dagger}(\mathbf{k}, z) + \underline{O}_{\mu} \underline{G}(\mathbf{k}, z) \underline{j}_{\nu} (\underline{G}(\mathbf{k}, z) - \underline{G}^{\dagger}(\mathbf{k}, z)))_c \\ & + \frac{1}{4\pi iV} \int_{-\infty}^{\infty} dE f_T(E) \text{Tr} \int_{\Omega_{\text{BZ}}} d\mathbf{k} \left(\left(\underline{O}_{\mu} \underline{G}(\mathbf{k}, z) \underline{j}_{\nu} \frac{d \underline{G}(\mathbf{k}, z)}{dE} - \underline{O}_{\mu} \frac{d \underline{G}(\mathbf{k}, z)}{dE} \underline{j}_{\nu} \underline{G}(\mathbf{k}, z) \right) \right. \\ & \left. - \left(\underline{O}_{\mu} \underline{G}^{\dagger}(\mathbf{k}, z) \underline{j}_{\nu} \frac{d \underline{G}^{\dagger}(\mathbf{k}, z)}{dE} - \underline{O}_{\mu} \frac{d \underline{G}^{\dagger}(\mathbf{k}, z)}{dE} \underline{j}_{\nu} \underline{G}^{\dagger}(\mathbf{k}, z) \right) \right)_c, \end{aligned} \quad (4)$$

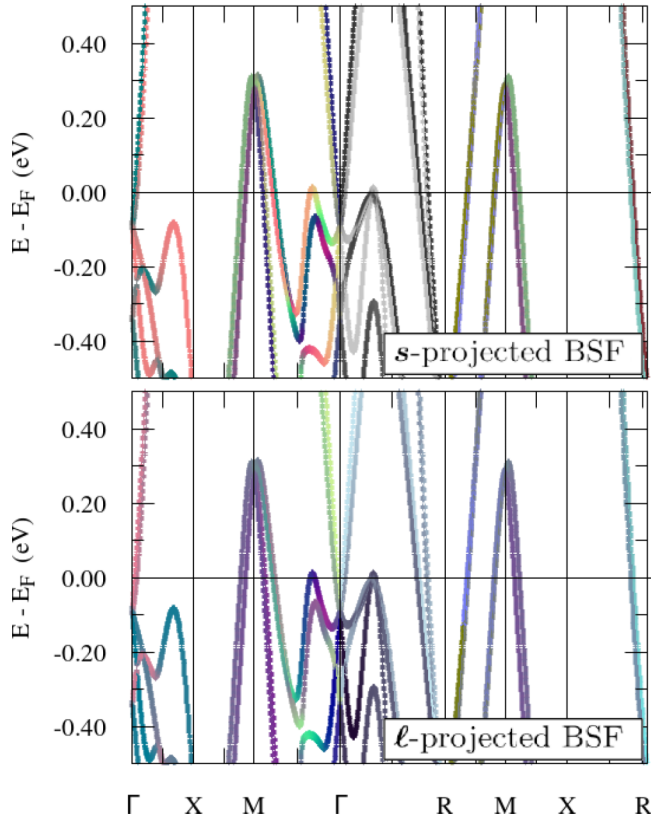


FIG. 2. BSF of AlPt, projected in terms of spin (top) or orbital (bottom) magnetic moment. The color encodes the variable $\nu = x, y, z$ components of either vector quantity as a mixture of red, green, and blue, see text.

in which O_μ stands for spin or for orbital magnetic moment matrix elements, similarly to Eq. (1). Angular brackets within the above Kubo-Bastin formula denote, as in Eq. (1), deployment of the AAM in order to include finite-temperature effects, beside their accounting through the Fermi-Dirac distribution function $f_T(E)$ [25]. The expression is here evaluated with the appropriate inclusion of disorder vertex corrections [36].

IV. AB INITIO RESULTS

A. Relevant features in the ground-state electronic structure

We adopt in this section the case of AlPt as a specific material example, although calculations confirm that the features of relevance for CISS effects discussed below are qualitatively shared across other compounds from Table I.

The electronic dispersion $\varepsilon(\mathbf{k})$ shows the SOC-induced splitting of various bands (Fig. 2). We adopt here a combination of red, green and blue primary colors each mixed with a weight proportional, respectively, to the $\nu = x, y, z$ component of either the spin $A_v^{(s)}(\mathbf{k}, E)$ (top panel) or the orbital $A_v^{(l)}(\mathbf{k}, E)$ (bottom panel) magnetic moment vectors.

The variation of this aggregated color as a function of $\mathbf{k}$ point and energy E indicates a nontrivial spin and orbital magnetic moment texture, in which each ν component is in general nonzero. This is more easily visualized for fixed $k_z = 0$ and considering just the Fermi energy E_F , i.e., focusing

on sections of the Fermi surface (Fig. 3 and Fig. 4). It is sufficient to plot only the $0 \leq k_x < \pi/A_{\text{lat}}$, $0 \leq k_y < \pi/A_{\text{lat}}$ quadrant thanks to the symmetry of the lattice. Results in the other quadrants can be obtained according to the space group of the crystals.

Within this $k_z = 0$ slice, the $\nu = z$ component of $A^{(s)}(\mathbf{k}, E)$ and of $A^{(l)}(\mathbf{k}, E)$ are all zero. We represent direction and magnitude of the remaining $\nu = x, y$ components of spin and of orbital magnetic moments contributions as 2D arrows, colored according to their orientation.

Lifting of energy degeneracy due to spin-orbit coupling appears, in this AlPt example, around the Γ and the M points (Fig. 4, top row). For the examined compounds from Table I, the direction of contributions to the spin magnetic moment across these SOC-split states is antiparallel. The orbital magnetic moment instead shows a more complex $\mathbf{k}$ dependence. On the other hand, the current density at the Fermi level is simply orthogonal to each element of the Fermi surface following the direction of steepest variation for electronic bands at E_F .

We can relate these features to the lattice geometry by examining in the same fashion the artificial cases of B20 AlPt turned into its nonchiral rocksalt (B1) or zincblende (B3) counterparts of Table II. Although this crystal manipulation modifies the outlook of the band structure and in particular of the $k_z = 0$ and $k_x, k_y \in [0, \pi/A_{\text{lat}}]$ slices of the Fermi surface, the qualitative feature of spin and of orbital magnetic moment-split electronic states can still be identified for the noncentrosymmetric *Strukturbericht* B3 (Fig. 3, bottom row). It is instead absent in the centrosymmetric B1 case (Fig. 3, top row).

We then return to the experimental *Strukturbericht* B20 geometry of AlPt, and we examine instead the role of spin-orbit coupling on the band structure and in particular on spin and on orbital polarization of each electronic state. A rewriting of Dirac's equation [37] allows to artificially manipulate its strength. Reducing SOC to 0% recovers energy degeneracy across relativistically split bands. The merge of antiparallel contributions to the spin magnetic moment, together with the shrinking of the hole pocket midway between the Γ and M points, suppresses the spin $\mathbf{k}$ texture. Interestingly, the orbital magnetic moment $\mathbf{k}$ texture instead persists (Fig. 4). This holds also in terms of Eq. (2) for the average length of contributions over the whole Brillouin zone (Fig. 5). The magnitude of the spin texture depends on SOC almost linearly whereas the magnitude of orbital texture is practically independent of SOC, in agreement with the trend shown in Fig. 4. In both cases of spin and of orbital magnetic moment we have, however, punctual cancellation of these vector quantities around the Γ point, i.e., $\int_{\Omega_{\text{BZ}}} \mathbf{A}^{(o)}(\mathbf{k}, E_F) d\mathbf{k} = 0$. This is the case at all energies, and there is no net spin or orbital magnetic moment per atom. The system fulfills time-reversal symmetry. Finally, we keep the physical AlPt lattice parameters and SOC magnitude fixed to realistic values, and we examine the possible role of finite temperature. Within the AAM scheme and in the absence of atomic exchange splitting, as temperature gets higher we have larger RMS for atomic displacements from their equilibrium positions. This increase in the average length of deviations from perfect lattice periodicity shows up as a progressively broadened electronic dispersion. Again we

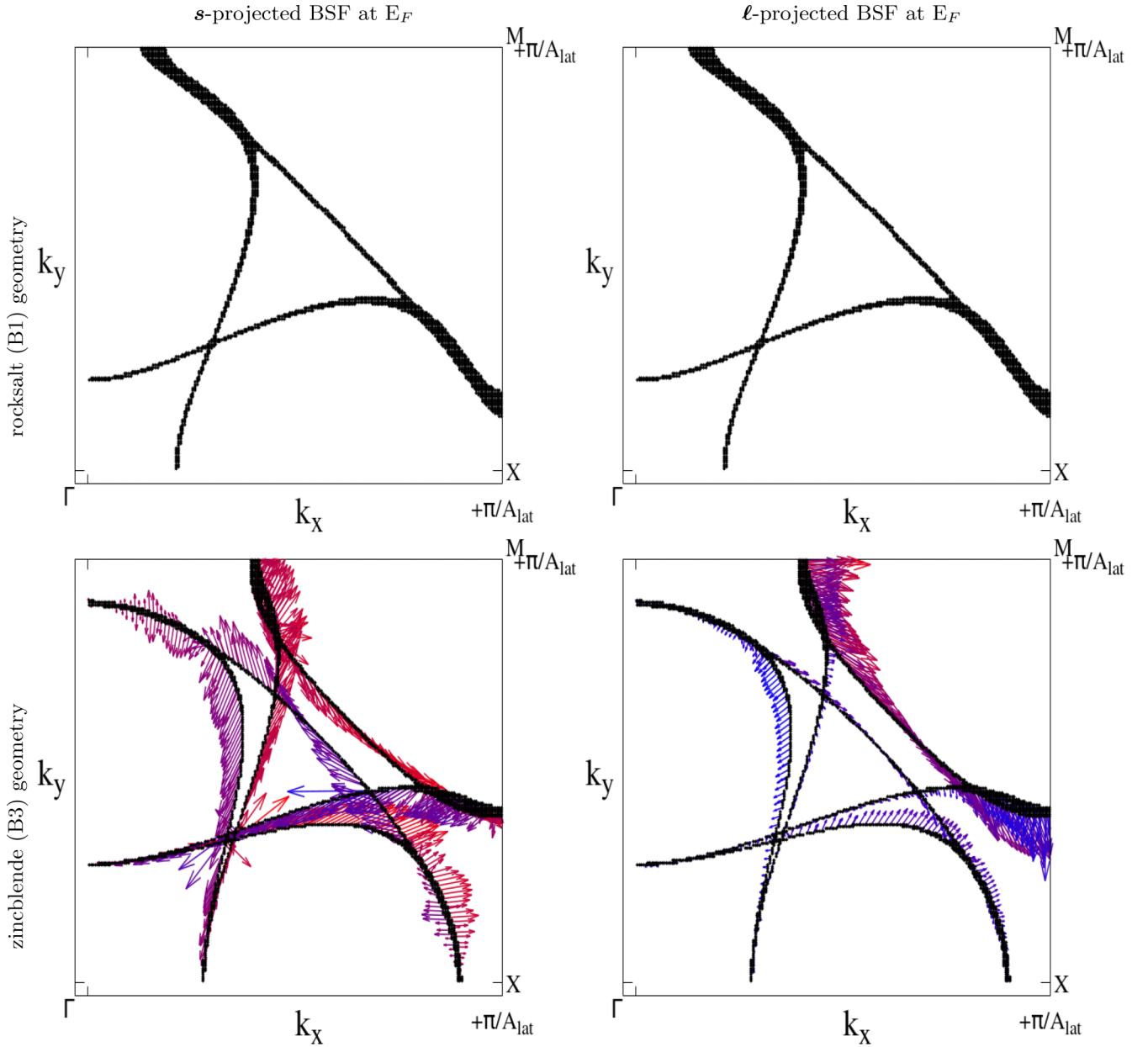


FIG. 3. Spin- (left) and orbital magnetic moment (right, scaled $2\times$ for better visibility)-projected BSF for AlPt in the artificial unit cell geometries of Table II: *Strukturbericht* B1, centrosymmetric (top row), and *Strukturbericht* B3, noncentrosymmetric (bottom row). Arrows colored according to their angle.

focus here on AlPt as example CISS material from the list of Table I. As fairly typical in the presence of only thermally induced positional disorder, its BSF shows a slowly increasing full width at half-maximum (FWHM) as the temperature increases (Fig. 6, with a fixed, arbitrary $\mathbf{k}$ point section highlighted in red for better visibility).

Evaluation of Eq. (2) to estimate the average magnitude of contributions to spin or to orbital magnetic moment also shows a linear and slow decrease with increasing temperature. This is more pronounced for the spin than for the orbital $\mathbf{k}$ texture (Fig. 7). There is no indication of a critical temperature and associated phase transition, which could be compared to the Curie or Néel point, respectively, in ferromagnets or antiferromagnets.

This observation leads to anticipate a certain degree of robustness of specific CISS properties, such as in particular the Edelstein effect. We explore this expectation first at the level of a simplified Boltzmann approach in terms of prior results from Eq. (1), i.e., at the level of only intraband contributions and adopting a temperature-independent constant relaxation time approximation. We then reevaluate it in better detail, through the full linear response expression of Eq. (4) (Sec. IV C).

B. Trends in the total Edelstein response across different B20 materials

The spin and the orbital magnetic moment $\mathbf{k}$ textures shown in Sec. III A are odd with respect to the

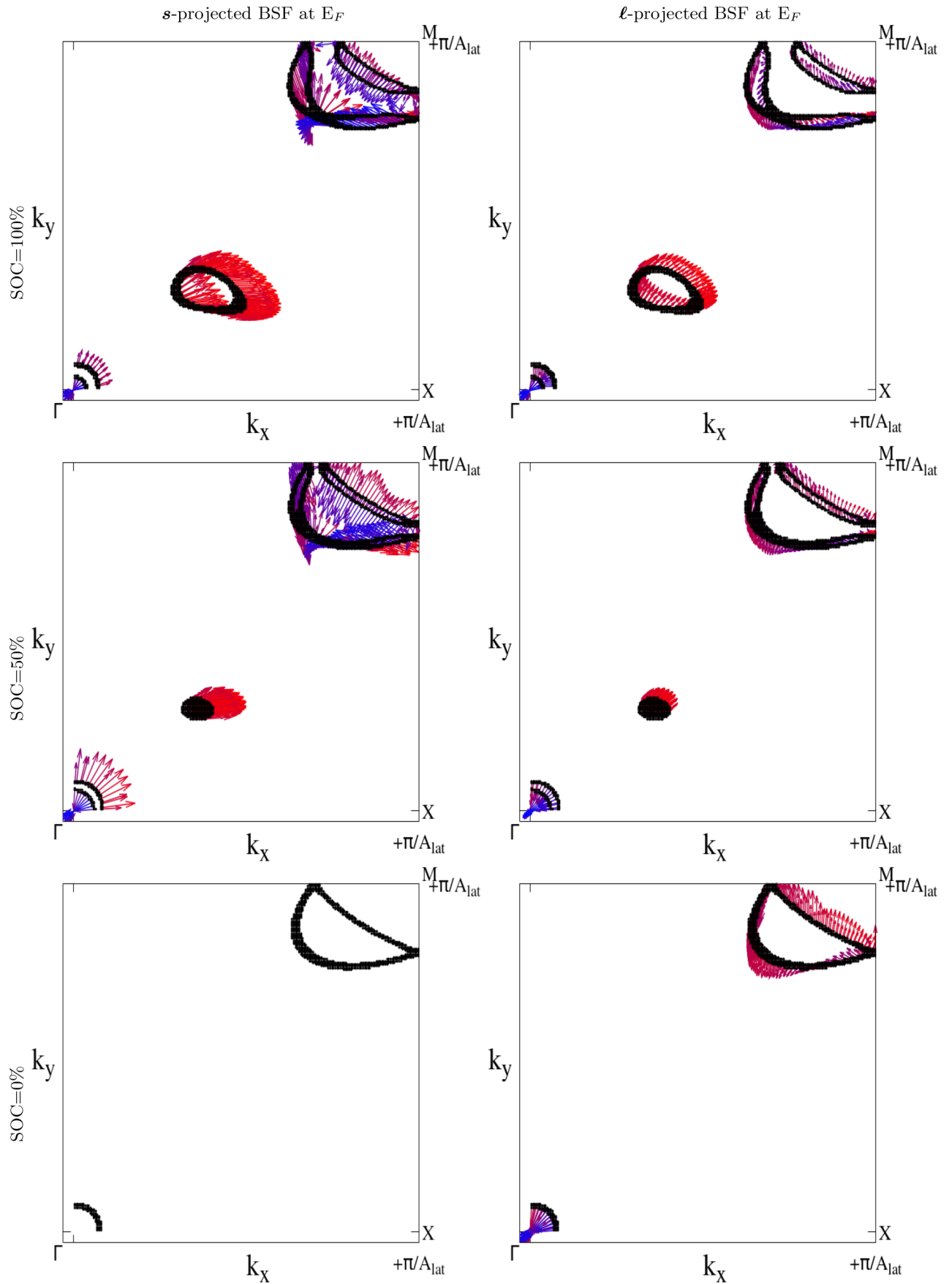


FIG. 4. Spin- (left) and orbital magnetic moment (right, scaled $2\times$ for better visibility)-projected BSF for AlPt as a function of artificial SOC scaling (top to bottom rows).

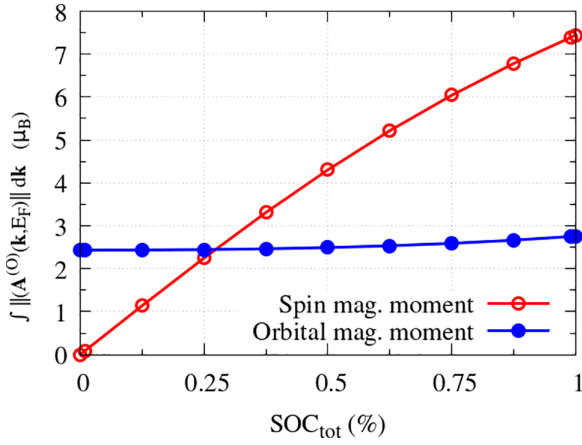


FIG. 5. Average magnitude of the spin (red empty circles) and of the orbital (blue filled circles) magnetic moment $\mathbf{k}$ textures in a AlPt unit cell as a function of artificial SOC scaling, from Eq. (2).

Γ point, i.e., $A^{(O)}(+\mathbf{k}, E_F) = -A^{(O)}(-\mathbf{k}, E_F)$ for $\hat{O} = \hat{s}$ or $\hat{\ell}$.

Integrating Eq. (1) across the whole Brillouin zone gives therefore net zero contributions to the spin and to the orbital magnetization at each energy. Repeating this over all valence bands confirms that indeed our DFT treatment assigns zero atomic magnetic moment for all materials of Table I. Compared to an antiferromagnet, this result holds also upon considering sublattice-resolved integrations. The above compensation takes place in a punctual fashion across $+\mathbf{k}$ and $-\mathbf{k}$, not just across different atoms, which would have in that case a finite exchange splitting, mutually compensating only across Wigner-Seitz cells.

Taking into consideration also the current density $\mathbf{j}$ and evaluating Eq. (3) confirms numerically that only the $\mu = \nu$, i.e., only the diagonal components of the spin and of the orbital Edelstein response tensors are nonzero, and that they are all equal, as a consequence of symmetries [38,39] fulfilled by all *Strukturbericht* B20 materials of Table I. In other words, a nonmagnetic group No. 198 lattice only allows an isotropic and longitudinal Edelstein response, with magnetization either parallel or antiparallel to the electric field, in whatever direction this is applied to bring the system out of equilibrium.

We expect the magnitude of this response to reflect the strength of spin and of orbital polarization of electronic states. As discussed in Sec. III A, both geometry and SOC magnitude play a crucial role in controlling this feature.

To further investigate the underlying mechanism, we evaluate the SOC energy $\xi_W(E_F)$ associated with atoms $W = A$ or B using the approach of Ref. [40] to isolate the corresponding contribution in terms of the gradient of the effective potential for either species. From the geometrical point of view, we focus our attention on the helical atomic arrangement of the two atomic species around the *Strukturbericht* B20 chiral axis (Sec. II). Their positions, projected on the orthogonal plane, forms an equilateral triangle with an inscribed circle, which would have zero radius in the absence of helicity, i.e., for a more symmetric lattice structure. Due to the compensated, antiparallel winding of the two atomic species, we examine

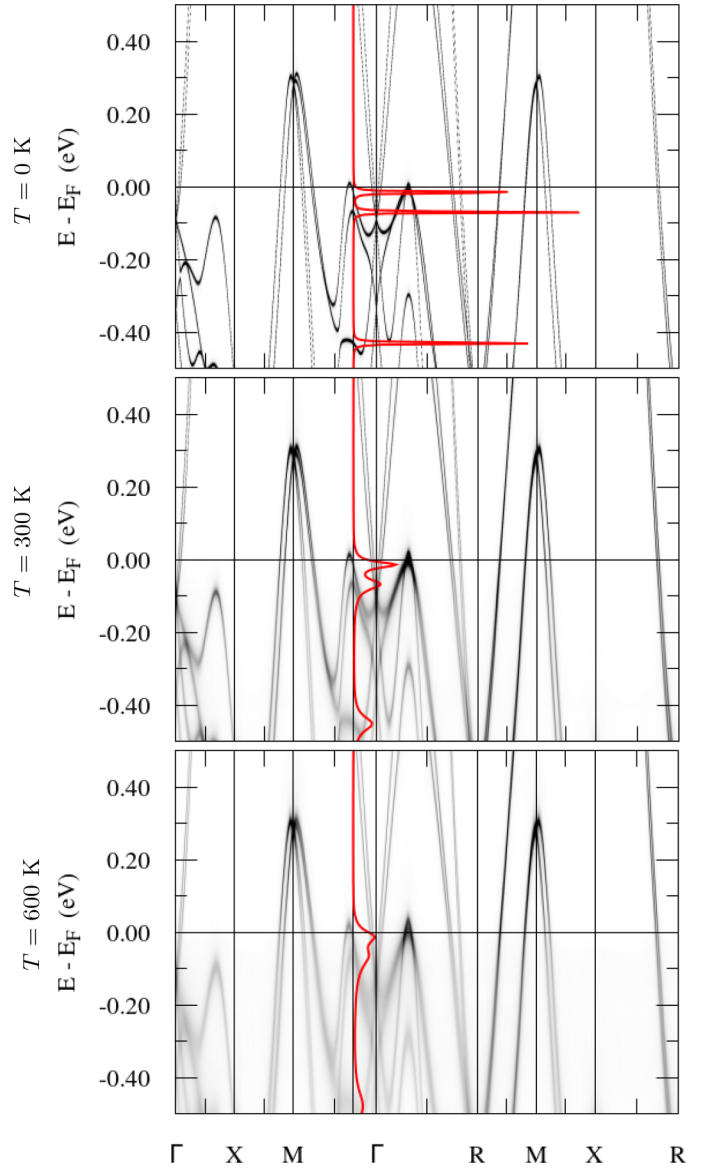


FIG. 6. Total BSEF of AlPt as a function of temperature. The intensity is also plotted as a function of energy alone, i.e., as a slice at a fixed $\mathbf{k}$ point, arbitrarily chosen between M and Γ (vertical red line, with a peak wherever a band is intercepted).

this feature across the compounds of Table I, adopting the convention of an opposite sign for the winding radius of species A or B.

Results from Eq. (3) show a fairly systematic, linear relationship between this estimate of the total Edelstein response, and a combination of the above two SOC and geometry-derived quantities (Fig. 8). Other geometrical measures for chirality, i.e., for the deviation of a specific B20 unit cell from a more symmetric lattice structure could also be adopted [4]. Finally, to study the influence of temperature on the representative example of AlPt, we deploy the more comprehensive but numerically demanding Kubo formulation for the Edelstein response of Eq. (4).

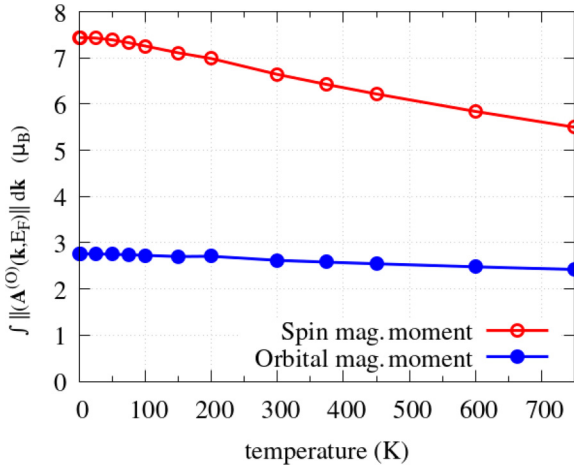


FIG. 7. Average length of the spin (red empty circles) and of the orbital (blue filled circles) magnetic moment $\mathbf{k}$ textures in AlPt as a function of temperature, from Eq. (2).

C. Temperature-dependent results for AlPt

We use for each temperature the same reconverged SCF-DFT solutions already used for the results of Fig. 6 and Fig. 7. Since in the low-temperature limit the Fermi-Dirac distribution $f_T(E) = 1/(e^{(E-E_F)/(k_B T)} + 1)$ progressively reduces to a Heaviside theta, with a Dirac delta as energy derivative, we consider here only the first, i.e., only the Fermi surface term of Eq. (4). Numerical tests confirm the negligible impact of the Fermi sea term for the particular material up to $T \leq 750$ K. We study in particular the diagonal terms of the 3×3 linear response transport tensors, that describe the response to an applied electric field in terms of charge, of spin, and of orbital magnetic moment (respectively, black, blue, and red points in Fig. 9). Other entries are zero in the particu-

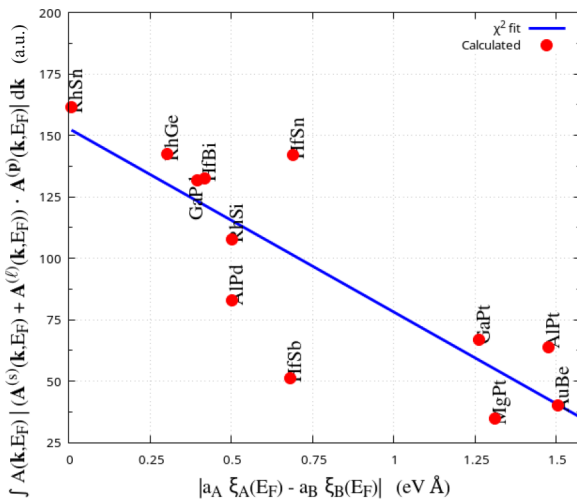


FIG. 8. Results from the Boltzmann-level estimate of total (i.e., spin and orbital) Edelstein response given by Eq. (3) for the B20 compounds of Table I. A least- χ^2 fit highlights distribution of numerical outcomes in linear fashion, with respect to a combination of atom-resolved winding radius a_A , a_B , and SOC magnitude at the Fermi level $\xi_A(E_F)$, $\xi_B(E_F)$ according to Ref. [40], see text.

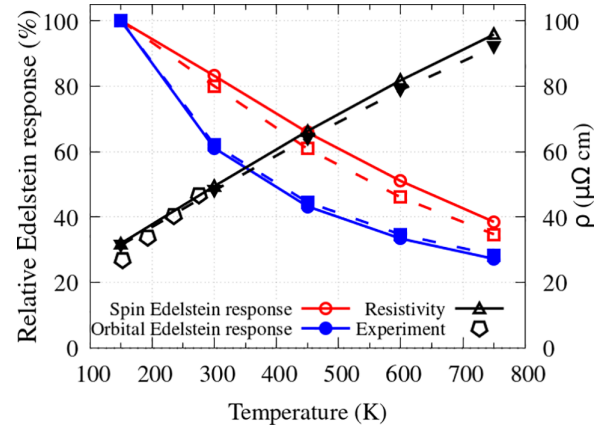


FIG. 9. Spin- (red empty points) and orbital (blue full points)-Edelstein response (left scale, in percentage of the $T \rightarrow 0$ K outcome), and electric resistivity (black points, right scale) vs temperature for AlPt. Results from Eq. (4) are given with (full lines) or without (dashed lines) disorder vertex corrections. Electrical conductivity measurements from Fig. 1(a) of Ref. [41] are also plotted (empty pentagons).

lar lattice geometry here under consideration [38]. Available measurements for electric resistivity [41] are in good agreement with calculations, which furthermore predict a nonzero but decreasing spin and the orbital Edelstein response for larger thermal disorder (Fig. 9). This trend is qualitatively consistent with the reduction in average magnitude for the spin and orbital magnetic moment $\mathbf{k}$ textures of Fig. 7. The Kubo formula, however, predicts a different dependence for the two components of magnetization in response to the applied electric field. While the spin-Edelstein response decreases linearly, the orbital Edelstein response goes to zero with a nonlinear and faster decay. In relative terms, in both cases there should still be more than 50% of the signal expected from $T = 0$ K calculation for an ideal, i.e., long-range ordered (LRO) single-domain crystal, even at a conventional room temperature of 300 K.

V. DISCUSSION

A. Spin and orbital magnetic moment $\vec{k}$ textures

1. Role of geometry

Spin-polarized ARPES experiments [24] offer some direct evidence for the radial magnetic moment $\mathbf{k}$ textures of Sec. III A. The study of such electronic structure features also assists in interpreting more complex transport properties, e.g., the Edelstein response of Sec. IV B and IV C.

Alike the case of noncentrosymmetric but nonchiral zincblende lattice geometry [42], spin-orbit splitting lifts the degeneracy of electronic states. It opens in particular an energy gap between bands, which have different spin and orbital magnetic polarization (Fig. 2 and Fig. 3).

A noncentrosymmetric lattice geometry leads to an orbital magnetic moment $\mathbf{k}$ texture. In the examined case of *Strukturbericht* B20 AlPt, the average magnitude of contributions to ℓ is finite, even for an artificially scaled-down SOC (Fig. 5). A similar outcome appears also upon artificially

arranging the same chemical elements in a *Strukturbericht* B3, i.e., zincblende unit cell. It is not present instead for the centrosymmetric case of *Strukturbericht* B1, i.e., rocksalt unit cell (Fig. 3), as a consequence of Kramers' theorem, i.e., of twofold degeneracy of the electronic Hamiltonian's eigenvalues for systems with spatial inversion (see also the Supplemental Material [43] for a model Hamiltonian derivation of this feature).

In the case of a *Strukturbericht* B3 unit cell, each of the two chemical constituents is arranged into a highly isotropic fcc sublattice, which would fulfill by itself inversion symmetry. In a group No. 198 representation of this B3, i.e., zincblende geometry (Table II), the atomic species A can be assigned to Wyckoff position 4a: (x, x, x) with $x = 0$. The other element B then lies at Wyckoff position 4a: (x', x', x') with $x' = \pm 0.25$. Changing the sign leaves the length of the spin and of the orbital magnetic moment contributions unchanged at each $\mathbf{k}$ point, but it inverts the direction of such vectors.

These two *Strukturbericht* B3 realizations remain, however, superimposable by simple 90° rotation around the central $\hat{z}$ axis. This is not the case for the *Strukturbericht* B20 examples from Table I. As noted in Sec. II, each A and B chemical constituent forms already by itself a winding atomic arrangement, antiparallel with respect to the other species. A swap in sign for both their Wyckoff positions 4a: (x, x, x) and 4a: (x', x', x') again inverts the sign of both $A^{(s)}(\mathbf{k}, E)$ and $A^{(l)}(\mathbf{k}, E)$ across the whole Brillouin zone.

The winding radius offers an intuitive but not unique measure of how much each compenetrated sublattice deviates from a higher-symmetry geometry [4]. When this radius is the same due to a $x = -x'$ offset across the two Wyckoff 4a positions, such as for materials such as HfSn (Table I), it is only the distinctiveness across the two chemical elements that generates the $\mathbf{k}$ textures in spin and orbital polarization. These would then vanish in the limit $A = B$ of equal occupancy for both sets of sublattices, which would be a realization of the higher-symmetry group No. 205 crystal structure. As further discussed in Sec. VB1 below, such geometrical considerations suggest the attempt reported in Fig. 8, to highlight how mutually antiparallel helical windings of the two A and B constituents contribute to the total Edelstein response through a difference, rather than a sum.

2. Effects of SOC and of thermal disorder

After fixing the lattice and the composition, numerical calculations suggest that the strength of SOC controls in linear fashion the average length of $A^{(s)}(\mathbf{k}, E)$ across the Brillouin zone, for both the physical B20 (Fig. 5) or for the artificial B3 (not shown here) AlPt unit cells. The average length of $A^{(l)}(\mathbf{k}, E)$ is instead hardly affected. In both cases, Brillouin zone integrations give zero atomic magnetic moments at equilibrium.

Before discussing how an applied electric field perturbation modifies this scenario and gives raise, for instance, to a finite Edelstein response (Sec. VB2), we examine how temperature can affect the above average length of spin and of orbital contributions across electronic bands intercepting the Fermi level. When the temperature increases, the progressive broadening of the total BSF is a general consequence of ran-

dom atomic displacements from equilibrium positions within the AAM (Fig. 6, red highlight). On the time scale of electrons hopping from site to site, much faster than the time needed for heavier atoms to move, the lattice is no longer periodic. The situation is well approximated by a positional alloy model with its corresponding disorder self-energy [29].

On the other hand, the distinct trends for $\hat{s}$ and $\hat{l}$ (Fig. 7) are more peculiar. As possible explanation, we recall how for the compounds from Table I SOC-split electronic states appear to have always antiparallel $A^{(s)}(\mathbf{k}, E_F)$ sign, while this is not always the case for $A^{(l)}(\mathbf{k}, E_F)$ (Fig. 4 top row, left vs right panels).

When higher temperature increases the FWHM of the BSF, the resulting mix of spectral weight leads therefore to partial cancellation of spin polarization. The average decrease is smaller for the orbital magnetic moment, for which the gradual filling of SOC-induced bands' splittings can mix states, which have the same $\hat{l}$ orientation (Sec. III A).

Ultimately both contributions persist fairly unaffected by finite temperature (Fig. 7). This can be compared with the different outlook of the rapid $(1 - T/T_c)^\beta$ reduction of average atomic magnetic moment in ferromagnets, upon approaching their critical temperature T_c . In the materials here under consideration, CISS effects originate instead, beside SOC, from the relative atomic positions. Their thermal shaking away from equilibrium lattice sites progressively reduces LRO. However chirality, or more generally lack of centrosymmetric invariance, are geometrical features that persist until uncorrelated displacement of individual atoms (i.e., simulated finite temperature within the AAM) become very large. For comparison, within the disordered local moment (DLM) description of finite temperature magnetism, the uncorrelated upside-down flip of single-site exchange splitting has a larger and more immediate impact on the electronic structure.

B. Edelstein response

1. Comparison across different materials

An externally applied electric field shifts spin- and orbital-polarized spectral weight across the Brillouin zone. This makes the spin and the orbital $\mathbf{k}$ textures no longer odd around the Γ point, breaking compensation. The Edelstein response then emerges, as first described in Sec. IV B, already in terms of an intraband and constant relaxation time treatment. The current density $\mathbf{j}$ quantifies how the electric field perturbation couples to electronic states at each $\mathbf{k}$ point. A magnetic response develops proportionally to the resulting unbalance in spin and in orbital magnetic moment contributions. Given the approximately radial character of these $\mathbf{k}$ textures (Fig. 4, top row), in contrast for instance with a tangential magnetic polarization of electronic states in the case Rashba effect, the spin and orbital response in AlPt and other *Strukturbericht* B20 materials are aligned rather than transverse with respect to the direction of an applied electric field perturbation. We numerically recover a longitudinal, isotropic response tensor, in agreement with symmetry considerations.

As noted in Sec. II, the *Strukturbericht* B20 geometry of materials from Table I is the result of two compenetrated lattices of atomic species A or B, arranged in antiparallel

chirality. Each of the two would produce already by itself an Edelstein response. Its magnitude and sign reflect the deviation of the helical atomic placement around the chiral axis, away from a centrosymmetric arrangement, (Sec. V A). From this originates the linear trend approximately fulfilled by the *Strukturbericht* B20 compounds here examined (Fig. 8).

This situation can be compared to the cases where it is a noncollinear ordering of atomic magnetic moments to break spatial inversion symmetry. We can consider the example of Mn_3Ge in *Strukturbericht* L1₂, i.e., with a cubic Cu_3Au -like unit cell [44] as reference. Adopting an artificial noncollinear magnetic order with the Mn moments arranged in coplanar, equilateral triangular fashion orthogonally to the [111] cubic body diagonal, a finite component of the atomic orbital and spin magnetic moment gets generated along such direction. The other two Cartesian components of s and ℓ remain instead compensated to zero upon adding up across the three transition metal atoms. In such example as well the magnitude of the effect scales with the SOC strength. It also depends in sign, similar to the case of *Strukturbericht* B20 or B3 materials, on how inversion symmetry has been broken.

The necessary noncollinear magnetic order may, however, not be the ground state, or may not remain stable up to high enough temperature. On the other hand, all *Strukturbericht* B20 materials from Table I are already experimentally reported as synthesized with the desired lattice structure. Atomic positions fulfill the necessary geometrical condition already in the absence of any atomic magnetic moment. The robustness for $T > 0$ K of the Edelstein response from Kubo's formula results for the example case of *Strukturbericht* B20 AlPt is discussed below.

2. Temperature dependence in the AlPt example

The approach of Eq. (4) is more comprehensive but numerically demanding than the Boltzmann approximation of Sec. V B 1. As a basic benchmark, we also compare its predictions for electrical resistivity with available measurements up to 300 K from Ref. [41]. Although included for all the results of Fig. 9, numerical tests suggest that neglecting disorder vertex corrections does not change much the electric resistivity as a function of thermal deviations from LRO. In contrast to the case of an actual alloy, the on-average periodic lattice does not mix chemical elements with very different orbitals, such as Al and Pt. It keeps each atom within its repeating Wigner-Seitz region, with just a random RMS displacement proportional to the finite temperature. This does not change very much the effective phase shift of the electronic wave function [45]. The BSF gets broadened, but separate peaks associated with distinct bands remain recognizable (Fig. 6). In terms of resistivity, the numerical scheme of Eq. (4) gives good agreement with expectation of a metallic outlook, approaching experimental reports even in absolute value, although with a slightly different slope.

The slightly larger spread for the spin than for the orbital Edelstein response, upon including or not including disorder vertex corrections, appears in line with the different sensitivity to finite temperature of $||\mathbf{A}^{(s)}(\mathbf{k}, E_F)||$ and of $||\mathbf{A}^{(\ell)}(\mathbf{k}, E_F)||$ from Eq. (2). Upon examining numerical outcome of Eq. (4) also with or without the second, i.e., Fermi sea term, we find

that this plays a negligible role, even up to fairly elevated temperature. The outcome is not unusual for longitudinal response function in generalized linear response transport [45]. Other transverse quantities such as the anomalous Hall conductivity or the spin anomalous Hall conductivity can be generally more sensitive, with large mutual cancellation between Fermi surface and Fermi sea terms in case of disorder. Symmetry considerations [38] lead, however, to only diagonal nonzero entries in the response tensors examined here for the materials of Table I.

When thermal disorder increases, both components of the Edelstein response get quenched. The decay is faster in particular for the orbital term (Fig. 9, blue full symbols). In the case of the spin term, an almost linear decay rate remains qualitatively confirmed as in the cruder estimate based on Boltzmann-like extrapolation of the trends from Fig. 7. The orbital Edelstein response would appear instead rapidly reduced up to room temperature, but then tapering off toward a finite asymptotic value.

VI. CONCLUSIONS

We have numerically investigated how some chirality induced spin and orbital selectivity effects emerge within the electronic structure of nonmagnetic chiral crystals with *Strukturbericht* B20 and binary AB composition. Focusing in particular on the prototypical AlPt example, we obtain approximately radial spin and orbital magnetic moment $\mathbf{k}$ textures near the Fermi level, in qualitative agreement with available ARPES measurements [24]. The roles of SOC and of the noncentrosymmetric (and furthermore chiral) unit cell geometry in determining this basic feature are highlighted. We also explore its robustness with respect to finite-temperature disorder.

An externally applied electric field should produce a longitudinal Edelstein response due to lifted compensation of the above $\mathbf{k}$ -resolved contributions to spin and orbital magnetic moments across the Brillouin zone. Approximated Boltzmann transport results suggest that the magnitude of this effect reflects how *Strukturbericht* B20 materials contain two compensated, antiparallel helical windings of A and B atoms along the chiral axis.

Finally, we deploy a more comprehensive Kubo approach again in the prototypical case of AlPt. Trends of temperature dependence for electric resistivity appear in agreement with available experiments. Calculations predict that the spin and the orbital Edelstein response should maintain a fair degree of robustness against thermal disorder.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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