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# Unconventional metallic magnetism in $LaCrSb_3$

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**Abstract**

The compound $LaCrSb_3$ is a non-collinear ferromagnet with a spin reorientation at $T_{sr} \approx 95$ K. Coexistence of itinerant and localized spins at one and the same Cr site was suggested to explain the experimental findings. Here, arguments against this model are provided on the basis of electronic structure calculations and re-considered experimental information. An alternative model is proposed.


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The field of metallic magnetism in bulk compounds is still a rich source of surprises. As an example, results on the compound $LaCrSb_3$ have recently been reported that led the authors to speculate about a possible coexistence of itinerant and localized spins belonging to one and the same Cr site [1]. The present contribution aims at providing arguments against this hypothesis on the basis of electronic structure calculations and re-consideration of experimental data from Ref. [1].

Fig. 1 shows the orthorhombic structure of $LaCrSb_3$ with the (distorted) octahedral coordination of Cr indicated. The system is ferromagnetic below $T_C \approx 126$ K with an ordered moment of about 1.8 $\mu_B$ per Cr atom along the *b*-direction and a smaller antiferromagnetic component ($\approx 0.5$ $\mu_B$). Both components add to a canted arrangement ($\approx 1.9$ $\mu_B$), where the angle between successive moments and crystallographic *b*-direction amounts to $\pm 18°$.

An astonishing finding is the abrupt spin reorientation at $T_{sr} \approx 95$ K. At this temperature, the moments switch into the *c*-direction while preserving their canting within experimental error bounds. Such a behavior is commonly observed in compounds with competing spin anisotropies from different Wyckoff positions. For example, rare earth—transition metal compounds may exhibit crystal field anisotropy at the rare earth site with a strong temperature dependence that competes with a weakly temperature-dependent itinerant contribution of the transition metal. In the present case, however, there is only one magnetic site existing. On this basis, coexistence of itinerant and localized Cr spins was postulated to arise from anisotropic hybridization [1].

To check this idea, calculations in local spin density approximation [2] have been carried out in the present work. The full-potential local-orbital (FPLO) method [3] was employed with the following states included in the valence basis: Cr-3spd and 4sp; La-4f, 5spd, and 6sp; Sb-4spd and 5sp; **k**-space integration was performed using 500 points in the irreducible part of the Brillouin zone; experimental structure parameters have been used. Assuming a strictly ferromagnetic arrangement, a spin moment of 2.1 $\mu_B$ per formula unit was found in reasonable agreement with the experiment.

It should be noted that the present calculation relies on the assumption of completely itinerant Cr-3d states. The assumption can be supported a posteriori by

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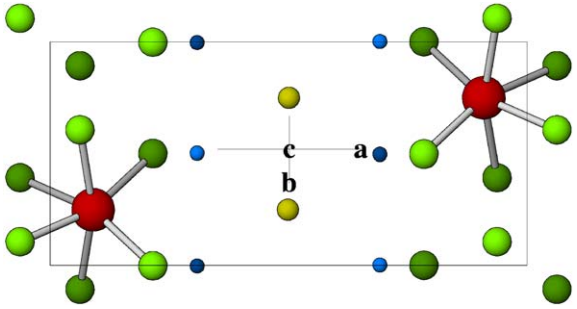


Fig. 1. Orthorhombic structure of $LaCrSb_3$, view onto the $a$–$b$-plane. The coordination of Cr inside Sb-octahedra is indicated.

checking band dispersions and projected densities of states (DOS). While flat bands of predominating Cr-3d($m_l = \pm 1$)-character exist in a part of the Brillouin zone (not shown), the related $m_l$-projected DOS discloses a total dispersion of about 3 eV (Fig. 2) in the majority spin band. This value exceeds the magnitude of screened intra-atomic Coulomb interaction on the Cr-3d states ($\simeq 2$ eV) and thus does not give a clue for localized behavior. All other $m_l$-projected DOS show a similar dispersion, disproving the assumption of anisotropic hybridization. An octahedral coordination, though slightly distorted, should indeed rather result in a more or less isotropic hybridization.

How could the spin reorientation be understood if the previously suggested model would not be applicable? One possibility would be a competition between itinerant and dipole anisotropies that exhibit different dependencies on the lattice geometry, being subject to a magnetostrictive temperature dependence close to $T_C$. In many systems, the bulk dipole anisotropy is much smaller than the itinerant anisotropy. Here, the former can be considerable due to the low symmetry; the latter will be quite small, since the almost half-filled Cr-3d shell shows only marginal spin–orbit effects. This idea is supported by fully relativistic [4] FPLO calculations yielding an orbital moment of only 0.003 $\mu_B$ per Cr atom.

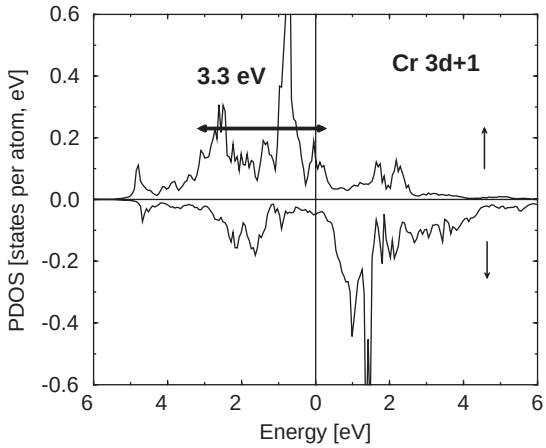


Fig. 2. Orbital-projected density of states: Cr-3d, $m_l = 1$.

Finally, there is no lattice anomaly observed at the spin reorientation [1]. This fact also points to itinerant magnetism with marginal spin–orbit coupling. Magneto-crystalline anisotropy by localized magnetic moments arises from multi-polar interactions of non-spherical electron densities with the crystal field. A reorientation would be connected with considerable magnetostriction in this case.

Summarizing, arguments have been provided in favor of completely itinerant magnetism in $LaCrSb_3$. A related model for the observed spin reorientation is suggested.

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