DFT study for novel noncollinear magnets

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Noncollinear magnetism (NCM) has been a very active research field. It is known that the emergence of NCM may provide unusual physical properties such as anomalous transport propertiesin metals and ferroelectric polarizationin insulators. NCM includes the magnetic skyrmions and the chiral spin solitons, which are extensively studied now.

In this talk we will pick up two materials exhibiting NCM, $PdCrO_2$ and $Cr(NbS_2)_3$, and will see how important the theoretical study based on the density functional theory (DFT) is to understand their physical properties.

$PdCrO_2$[1] crystallizes in the delafossite structure, which is made of alternating stack of triangular layers of Pd and Cr. The Cr^{3+} localized moments (S=3/2) show antiferromagnetic ordering at T_N=37.5K, forming 120 degree noncollinear spin structure.Due to the Pd 4d electrons it shows metallic conductivity bearing strong two-dimensional anisotropy. At temperatures lower than T_N, unusual Hall resistivity was measured[2]. It displays very strong dependence on the temperature and external magnetic field. Its microscopic mechanism has been unclear for a while. We carried out first-principles DFT calculations and measurements of de Haas-van Alphen oscillations[3]. We found thatthe Fermi surface reconstruction and the magnetic breakdown at high fields play essential role in the Hall resistivity.

The layered intercalated compound $Cr(NbS_2)_3$ has been attracting extensive interest. The Cr local moments, whose directions are confined in the *c*-plane, show a spiral magnetic structure of very long periodicity (L=48nm) with a handedness being in a one-to-one correspondence to the crystal chirality. It has been theoretically predicted [4] and experimentally confirmed [5] that a small external magnetic field perpendicular to the *c*-axis can lead to an emergence of a noble chiral spin soliton lattice. In accord with this intriguing soliton formation, an anomaly in the electrical conductivity has also been observed [6]. In the talk, we will present our DFT calculations and discuss the crystal chirality, fundamental electronic structure, magnetocrystalline anisotropy, and various magnetic interactions between the Cr moments.

References

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