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Magnetic and transport properties of NbS2 intercalated by 3d-elements

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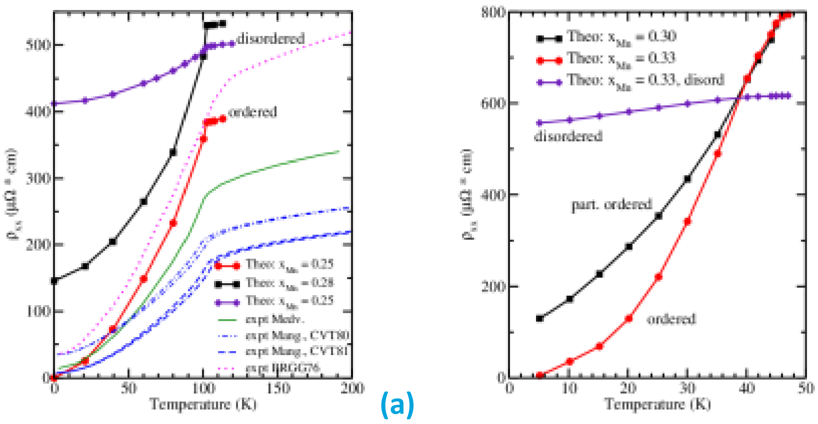
The magnetic and transport properties of the 2H-NbS_2 compound intercalated by 3d-elements, Cr and Mn, have been investigated based on first-principles calculations of the electronic structure by means of the Korringa-Kohn-Rostoker (KKR) method. We focus on the systems with 33% and 25% of intercalation which allow the formation of ordered phases characterized by $\sqrt{3} \times \sqrt{3}$ and 2×2 in-plane arrangements of the magnetic atoms, respectively. The calculations have been performed both for stoichiometric composition as well as taking into account small deviations from stoichiometry to investigate its impact on the magnetic and transport properties. The ground state magnetic structure as well as finite temperature magnetic properties have been studied via Monte Carlo simulations using exchange coupling parameters calculated from first principles. In the case of 33%-intercalation, we discuss the impact of the Dzyaloshinskii-Moriya interaction responsible for the formation of a helimagnetic structure in the system, which can be transformed into the so-called chiral soliton lattice in the presence of an external magnetic field. This property allows to tune the magneto-resistance of the material by varying the strength of the magnetic field.

The Kubo-Greenwood linear response formalism was used in addition to calculate the temperature dependent electrical resistivities of the systems (see Figure 1). The investigations have been performed both for ambient pressure as well the increasing pressure. The first-principles calculations in combination with Monte Carlo simulation demonstrate in the case of $Mn_{0.25}MbS_2$ a transition from the FM to AFM state upon an increasing pressure. Based on these results, calculations of the magneto-resistance (MR) for different pressures show a good agreement with the experimental results that allows us to make conclusions about the origin of different behavior of MR at different pressures.



(a) (b)

Figure 1: Electrical resistivity as a function of temperature calculated for $Mn_{0.25}NbS_2$ (a) and $Mn_{0.33}NbS_2$ (b).