Study of complex magnetic states and phase transitions with Lichtenstein method

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The first-principle calculations of the magnetic exchange constants using the magnetic force theorem (so-called Lichtenstein method) is allowed to investigate the microscopic mechanism of the complex magnetic phase formations and phase transitions. We illustrate this using as examples the complex non-collinear ground state in NpCoGe compound, predictions of novel type of meta-magnetic transition in (Mn,Cr)Au_2 alloy and evaluation of magnetic compensation temperature in $DyCo_5$ compound. On the basis of Lichtenstein method the state-of-the-art ab-initio calculations one may predict a novel materials with superior magnetic properties. The experimental invention of high-temperature antiferromagnets Mn_2Au (T_{Neel} > 1200K), which for over two decade has been regarded as non-magnetic compound, has been initiated by the theoretical predictions on the basis of Lichtenstein method. Another example is the prediction of the one-dimensional metallic ferromagnetism in MnB_4 will be discussed.