

**Title:**

First-principles investigation of electronic structures and transport properties of new half-metallic materials

**Abstract:**

Half-metallic system, i.e. metallic in one spin direction of electrons but insulating in the other spin direction, are one of the key materials in spintronics (spin-electronics). The purpose of the present study is to design new half-metallic systems that are chemically and magnetically stable, easy to fabricate, and opening up the possibilities for new spintronics devices. To this end, in the first step, the chemical stability and phase diagram of the diluted magnetic semiconductors (DMSs) are discussed on the basis of a newly developed method calculating atomic pair interactions starting from the completely disordered states. As the second step, a new type of ferrimagnetic half-metals, namely transition metal doped manganese chalcogenides (Mn, TM)X (TM=transition metal elements, X=chalcogen) is designed. In order to further widen the applicability of this type of the half-metallic systems, spin-compensated ferrimagnetic half-metals (so-called half-metallic antiferromagnets) are designed starting from the above ferrimagnetic systems. Thus designed intermetallic compounds (AB)X<sub>2</sub> have significant features of half-metallic antiferromagnets. Moreover, they are chemically stable and the magnetic transition temperature is relatively high. In fact, some of them have a Néel temperature that well exceeds 1000K. As the final step, the DC conductivity of these new half-metallic systems as well as the superstructure simulating GMR/TMR structures composed of these systems are investigated using Kubo-Greenwood formula. The results show that those systems function as the spintronics materials if used as components of GMR/TMR and magnetic random memory cells. Through the above study, the first-principles calculation based on the KKR-CPA method in the framework of local density approximation and its extension of the density functional method is used.