

Hfi/nqi 2007

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" Hyperfine interactions of half-metallic diluted antiferromagnetic semiconductors (p. 21-22) Abstract

Half-metallic diluted antiferromagnetic semiconductors (HM-AF-DMSs) are magnetic materials that are half-metallic and yet do not exhibit magnetization. The remarkable features of these materials and the possible experimental verifications for determining whether or not a material is a HM-AF-DMS by the detection of hyperfine interactions are discussed on the basis of the first-principles calculations of the electronic structure. Keywords Diluted magnetic semiconductor- Half-metal- Hyperfine field 1 Introduction

Spin-electronics (or spintronics), which is a technology that employs the spin state of electrons and provides a new degree of freedom for storing information, is among the most challenging strategies in the development of electronic devices. One of the key issues in spintronics is half-metallicity, i.e., the property of metallicity in one spin state (say, spin-up) of electrons but insulating in the opposite spin state (spin-down). Although all the half-metals known thus far are ferromagnetic, half-metallicity is not restricted to ferromagnets. The realization of half-metallic antiferromagnets (more precisely, half-metallic compensated ferrimagnets), which are half-metallic and yet do not exhibit magnetization, might be possible and these materials are expected to be used as a new type of spintronics materials. Since the past few years, several diluted ferromagnetic semiconductors (DMSs) have been theoretically designed (computational materials design). In these DMSs, local magnetic states are formed at the impurity bands that appear in a semiconductor gap. Similarly, half-metallic antiferromagnetic DMSs (HM-AF-DMSs) can be realized for the impurity bands in the gap. We have proposed such a new type of half-metallic antiferromagnets and named them half-metallic diluted antiferromagnetic semiconductors [2]. In order to realize such systems, we have to introduce at least two different types of magnetic ions into nonmagnetic hosts . In DMSs that contains two types of magnetic ions among which the electron occupation of one type of ion is more than half-filling and that of the other is less than half-filling, the local magnetic moments of the two ions can be coupled anti-parallel to each other. In most cases, such an anti-parallel coupling is more stable than the parallel coupling and also exhibits half-metallicity. Since half-metallic antiferromagnets do not exhibit magnetization, and moreover since they are disordered and diluted

systems, it could be rather difficult to observe their characteristics. In this study, we propose methods to verify whether or not a material is a half-metallic antiferromagnetic semiconductor. Magnetic circular dichroism (MCD) can be employed as one of the methods for detecting half-metallic antiferromagnetism. Another possible method for the verification of half-metallic antiferromagnetism is the detection of hyperfine interactions. In order to employ the latter method, we have performed the first-principles calculations of the electronic structure and hyperfine fields of half-metallic antiferromagnetic semiconductors. Although several examples indicate that HM-AF materials might be stable, the fabrications of materials based on group II-VI compounds appear to be relatively easy. As an example of such semiconductors, we consider $(\text{Cd}_{1-2x}\text{Cr}_x\text{Fe}_x)\text{Te}$ and discuss its hyperfine interactions." Hyperfine interactions of half-metallic diluted antiferromagnetic semiconductors (p. 21-22) Abstract Half-metallic diluted antiferromagnetic semiconductors (HM-AF-DMSs) are magnetic materials that are half-metallic and yet do not exhibit magnetization. The remarkable features of these materials and the possible experimental verifications for determining whether or not a material is a HM-AF-DMS by the detection of hyperfine interactions are discussed on the basis of the first-principles calculations of the electronic structure. Keywords Diluted magnetic semiconductor- Half-metal- Hyperfine field 1 Introduction Spin-electronics (or spintronics), which is a technology that employs the spin state of electrons and provides a new degree of freedom for storing information, is among the most challenging strategies in the development of electronic devices. One of the key issues in spintronics is half-metallicity, i.e., the property of metallicity in one spin state (say, spin-up) of electrons but insulating in the opposite spin state (spin-down). Although all the half-metals known thus far are ferromagnetic, half-metallicity is not restricted to ferromagnets. The realization of half-metallic antiferromagnets (more precisely, half-metallic compensated ferrimagnets), which are half-metallic and yet do not exhibit magnetization, might be possible and these materials are expected to be used as a new type of spintronics materials. Since the past few years, several diluted ferromagnetic semiconductors (DMSs) have been theoretically designed (computational materials design). In these DMSs, local magnetic states are formed at the impurity bands that appear in a semiconductor gap. Similarly, half-metallic antiferromagnetic DMSs (HM-AF-DMSs) can be realized for the impurity bands in the gap. We have proposed such a new type of half-metallic antiferromagnets and named them half-metallic diluted antiferromagnetic semiconductors [2]. In order to realize such systems, we have to introduce at least two different types of magnetic ions into nonmagnetic

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