GW study of half-metallic electronic structure of La$_{0.7}$Sr$_{0.3}$MnO$_3$

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Abstract

Half-metallic systems will be quite useful in future spin electronics. The GW approximation is employed to study electronic structure of half-metallic La$_{0.7}$Sr$_{0.3}$MnO$_3$, to show that the lowest quasiparticle energy of the unoccupied minority spin states is far above the Fermi energy compared to that in the LSDA. As a bulk, this system is predicted to be a fully spin-polarized half-metallic ferromagnet.

Key words: GW approximation; colossal-magnetoresistive manganites; half-metals

1. Introduction

Half-metallic systems\cite{1} attract much attention for possible applications to future spin electronics. A lot of works are executed to find out promising materials both in experiments and theories. Among them, La$_{0.7}$Sr$_{0.3}$MnO$_3$ is a material in dispute. The point is the degree of the spin polarization, which is important for device performance. But the experimental values of the spin polarization varies from 35% to 100%\cite{2}.

In the LSDA, this system is calculated to be a spin-polarized half-metal, but has non-zero density of states in the minority spin component as well as the majority spin component.\cite{3} However it is well known that the LSDA has difficulties in describing excited states: The LSDA underestimates band gaps in semiconductors and insulators. The GW approximation\cite{4} is a method which takes account of electron correlations within the RPA to give larger band gaps than those in the LSDA in most cases. In general, the calculated GW band gaps are in good agreement with the experimental ones.

In this study, GW quasiparticle energies are calculated to theoretically clarify electronic structure of La$_{0.7}$Sr$_{0.3}$MnO$_3$ including electron-electron correlations beyond the LSDA treatment. It is shown that the lowest energy of the unoccupied minority spin state is far above the Fermi energy compared to that in the LSDA. As a bulk, this system is predicted to be a fully-polarized half-metal in the first-principles calculation. This is the first study for the half-metallic system in the GW approximation.

2. Method of the Calculation and Results

In the GW approximation, quasiparticle energy $E_{kn}$ is calculated as

\[ E_{kn} = \epsilon_{kn}^{\text{LDA}} + \left( \langle \psi_{kn}^{\text{LDA}} | \Sigma(E_{kn}) - V_{xc} | \psi_{kn}^{\text{LDA}} \rangle \right) \]

where $\epsilon_{kn}^{\text{LDA}}$ and $| \psi_{kn}^{\text{LDA}} \rangle$ are the $n$th energy level and wave function at wave number $k$. They are given in the LMTO-ASA in the LSDA. $\Sigma(E)$ is the self-energy in the RPA and $V_{xc}$ is the LSDA exchange-correlation potential. The virtual crystal approximation\cite{5} is employed to simulate "Sr" doping to LaMnO$_3$. This is
the Fermi level crosses the majority spin Mn particle energies are shown in Fig. 1. [6] In the LSDA, gen 2 68%, as the additional energy splitting between oxy-
tation, these states are pushed up by about 2 eV above the Fermi level. Besides, the oxygen 2p band is shifted down that additionally increases the bang gap in the minority spin channel. The electron-electron correlations also reduces the band widths. So, the valence majority spin Mn eg band is shrunk by almost 50%. The conduction minority spin Mn t2g band is shrunk by 68%, as the additional energy splitting between oxygen 2p and Mn t2g levels suppresses the hybridization between these two states. Hence, we conclude that the system is a fully spin-polarized half-metallic ferromagnet, at least on the level of virtual crystal approxima-
tion for the analysis of magnetic phase diagram of La$_{1-x}$Sr$_x$MnO$_3$, which can be analyzed in terms of the Mn eg bandwidth (w) and the intra-atomic exchange splitting at the Mn sites ($\Delta_{rmex}$). [8] According to the GW calculations, w becomes smaller (in comparison with the LSDA), while $\Delta_{rmex}$ becomes larger due to the additional upward shift of the minority spin Mn t2g and Mn eg states. Therefore, the ratio w/$\Delta_{rmex}$ will further decrease in comparison with LSDA calculations. It will additionally stabilize the ferromagnetic phase for $x$=0.3 and justify the applicability of the double exchange limit, w/$\Delta_{rmex}$→0 for the analysis of other antiferromagnetic structures which typically appear for larger x.

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**References**


[5] Striktly speaking, the virtual crystal approximation can be applied only to La$_{1-x}$Ba$_x$MnO$_3$, and corresponds to the replacement of (La,Ba) sites by pseudatoms with the fractional atomic number $Z=57−x$. However, the exact chemical origin of the cation atoms seems to have only small effect on the electronic properties of perovskite manganites, and once the crystal structure is fixed, the alloys of the type (La,Ca), (La,Sr), and (La,Ba) exhibit very similar behavior.[8]

[6] The system is assumed to be cubic with the lattice parameter of 7.32 a.u. The mesh of 8×8×8 k-points is used both in LSDA and GW calculations.
