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Jahn-Teller effect and many-body correlation effect in $LaMnO_3$

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Effects of the Jahn-Teller (JT) distortion and the strong electron-electron correlation on the electronic structure of perovskite oxides $LaMnO_3$ are studied by using the linear muffin-tin orbital method. Results show that the Jahn-Teller distortion has evident influence on the electronic structure and its influence varies with different magnetic configurations. On the other hand, the effect of strong electron-electron correlation depends on crystal structures. For distorted $LaMnO_3$ structure, the strong correlation affects the density of states and the band structure lightly, while for undistorted structure, its effect is much stronger. Our calculations indicate that the effect of Jahn-Teller distortion is more pronounced than that of strong electron-electron correlation in $LaMnO_3$ but the latter is important for calculation of total energy. To get the correct ground state as experiments reported for $LaMnO_3$, it is necessary to take the Jahn-Teller distortion, the electron-electron correlation, and antiferromagnetic ordering into consideration simultaneously.

I. INTRODUCTION

In recent years, doped manganites systems such as $La_{1-x}A_xMnO_3$ ($A=$Ca, Ba, Sr, etc.) have attracted great attention due to their colossal magnetoresistance (CMR).[1,2] In these compounds, the trivalent La^{3+} ions are partially substituted by divalent A^{2+} ions, leading to the coexistence of mixed-valence Mn^{3+}/Mn^{4+}. Earlier a double exchange mechanism was proposed to explain the observed CMR phenomena.[3–5] However, recent studies indicate that the double exchange model alone cannot explain the existing experimental data,[6] and one must take the Jahn-Teller effects into account. In addition to the Jahn-Teller distortion, photoemission data also indicated that the electron-electron correlation effect with a value of $U=7.5$ eV for the Coulomb repulsion could be important.[7–9]

Experimentally it is observed that the undoped $LaMnO_3$ ($x=0$) is an A type antiferromagnetic insulator, i.e., the magnetic moments of Mn ions are aligned in the ab plane and antialigned between layers along the c axis.[10] It is also observed that $LaMnO_3$ is strongly distorted from its ideal perovskite structure to an orthorhombic $Pnma$ structure.[11] Early theoretical work focused on the undistorted perovskite structure and it was found that the usual local (spin) density approximation (LDA or LSDA) can not produce correct ground state for $LaMnO_3$.[12] The LDA or the LSDA calculations gave a metallic rather than an insulating ground state, in contrast to experiments. To overcome such difficulty, the effect of structural distortion and the effect of electron-electron correlation have been taken into consideration in the first-principle calculations by several groups. Pickett and Singh[13] have used the linearized augmented plane-wave (LAPW) method for the distorted $LaMnO_3$ caused by the Jahn-Teller effect and obtained a gap of 0.12 eV for the A-type antiferromagnet. It seems that the LSDA itself worked well to account for the antiferromagnetic insulating ground state after including the Jahn-Teller distortion. In their band studies of perovskite $LaMO_3$ ($M=$Mn, Fe, Co, Ni), Sarma *et al.*[14] also found that the Jahn-Teller distortion around Mn ions was important to account for a stable A-type antiferromagnetic structure, which is quite different from the other three compounds ($M=$Fe, Co, Ni). They also made the point that the electron-electron correlation is unimportant due to relative large hopping parameter t and large screening effect. Furthermore, work by Satpathy *et al.*[15] indicated that the distortion of the basal-plane mode was essential for the insulating gap within the LDA scheme. They have also applied the so-called LDA$+U$ approaches, in which the on-site Coulomb interaction was implemented in the ordinary LDA frame, to their linear muffin-tin orbital (LMTO) calculations for $LaMnO_3$ as well as $CaMnO_3$. In their work, the on-site Coulomb U and the exchange coupling J were chosen to be 10.1 and 0.88 eV for Mn ions in $LaMnO_3$, 10.0 and 0.86 eV for Mn ions in $CaMnO_3$, respectively. These large values of U and J, obtained from ''constrained'' LDA calculations, implied a strong correlation effect. They also reported that the variance of the valence-band spectra caused by LDA$+U$ correction was in agreement with experiments, but the obtained magnetic moments of Mn ions were overestimated in their calculations. In addition, Soloyev *et al.*[16] reported their calculations for $LaMO_3$ ($M=$Ti-Cu) and showed that the correlation correction was significant for Ti, V, Co, but less important for Mn.

Thus, previous theoretical studies of $LaMnO_3$ seem to indicate that once the structural distortion is taken into account, LSDA may work well to describe the electronic struc-

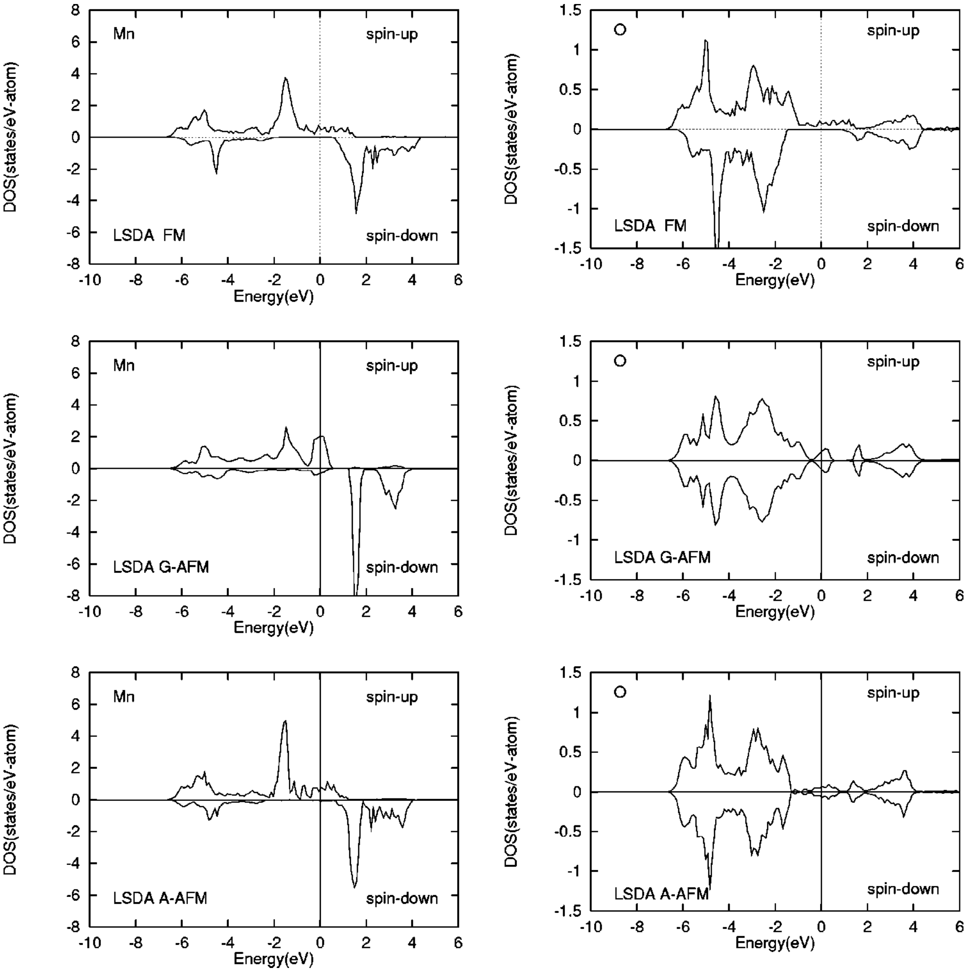


FIG. 1. Partial DOS for Mn and O of undistorted $LaMnO_3$ with three magnetic orders: FM, G-AFM, and A-AFM.

ture. The insulating ground state of $LaMnO_3$ is predicted correctly and the calculated total energy of the distorted A-type antiferromagnetic configuration is lower than that of the undistorted one. However, as to the question that whether $LaMnO_3$ is a strong correlated system, there seem to have two different opinions. In the view of Satpathy *et al.*,[15] the obtained large values of U and J from the ''constrained'' LDA calculations and the changes in one-electron spectra introduced by the LDA$+U$ correction suggested that the many-body interaction was strong in $LaMnO_3$. On the other hand, Pickett and Singh in their detailed studies of $La_{1-x}Ca_xMnO_3$ systems indicated that the failure of the LSDA method generally occurred towards the right end of the $3d$ transition-metal series, while for Mn which is in the middle of $3d$ series, no strong correlation interaction would be expected.

Recently, the phase diagram of $R_{1-x}A_xMnO_3$ (R $=$La, Pr, Nd, Sm; $A=$Ca, Sr, Ba) doped manganites was studied by several groups.[17–20] In their works, the competition among the ferromagnetic double exchange, the antiferromagnetic superexchange, the Jahn-Teller effect, the orbital correlation, as well as the electron-electron correlation were considered altogether. In the case of end point of $LaMnO_3$, Kugel and Khomsii pointed out that the observed orthorhombic distortion with $c<a$ cannot result from orbital ordering only and it is not obvious that the A-AFM phase is the most stable one. The cooperative Jahn-Teller effect could be a driving mechanism for orbital ordering which in turn controls the magnetic interactions. Maezono *et al.*[20] pointed out that the electron correlation remain strong even in the metallic state of doped manganites. The role of the JT distortion in this undoped case is also studied. They found that the global features of the phase diagram can be understood in terms of the superexchange and double exchange interactions. The electron correlation induces an orbital polarization which will affect the interactions. The JT distortion modifies the phase boundary between FM spin and AFM spin configuration then.

Therefore it is an important question that whether $LaMnO_3$, including $La_{1-x}A_xMnO_3$, is a strong correlated system. It is worth the effort to address this question in order to have a better understandings of this parent compound of CMR materials. In this work, we have performed the first-principle calculations for $LaMnO_3$ using the linear muffin-tin orbital method under the atomic sphere approximation (LMTO-ASA). We have also used the LSDA$+U$ method to include electron-electron correlation effects. In order to investigate whether the distortion effect is interrelated to the magnetic configuration of the compound, three types of magnetic configurations were considered: ferromagnetic (FM), a case of ferromagnetic alignment between nearest neighbor Mn spins; A-type antiferromagnetic (A-AFM), a case of ferromagnetic alignment of Mn spins on the ab plane and antiferromagnetic alignment along the c axis; and G-type antiferromagnetic (G-AFM), a case of antiferromagnetic alignment between nearest neighbor Mn spins, and four

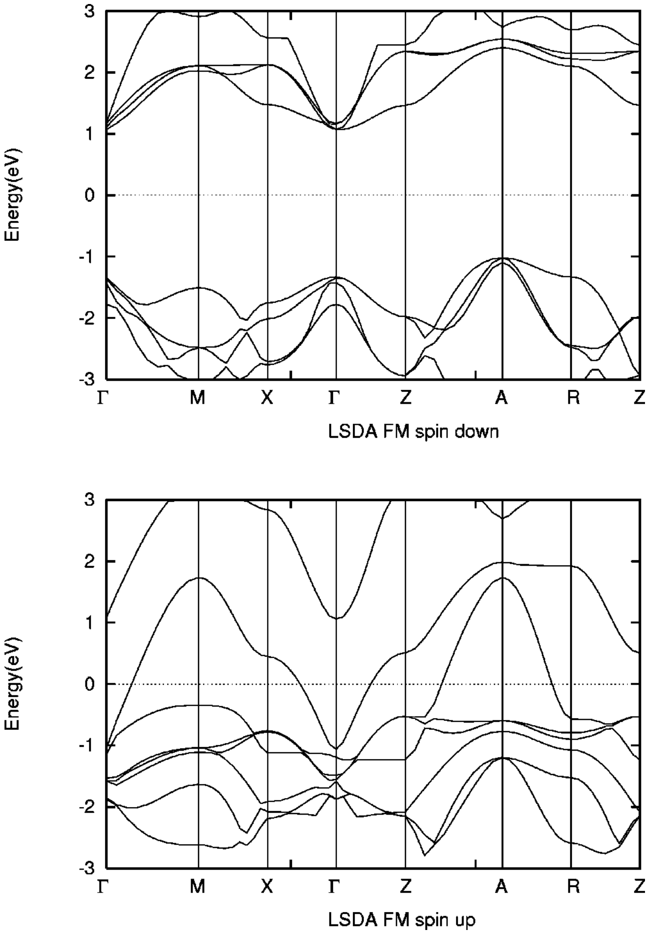


FIG. 2. Band structure of undistorted $LaMnO_3$ with FM order.

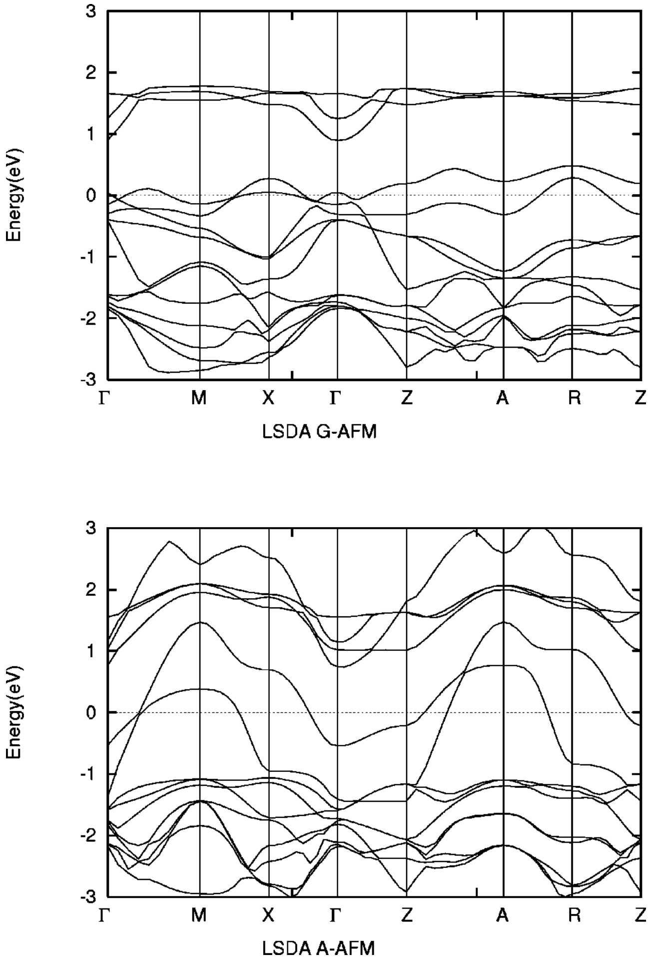


FIG. 3. Band structure of undistorted $LaMnO_3$ with G-AFM and A-AFM orders.

types of calculations were carried out: the LSDA calculation without distortion; the LSDA calculation with distortion (LSDA+JT); the LSDA+U calculation without distortion (LSDA+U); and the LSDA+U calculation with distortion (LSDA+U+JT). In the following section, we briefly describe the crystal structure and the method of calculation in our studies. Then we report our results for three magnetic configurations in Sec. III. Based on these calculations, effects of structural distortion and many-body interaction in $LaMnO_3$ are discussed. Finally, we summarize our findings in Sec. IV.

II. CRYSTAL STRUCTURE AND METHOD OF CALCULATION

Based on experimental observation that $LaMnO_3$ has a tetragonal perovskite crystal structure, we choose a tetragonal perovskite with $a=b=7.973$ a.u. and $c=7.693$ a.u. and identify it as the undistorted crystal structure even though it is already distorted from the ideal cubic perovskite structure. For this undistorted structure, the unit cell of the FM, the A-AFM, and the G-AFM state contains one, two, and four formulas, respectively. It is also reported that $LaMnO_3$ has a strongly distorted orthorhombic $Pnma$ structure with $a=10.8508$ a.u., $b=14.4904$ a.u., and $c=10.450$ a.u., containing four formulas in the A-type antiferromagnetic unit cell.[13] We have performed our calculations by using this distorted structure not only for the A-AFM order but also for the FM and the G-AFM orders to explore the effect of distortion (the static Jahn-Teller effect). The electronic structure is calculated using the LMTO-ASA band method. The valence orbitals are chosen as $6s$, $6p$, $5d$ for La; $4s$, $4p$, $3d$ for Mn; and $2s$, $2p$ for O. The muffin-tin sphere radii are taken to be 4.03 a.u. for La, 2.91 a.u. for Mn, and 2.07 a.u. for O atoms in the perovskite $LaMnO_3$. For distorted structure, the Muffin-Tin sphere radii are 3.75 a.u. for La, 2.70 a.u. for Mn, and 2.04 a.u. for O, respectively.

The standard LSDA theory does not treat many-body correlation between electrons properly. One can make improvement by including a term of on-site Coulomb interaction energy U in the density functional theory, the so-called LDA+U method.[21] In the LSDA+U approach, the effect of spin fluctuation due to the on-site Coulomb interaction is considered in a self-consistent way. Obviously this is a kind of mean-field approximations and it by no means treat many-body correlation truely. However, the system we are dealing with here is approximately three dimensional one and the quantum fluctuation neglected in the Hartree-Fock approximation may not be important, especially for total energy calculation. In spite of its limitations, the LSDA+U method has been applied to many compounds, such as the $3d$ transition metal oxides, La_2CuO_4, etc., and obtained correct energy band gap. Within this framework, the total energy functional of the system can be written as follows:

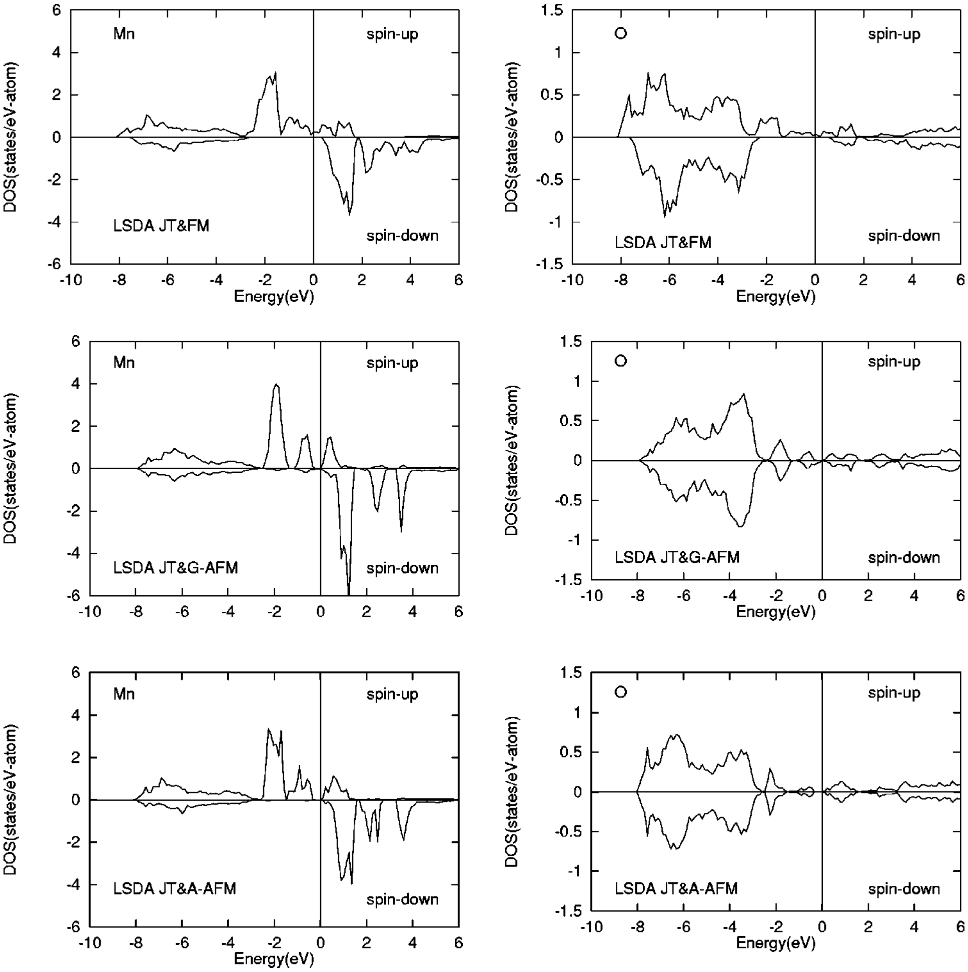


FIG. 4. Partial DOS for Mn and O of distorted $LaMnO_3$ with the three magnetic orders.

$$E=E^{\mathrm{LDA}}+\frac{1}{2}\sum_{m,m',\sigma}U(n_{m\sigma}-n^0)(n_{m'-\sigma}-n^0)$$
$$+\frac{1}{2}\sum_{m,m',\sigma}^{m\neq m'}(U-J)(n_{m\sigma}-n^0)(n_{m'\sigma}-n^0),\qquad(1)$$

where E^{LDA} is the energy and potential in the LDA calculation. U and J denote the Coulomb and exchange interactions, respectively. $n^0=[1/2(2l+1)]\Sigma_{m\sigma}n_{m\sigma}$ is the average occupancy of one d orbital, which should be replaced by the self-consistent occupancy number $n^0_{m\sigma}$ obtained from the LSDA calculation, as $n^0_\sigma=[1/(2l+1)]\Sigma_m n^0_{m\sigma}$. The total energy functional can be expressed as

$$E=E^{\mathrm{LSDA}}+\frac{1}{2}\sum_{m,m',\sigma}U(n_{m\sigma}-n^0_\sigma)(n_{m'-\sigma}-n^0_{-\sigma})$$
$$+\frac{1}{2}\sum_{m,m',\sigma}^{m\neq m'}(U-J)(n_{m\sigma}-n^0_\sigma)(n_{m'\sigma}-n^0_\sigma),\qquad(2)$$

and the corresponding potential in the one electron equation is

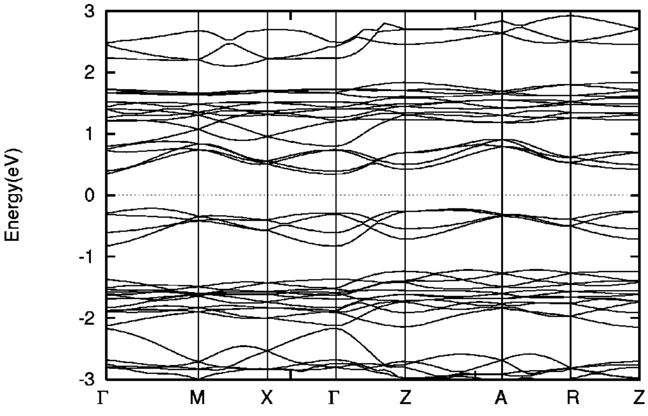
$$V_{m\sigma}=V_\sigma^{\mathrm{LSDA}}+U\sum_{m'}(n_{m'-\sigma}-n^0_{-\sigma})$$
$$+(U-J)\sum_{m'(\neq m)}(n_{m'\sigma}-n^0_\sigma).\qquad(3)$$

The on-site Coulomb energy $U=10.1$ eV and the exchange parameter $J=0.88$ eV for Mn atoms in $LaMnO_3$, used by Satpathy *et al.*[15] (obtained from the Slater's transition state calculations[11]), were also used in our LSDA+U calculations. Furthermore, values of $U=3.0$ eV and $J=0.3$ eV for O atoms, which are commonly used for the high-T_c superconducting oxides, were chosen for our calculations.

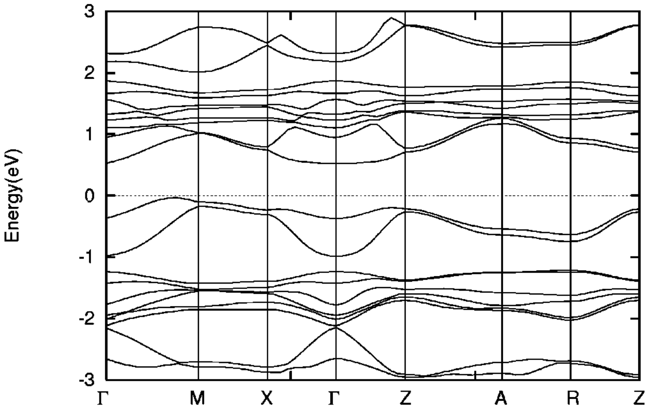
III. RESULTS AND DISCUSSIONS

A. The effect of distortion

Let us first discuss qualitative distinctions among the electronic band structures of $LaMnO_3$ with various magnetic configurations under the LSDA approximation without considering structural distortion and the on-site Coulomb interaction. For the undistorted tetragonal structure, the partial density of states (PDOS) are shown in Fig. 1 for the FM, the A-AFM, and the G-AFM spin configurations. Without lattice distortion caused by the static Jahn-Teller effect, the LSDA calculations show that $LaMnO_3$ is metallic for all three magnetic phases. The e_g orbitals of Mn $3d$ hybridize with O $2p$ orbitals. In all three cases, the Hund splitting is large and induces an empty minority spin bands. The difference among various magnetic configurations can be found from the PDOS curves of Mn and O ions in the figures. Calculations for the FM phase show a completely half-metallic character, that is, the PDOS around the Fermi energy (E_f) come from one spin state while there is a ''gap'' across the E_f for the



LSDA J-T & G-AFM



LSDA J-T & A-AFM

FIG. 5. Band structure of distorted $LaMnO_3$ with *G*-AFM and *A*-AFM orders.

other spin state. The E_f lies inside the majority spin (we label it spin-up) e_g state and this state overlaps with the empty minority spin (we label it spin-down) t_{2g} state. Both spin-up and spin-down e_g states extend over a wide energy range, more than 2.0 eV. For the *A*-AFM solution, its PDOS are somewhat similar to that of the FM case. Presumably due to the ferromagnetic ordering in the *ab* plane, the PDOS of Mn and O ions show quasi-half-metallic character. However, the PDOS of Mn and O for the *G*-AFM state where antiferromagnetic superexchange is dominant are quite different from that of the FM and the *A*-AFM phases. The partially occupied spin-up e_g state is separated from the empty spin-down t_{2g} state by an energy gap of 0.6 eV at about 0.6–1.2 eV above the E_f. The width of the e_g state is narrower than that in the FM or the *A*-AFM phase.

The corresponding LSDA band structures of the undistorted systems with FM order is shown in Fig. 2, where the upper plot is for the minority spin and the lower one is for the majority spin. The existing insulating spin-down bands and conducting spin-up bands clearly exhibit half-metallic character and the spin-up bands across the E_f is about 3.0 eV wide. Band structures for the *A*-AFM and *G*-AFM phases are shown in Fig. 3 for one spin state. It is the same for the other spin state because the two sublattices are equivalent. The width of the bands is about 2.0 eV wide for the *A*-AFM case. But for the *G*-AFM case, this width is much more narrow, only about 0.5 eV, which may easily give way to the opening of an insulating gap. This band came from the hybridized Mn $3d$ e_g and O $2p$ orbitals and the narrow width indicates a relative smaller effective transfer intensity. The calculated values of the magnetic moments for Mn ions are $3.81\mu_B$ for the FM and the *A*-AFM phases and $3.64\mu_B$ for the *G*-AFM phase. For the three magnetic phases considered here, the total energy calculations show that the FM phase has the lowest energy.

Examining differences among the three magnetic ordered states indicate that the spin interaction, which is related to the orbital configuration in $LaMnO_3$, plays an important role for their electronic band structures. Naturally, one expects that lattice distortion induced by the Jahn-Teller effect will affect the electronic band structures of $LaMnO_3$ with different magnetic orders differently because its influence on the stability of orbital configuration and then on the spin-spin interactions are different. So we next turn our attention to the distorted $LaMnO_3$.

Due to the strong Jahn-Teller effect, lattice structure of $LaMnO_3$ is distorted from ideal perovskite to an orthorhombic *Pnma* structure,[11] and its two degenerate e_g states split into nondegenerate e_g^1 and e_g^2 states. The PDOS of Mn and O for the *Pnma* structure with the above discussed three magnetic phases are shown in Fig. 4 and their corresponding band structures are shown in Fig. 5. Evidently, we observe different influence of lattice distortion on the electronic structure with different magnetic ordering.

For the *A*-AFM state, an insulating energy gap about 0.34 eV is obtained after the consideration of structural distortion. From its PDOS plot, it can be seen that the change from the partially occupied doubly degenerate $e_g\uparrow$ state in the undistorted structure (also the *A*-AFM order) to the split $e_g^1\uparrow$ (occupied) and $e_g^2\uparrow$ (empty) states in the distorted structure is the origin of this insulating gap. Symmetry reduction by the static JT effect opens an energy gap and the calculated magnetic moment of Mn ions is $3.73\mu_B$. The energy per formula is lower than that of the lowest FM state in the undistorted system. Our calculations of the distorted *A*-AFM $LaMnO_3$ are similar to other groups.[13]

For the FM state, the introduction of the distortion does not change the main features of the band structure. The distorted $LaMnO_3$ with FM order remains to be half-metallic as for the undistorted case. Although the separation of the occupied $e_g^1\uparrow$ states from the empty $e_g^2\uparrow$ states becomes more evident than that for the undistorted case, it is not sufficient to open a gap around the E_f. In the FM case, this band is a $3d$-$2p$ hybridized band rather than a pure $3d$-e_g band. The width of the bands becomes more narrow but the partial splitting around $\Gamma(0,0,0)$ point of the reciprocal lattice leads to the metallic behavior instead of the insulating behavior for the *A*-AFM phase.

For the *G*-AFM state, although the PDOS is zero at the E_f, the gap is smaller than that for the *A*-AFM state. Our calculations reveal that the splittings between the spin-up and the spin-down states are slightly unsymmetric for the two types of Mn ions because of the introduction of distortion. One of them shows a gap of 0.2 eV while the other shows zero gap. Similar situation occurs for the O ions. The net effect is that there exists very small gap for the *G*-AFM state.

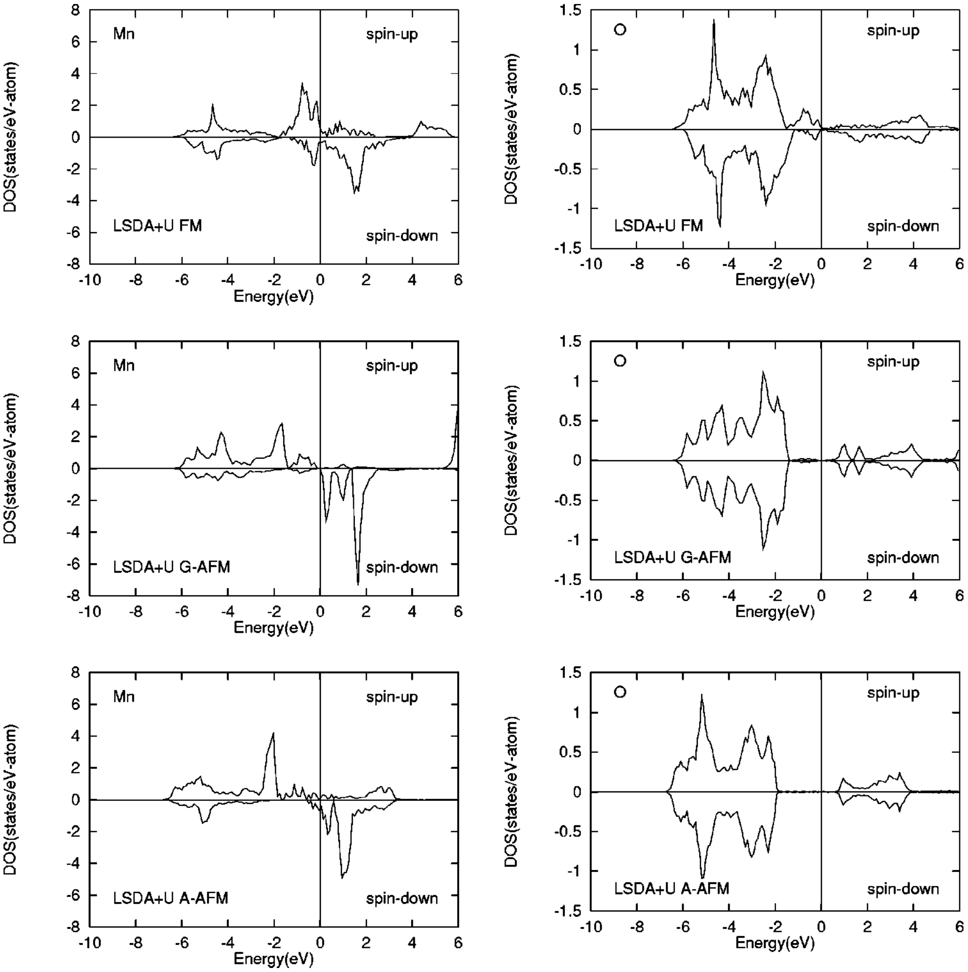


FIG. 6. Partial DOS for Mn and O of undistorted $LaMnO_3$ with three magnetic orders within the LSDA+ U scheme.

In conclusion, our calculations reveal that after using the reported distorted crystal structure, LSDA is successful in describing the insulating gap and magnetic moments of Mn ions. We also find that the effect of the structural distortion has a close relation with the underline magnetic configurations. The combination of spin interaction and the crystal field splitting has played an important role in opening the insulating gap. In the meantime, although the calculated total energy per formula for the distorted $Pnma$ structure with A-AFM order is lower than that of the lowest FM phase for the undistorted systems, the A-AFM phase is still not the lowest energy phase for the distorted systems. The energy of the FM state is lower than that of the A-AFM state by a value about 15 meV. The energy of the G-AFM state is the highest one, 110 meV higher than that of the FM state. These results imply that the LSD approximation plus structural distortion cannot give a good account for the ground state. Fortunately, such discrepancy can be improved by considering the electron-electron interaction corrections, as discussed below.

B. The effect of strong correlation

The LSDA+ U method was introduced to account for the electron correlation in band structure calculations.[21] Within the LSDA+ U framework, the on-site Coulomb energy U and the exchange interaction J are taken into consideration in the calculations. As pointed out by Koshibae *et al.*,[22] the on-site Coulomb interaction gives rise to a coupling between spin and orbital which may modify the double exchange and the superexchange. These arguments suggest that effects of the on-site Coulomb interaction for the three magnetic ordering phases are different. We have carried out band structure calculation by using the LSDA+ U method and results for the undistorted tetragonal $LaMnO_3$ with various magnetic configurations are shown in Figs. 6 and 7, where qualitative changes are evident.

Comparing with the LSDA results, the half-metallic character for the FM phase and the quasi half-metallic character for the A-AFM phase disappear in the LSDA+ U calculations, giving typical metallic behaviors. For these two phases, the changes for the occupied spin-up states are small but the spin-down states are shifted towards the E_f, leading to the reduction of the magnetic moments of Mn ions and nonzero density of states at the E_f. From the band structure shown in Fig. 6 for the A-AFM state, one can see that one of the two bands crossing the E_f is pulled up to higher energy region while the other one is pulled down to lower energy region in the LSDA+ U calculations. However, this separation is not strong enough to produce an insulating gap. In fact, the band structures obtained from the LSDA and the LSDA+ U calculations for the A-AFM state are quite alike.

On the other hand, U correction alone is able to open an insulating gap in the G-AFM phase. The gap is about 0.2 eV. The corresponding band structure shows a direct gap where conduction-band minimum and valence-band maximum are

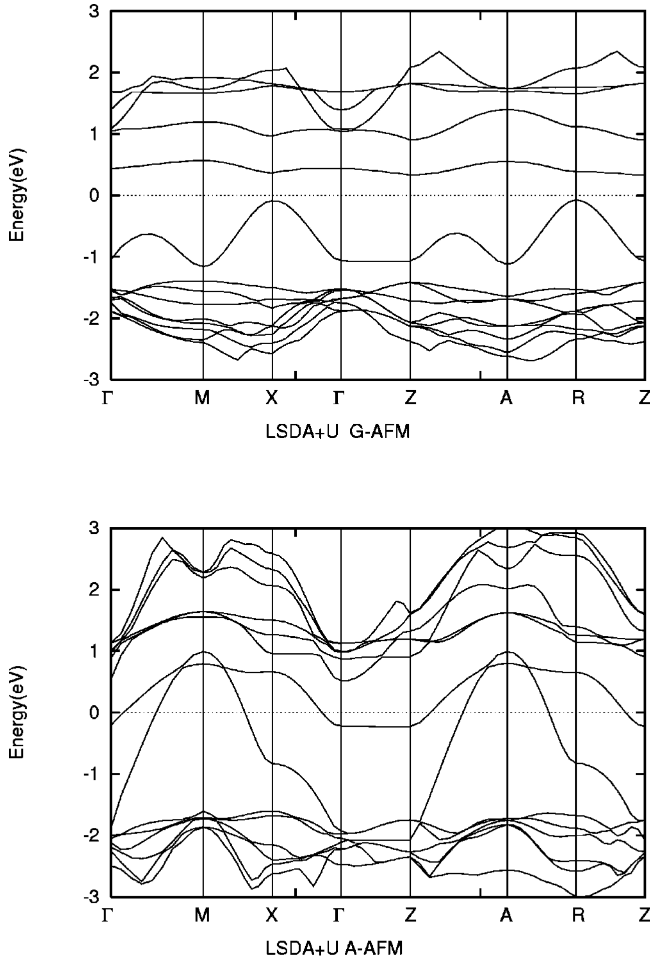


FIG. 7. Band structure of undistorted $LaMnO_3$ with G-AFM and A-AFM orders within the LSDA$+U$ scheme.

both at the $X(1,0,0)$ point. Notice that in the LSDA calculation with distortion there is an indirect energy gap in the A-AFM phase (Fig. 5).

After the inclusion of the on-site Coulomb energy U and the exchange interaction J, the lowest energy state for the undistorted systems is a metallic A-AFM state instead of previous half-metallic FM state. This result is consistent with the results obtained by Maezono *et al.*[20] that the electron correlation can induce an orbital ordering in favor of the A-AFM phase. Without considering lattice distortion, our LSDA$+U$ calculations indicate that the electron correlation correction has great influence on the electronic structures and it can give an A-AFM type ground state with zero gap. The LSDA$+U$ approach is able to obtain a nonzero gap only for the G-AFM state, which is similar to what people have seen in the Hubbard model. However, either the G-AFM phase with gap or the A-AFM phase without gap is not the experimentally observed magnetic structure. Hence we conclude that the LSDA$+U$ calculation without considering lattice distortion is not capable of giving a correct account to the ground state of $LaMnO_3$.

C. The combination of Jahn-Teller effect and strong correlation effect

In previous sections, we have discussed effects of crystal distortion and strong electron correlation separately. As our calculations indicated above, both effects seem to be important yet including either one of them while neglect the other could not yield correct answer as compared with experiments. Naturally, one may think of combining the two effects together in order to obtain results consistent with experimental data. To complete our investigation, we have applied the LSDA$+U$ method to the distorted $LaMnO_3$ and we show the PDOS for the three magnetic ordered states in Fig. 8. Comparing with LSDA calculations of distorted $LaMnO_3$, there seems not much changes in the PDOS spectra except that the hybridization between Mn $3d$ e_g and O $2p$ orbitals is increased. However, the A-AFM phase opens an insulating gap (about 0.40 eV) and its total energy per formula is the lowest one now. In another words, the ground state is insulating with A-AFM type ordering, just as what experiments reported. For the FM and the G-AFM phases, the energy per formula are 34 and 204 meV higher than that of the A-AFM phase, respectively. The distortion of crystal decreases the total energy by 150 meV per formula for the A-AFM state. These results clearly show that in $LaMnO_3$, antiferromagnetic order, crystal distortion caused by the Jahn-Teller effect, and the strong electron-electron correlations, are all essential ingredients in electronic band structure calculations. The A-type antiferromagnetic order reduces the size of the Brillouin zone along the c axis, inducing the spin-up e_g states of Mn ions to become half occupied. The distortion of crystal structure leads to the splitting of the two degenerate e_g states and opens up an energy gap. Finally, the strong correlation effect enlarges the gap and in the meantime prevents the charge transfer to the $3d$ states of Mn ions. Band structure of the A-AFM phase is shown in Fig. 9.

Satpathy *et al.* have also used the LSDA$+U$ method for the distorted $LaMnO_3$ and their calculations somehow overestimated the magnetic moments of Mn ions.[15] Their approach is different from us. For the LSDA$+U$ approach used in this study n_σ^0 [see Eqs. (2) and (3)] are taken for each spin independently, while E^{LDA} and V^{LDA} are replaced by E^{LSDA} and V^{LSDA}. The obtained magnetic moment per Mn is about $3.73\mu_B$, close to the reported data. The large values of Coulomb repulsion U and exchange parameter J have little influence on its value.

IV. SUMMARY

We have investigated the Jahn-Teller effect and the electron-electron correlation effect in $LaMnO_3$ by using the LMTO-ASA band structure method under the LSD approximation and the LSDA$+U$ approach, respectively. Structural distortion in the A-type AFM phase plays a crucial role in opening an insulating gap, which implies that the Jahn-Teller effect is more important than the strong correlation effect in generating an energy gap. The inclusion of structural distortion alone can give a good description of DOS spectrum, magnetic moments, and band structures but it fails in getting the correct ground state by total energy criteria.

The on-site Coulomb energy U correction leads to explicit changes on the electronic structure for the undistorted $LaMnO_3$ and it does not influence the electronic structure very much for the distorted systems. However the inclusion of U lowers the total energy per formula for the A-AFM

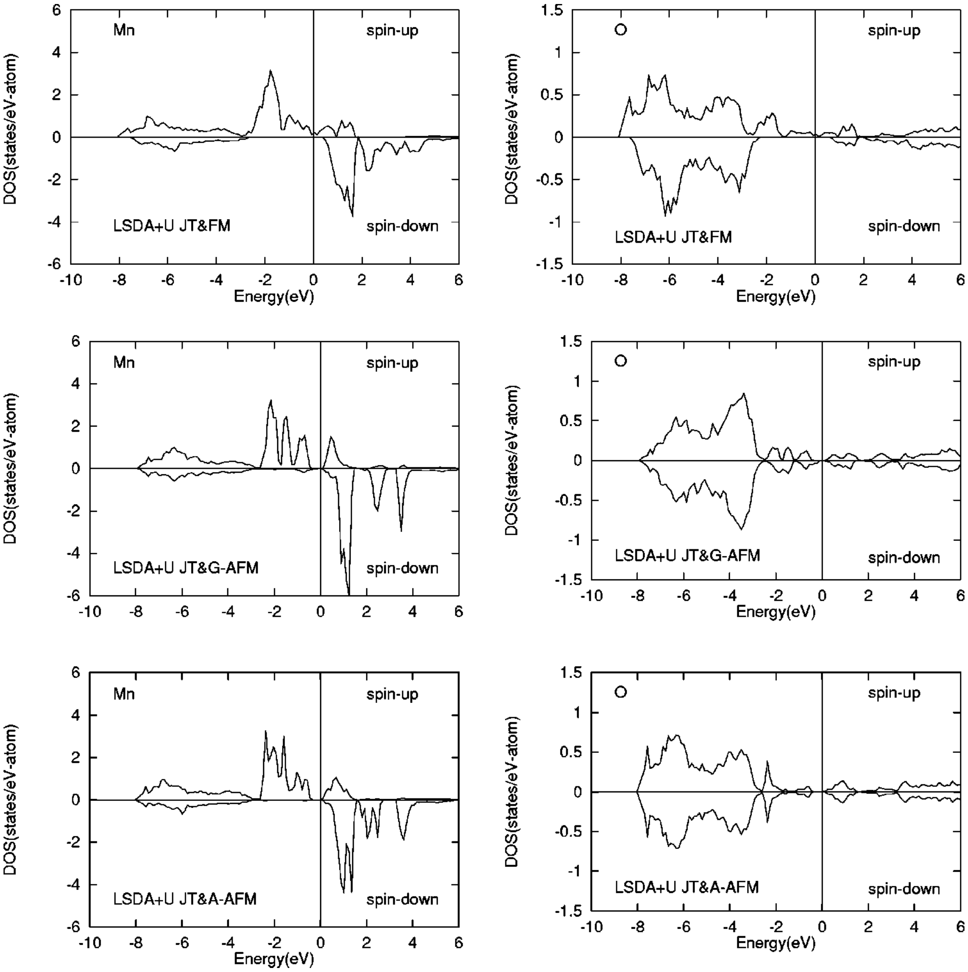


FIG. 8. Partial DOS for Mn and O with correlation and JT effects for the three magnetic orders.

ordered phase, makes it to be the ground state consistent with experimental data.

To summarize, we listed some of our results in Table I in which the relative total energy per unit cell for the three magnetic ordering phases we have discussed, the energy gap, and the magnetic moments of Mn of $\mathrm{LaMnO_3}$ are presented. The conclusions are (1) for $\mathrm{LaMnO_3}$ with tetragonal perovskite structure, we obtain metallic solutions for all three magnetic phases (FM, *A*-AFM, and *G*-AFM) within the LSDA regime. (2) After the consideration of the electron correlation interaction for these undistorted systems, we find that $\mathrm{LaMnO_3}$ remains metallic for the FM or the *A*-AFM phase while it opens an energy gap of 0.2 eV for the *G*-AFM phase. (3) For the LSDA description of $\mathrm{LaMnO_3}$ with observed crystal structure, i.e., the orthorhombic *Pnma* structure due to the Jahn-Teller distortion, the FM phase is metallic while the other two antiferromagnetic phases are insulating. The result that the total energy of the FM state is

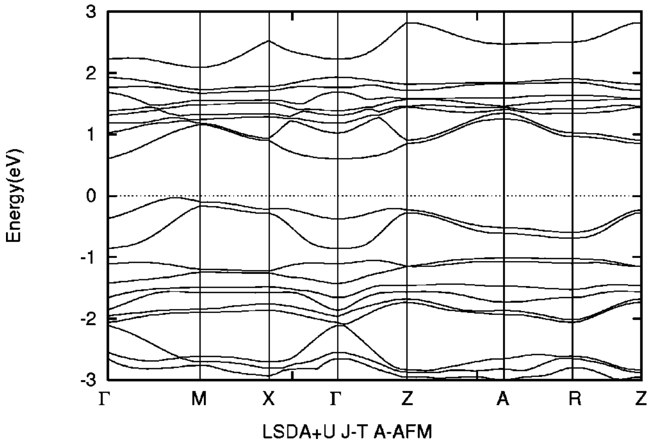


FIG. 9. Band structure for the *A*-AFM ordering with correlation and JT effects.

TABLE I. Total energy (relative to the lowest state) per unit cell, energy gap, and magnetic moment of Mn in $\mathrm{LaMnO_3}$ for the FM, the *A*-AFM, and the *G*-AFM order phases.

		Total energy (meV/formula)	Energy gap (eV)	Magnetic moments (μ)
	FM	0	0.0	3.81
LSDA	*A*-AFM	15	0.0	3.81
	G-AFM	125	0.0	3.64
	FM	0	0.0	3.76
LSDA	*A*-AFM	15	0.34	3.73
distorted	*G*-AFM	110	0.20	3.63
	FM	1076	0.0	
LSDA+*U*	*A*-AFM	0	0.0	
	G-AFM	2042	0.2	
	FM	34	0.0	3.76
LSDA+*U*	*A*-AFM	0	0.4	3.72
distorted	*G*-AFM	204	0.2	3.63

the lowest one dose not agree with existing experiments. (4) Applying the LSDA$+U$ method to the observed structure, in which both the Jahn-Teller distortion and the strong correlation are considered, we find that the A-AFM phase is the lowest in total energy per formula, with an insulating gap of 0.40 eV and the magnetic moments of Mn ion $3.72\mu_B$. (5) In the case of LSDA$+U+$JT, the hybridization between Mn $3d$ and O $2p$ is enhanced.

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