Weak ferromagnetic insulator with huge coercivity in monoclinic double perovskite La$_2$CuIrO$_6$

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Abstract

Insulating ferromagnets with high $T_C$ are required for many new magnetic devices. More complexity arises when strongly correlated 3d ions coexist with strongly spin–orbit coupled 5d ones in a double perovskite. Here, we perform the structural, magnetic, and density functional theory (DFT) study of such double perovskite La$_2$CuIrO$_6$. A new $P2_1/n$ polymorph is found according to the comprehensive analysis of x-ray, Raman scattering and phonon spectrum. The magnetization reveals a weak ferromagnetic (FM) transition at $T_C = 62$ K and short range FM order in higher temperature range. A huge coercivity is found as high as $H_C \sim 11.96$ kOe at 10 K, which, in combination with the negative trapped field, results in the magnetization reversal in the zero field cooling measurement. The first principle calculations confirm the observed FM state and suggest La$_2$CuIrO$_6$ of this polymorph is a Mott insulating ferromagnet assisted by the spin–orbit coupling.

Keywords: ferromagnetic insulator, spin–orbit coupling, double perovskite iridates, huge coercivity

(Some figures may appear in colour only in the online journal)

1. Introduction

Transition-metal oxides (TMOs) are usually correlated electron systems that offer many multifunctional properties, such as superconductivity, colossal magnetoresistance, and multiferroicity [1–3]. Searching for magnetic TMOs has lasted for over 100 years because of the wide range of applications in microwave devices, permanent magnets, and spintronic devices [4–10]. Moreover, TMOs become a renewed focus since a record of highest magnetic order temperature ($T_C \sim 1060$ K) has been found in the 5d TMO insulator Sr$_3$OsO$_6$ very recently [11].

5d TMOs have drawn considerable research interest in the condensed matter physics recent years, due to their comparable energy scales of strong spin–orbit coupling (SOC), electron correlation, crystal field and exchange interactions. In such systems, many novel quantum phases have been realized [12, 13], such as spin–orbit coupled Mott insulators [14], topological Mott insulators [15], superconductivity [16, 17], Weyl semimetals [18], axion insulators [19] and quantum spin liquid phases [19]. An interesting scenario appears in the perovskite iridates, where the 5d orbitals of iridium are split into $e_g$ and $t_{2g}$ states by the strong crystal field. The $t_{2g}$ state further...
forms a \( J_{\text{eff}} = 1/2 \) doublet and a \( J_{\text{eff}} = 3/2 \) quartet as a result of large SOC [14]. For systems with Ir\(^{4+}\) ions, the partially occupied \( J_{\text{eff}} = 1/2 \) state has properties very different from that of the spin-only \( s = 1/2 \) state. In fact, the detailed interplay of the aforesaid comparable energy scales is still not clear and under investigation.

Double perovskite TMOs provide additional degrees of freedom to choose different transition metal ions over the normal perovskite family, which have huge variety of properties such as high Curie temperature [20, 21], high magnetoresistance [20], metal–insulator transition [22] and half-metal [23]. More complexity arises when strongly correlated 3d ions coexist with strongly spin–orbit coupled 5d ones in a double perovskite. For instance, among the La\(_2\)IrO\(_6\) compounds, \( B = \) Fe, Co, Ni are reported to be noncollinear magnetism [7, 24, 25], \( B = \) Mn is FM [26], and \( B = \) Zn, Mg show canted antiferromagnetism with unconventional Kitaev interaction [27–30]. Thus, these compounds promise new ways to develop desired magnetic functional materials for advanced technological applications.

The situation of double perovskite La\(_2\)CuIrO\(_6\) is extremely complicated and in high debate. First of all, different crystal structures are reported by various groups. It is found that La\(_2\)CuIrO\(_6\) forms a monoclinic P\(_{2}/n\) (No. 14) space group with \( \beta \) near 90° in early reports [31–33] and a recent pre-printed paper [34], while a triclinic P\(_1\) (No. 2) space group is also observed by x-ray diffraction (XRD) and neutron diffraction experiments [35]. Density functional theory (DFT) calculations show that the energetics of these two structures are comparable, with the energy slightly lower in P\(_1\) structure than in P\(_{2}/n\), and the energy difference only being \( \approx 2 \) meV f.u.\(^{-1}\) [36]. Then, the magnetic behavior of La\(_2\)CuIrO\(_6\) is also controversial. Magnetic susceptibility measurements find an AFM transition at \( T_N \) around \( \approx 70 \) K and a weak FM behavior below \( \approx 50 \) K [32, 34, 35]. Neutron diffraction suggests a possible spin configuration with collinear AFM spin arrangement in every \( ac \) plane and mutually orthogonal spin orientations in neighboring planes [35]. On the other hand, various spin structures have been proposed based on first principle calculations, such as a canted AFM [34] and a C-type AFM with the Cu and Ir spins anti-parallel in a given \( ac \) plane, while paralleled in out-of-plane [36]. Therefore, the crystal structure and the magnetic properties remain to be fully understood.

### 2. Experimental and computational details

Polycrystalline samples of La\(_2\)CuIrO\(_6\) are synthesized through the conventional solid state reaction method [34, 35]. The starting materials are IrO\(_2\) (99.99%), CuO (99.99%) and La\(_2\)O\(_3\) (99.99%). These mixtures are sufficiently grinded for 12 h and heated in air at 900, 1100, 1150 °C for 60 h by a cooling of the furnace at a rate of 300 °C h\(^{-1}\) with several intermediate grindings. The phase of all samples is checked by XRD on a Bruker diffractometer with Cu K\(_\alpha\) radiation. The structural investigations have been done by Rietveld analysis using the EXPGUI program. Electronic Raman scattering is performed at room temperature for the samples with a confocal microscope Raman spectrometer (Horiba HR-800). Magnetic properties are determined through a quantum design physical properties measurement system (PPMS). Electronic structure calculations high accuracy are performed by the full-potential linearized augmented plane wave (FP-LAPW) method implemented with the WIEN2K code [37]. The generalized gradient approximation (GGA) [38] is applied to the exchange-correlation potential calculation. The muffin tin radii are chosen to be 2.37 a.u. for La, 1.65 a.u. for O, 2.0 a.u. for both Cu and Ir atoms. The plane-wave cutoff is defined by

### Table 1. Structural parameters of obtained from Rietveld refinements of powder XRD data. Space group: P\(_{2}/n\), \( a = 5.60586(8) \) Å, \( b = 5.77985(9) \) Å, \( c = 9.57670(4) \) Å, \( \beta = 125.91^\circ \), \( V = 251.32(5) \) Å\(^3\).

| Atom | \( x/a \) | \( y/b \) | \( z/c \) |
|------|----------|----------|----------|
| La   | 0.26489(9) | 0.45059(5) | 0.25385(4) |
| Cu   | 0.500000  | 0.000000  | 0.500000  |
| Ir   | 0.000000  | 0.000000  | 0.000000  |
| O1   | 0.17614(2) | 0.01098(4) | 0.24828(9) |
| O2   | 0.23012(3) | 0.69304(9) | 0.02923(4) |
| O3   | 0.34863(1) | 0.21278(1) | 0.07246(7) |

wRp 5.37% \( R_p \) 3.84% \( \chi^2 \) 3.08
and orthorhombic phases [39]. Moreover, cation vacancies conditions, known as corundum, monoclinic, defective spinel, to ~550 cm\(^{-1}\) indicate that there are 60 phonon bands extending up new polymorph structure. The calculated phonon disper-
sions indicate that there are 60 phonon bands extending up to ~550 cm\(^{-1}\) and the point group is \(C_{2h}\), \(C_{2h}\) is Abelian group with 4 irreducible representations. The modes at \(\Gamma\) can be decomposed as \(\Gamma = 18A_{g} \oplus 18B_{g} \oplus 12A_{g} \oplus 12B_{g}\), in which \(A_{g}\) and \(B_{g}\) modes are infrared active, \(A_{g}\) and \(B_{g}\) are Raman active. Thus, twenty-four Raman active modes are expected according to the calculation, as presented in table 2. To compare with experiments, electronic Raman scattering is carried out at room temperature. As shown in figure 3, four peaks at 205.8, 278.4, 385.9 and 530.3 cm\(^{-1}\), labeled as \(M_{1} \sim M_{4}\), dominate the spectrum. A comparison with the calculation suggests that peak \(M_{1}\) is a mode with \(A_{g}\) symmetry, peaks \(M_{3}\) and \(M_{4}\) are \(B_{g}\) modes, and peak \(M_{2}\) (hereby termed \(M_{2}^{i}/M_{1}^{i}\)) is a superposition of an \(A_{g}\) and a \(B_{g}\) mode at nearby frequencies. Indeed, our calculations indicate \(A_{g}\) modes at 209.3, and 272.3 cm\(^{-1}\) and \(B_{g}\) modes at 201.0, 386.2 and 522.4 cm\(^{-1}\) in good agreement with the observed frequencies. The vibration representations of \(A_{g}\) and \(B_{g}\) modes are given in figure 4. Since these modes all correspond with \(Cu-O\) and \(Ir-O\) vibrations, only the patterns of the \(Cu/\text{Ir}O_{6}\) octahedra are given for clarity. The mode \(M_{2}\) corresponds to an out-of-phase asymmetric stretching. While in mode \(M_{4}\), vibration of \(CuO_{6}\) octahedra corresponds to an out-of-phase symmetric breathing, and \(\text{IrO}_{6}\) octahedra vibrates in an asymmetric stretching way.

### 3. Results and discussion

#### 3.1. Crystal structure

Powder XRD data of polycrystalline \(La_{2}CuIrO_{6}\) are presented in figure 1. All the lines in this pattern could be indexed to the monoclinic \(P_{2}/n\) structure [31–34]. This monoclinic double perovskite structure is derived from the perovskite structure by alternatingly placing \(Cu\) and \(Ir\) at the \(B\) site so that \(Cu\) and \(Ir\) ions form the fcc lattice respectively. The resulted lattice parameters are listed in table 1 from the Rietveld refinements. The obtained lattice parameters are different from those in \(P_{2}/n\) structure of \(La_{2}CuIrO_{6}\), although the cell volume is comparable with that of the literature [33]. For example, \(\beta \sim 126^\circ\) is larger than ~87° in early works [32, 33], indicating a considerably tilted crystal cell resulting in a much longer \(c\)-axis parameter. The attempts to fit the XRD data with earlier \(P_{2}/n\) and \(P1\) structures (not shown for simplicity) have failed since very large values of \(\chi^2\) are obtained. Hence, a new polymorph is found in this \(La_{2}CuIrO_{6}\) double perovskite due to different growth conditions. In fact, polymorphs have been found in various oxides. For example, there are five identified polymorphs of \(Ga_{2}O_{3}\) depending on various growth conditions, known as corundum, monoclinic, defective spinel, and orthorhombic phases [39]. Moreover, cation vacancies can weaken the interaction between \(Cs\) and \(PbO_{6}\) octahedra in \(CsPbI_{3}\), stabilizing the Cubic Perovskite Polyphased [40]. In addition, polymorphs are also found in double perovskite \(Sr_{2}FeMoO_{6}\) driven by defects [41].

To verify this new polymorph, the phonon spectrum is calc-
dulated based on GGA according to the lattice constants from the above XRD Rietveld refinements. As shown in figure 2, there are no imaginary frequencies over the Brillouin zone and thus the \(La_{2}CuIrO_{6}\) would be dynamically stable in this new polymorph structure. The calculated phonon disper-
sions indicate that there are 60 phonon bands extending up to ~550 cm\(^{-1}\) and the point group is \(C_{2h}\), \(C_{2h}\) is Abelian group with 4 irreducible representations. The modes at \(\Gamma\) can be

| Mode | Calc (cm\(^{-1}\)) | Observ. (cm\(^{-1}\)) | Mode | Calc (cm\(^{-1}\)) | Observ. (cm\(^{-1}\)) |
|------|-------------------|----------------------|------|-------------------|----------------------|
| \(A_{g}(1)\) | 92.6 | | \(B_{g}(1)\) | 87.6 | |
| \(A_{g}(2)\) | 123.1 | | \(B_{g}(2)\) | 127.0 | |
| \(A_{g}(3)\) | 131.3 | | \(B_{g}(3)\) | 143.7 | |
| \(A_{g}(4)\) | 209.3 | | \(B_{g}(4)\) | 201.0 | |

\(^{a}\) Indicates the superposition of these two modes.

\[ R \cdot K_{max} = 7.0, \text{ where } R \text{ is the minimum LAPW sphere radius and } K_{max} \text{ is the plane-wave vector cutoff.}\]

### 3.2. Magnetic behavior

The magnetic behavior of \(La_{2}CuIrO_{6}\) is very interesting. Double magnetic phase transitions in both \(P1\) and \(P2_{1}/n\) structures are reported by literatures [34, 35], namely a paramagnetic to AFM phase transition at \(T_{N} \sim 74 K\) and a weak FM transition below 60 K. A similar kind of double transition behavior is also observed for \(La_{2}ZnIrO_{6}\) [29]. Figure 5 illustrates the temperature dependent field cooled (FC) and zero field cooled (ZFC) magnetization (\(M-T\)) for our new polymorph of \(La_{2}CuIrO_{6}\) sample. As the sample is cooled from high temperatures is noteworthy, which will be discussed later.
Moreover, there is a distinct bifurcation between ZFC and FC curves when cooling below about 250 K as shown in the upper inset of figure 5 with an enlarged plot of the magnetization data, which can also be observed in the reciprocal susceptibility plot in the lower inset. Similar phenomena are observed in other ferro/ferri-magnets, such as Pr$_{1-x}$Ca$_x$CoO$_3$ [42] and Nd$_{1-x}$Ca$_x$CoO$_3$$_{δ}$ [43], which is usually interpreted as a short-range FM order. The paramagnetic phase is further analyzed by plotting the temperature dependent inverse susceptibility in the lower inset of figure 5. The high temperature data, in the $260 \text{ K} < T < 300 \text{ K}$ window, nicely fit with the Curie–Weiss law yielding an effective magnetic moment of $μ_{\text{eff}} = 2.54 \mu_B \text{ f.u.}^{-1}$. This is consistent with previous result of P2/n structure [34] but larger than that of P1 one [35]. Note that the obtained effective magnetic moment $μ_{\text{eff}} = 2.54 \mu_B \text{ f.u.}^{-1}$ is very close to the ideal value $\sqrt{μ_{\text{Cu}}^2 + μ_{\text{Ir}}^2} = 2.449 \mu_B$ with $μ_{\text{Cu}} = μ_{\text{Ir}} = \sqrt{n(n+2)} \mu_B$ in the ‘spin only’ model if considering the spin configuration of Cu$^{2+}$/Ir$^{4+}$ ions. Interestingly the Curie–Weiss temperature is found to be $θ_{\text{CW}} = +147 \text{ K}$, consistent with the FM interaction.

To further understand the magnetic phases, magnetic isothermal ($M$–$H$) measurements are performed at several temperatures in figure 6. In earlier reports [34, 35], it is found that the magnetization of La$_2$CuIrO$_6$ system with both P1 and P2/n structures exhibits a small but visible hysteresis loop with the coercivity $H_C$ equaling to several hundreds of Oe, and linearily increases with the applied magnetic field as usually seen in other AFM materials. On the contrary, the $M$–$H$ curves show large hysteresis loops of our new polymorph, indicating obvious FM order. Note that the magnetic hysteresis loop can still be observed at $T = 70 \text{ K}$ as shown in the inset of figure 6, where the temperature is above the FM transition temperature $T_{\text{C}} = 62 \text{ K}$, consistent with the framework of short-range FM order. Particularly, a huge coercivity of $H_C \sim 11.96 \text{ kOe}$ at 10 K is found, which is larger than ~2.5 kOe, the highest
value for hard magnetic ferrites, and is similar to a very recent YMn0.5Cr0.5O3 system [44]. As the temperature increases, the hysteresis loop shrinks and $H_C$ decreases significantly to ~580 Oe at $T = 50$ K, as shown in the inset of figure 7. The huge coercivity could be relevant to the magnetocrystalline anisotropy, since uniaxial magnetocrystalline anisotropy usually corresponds with a higher coercivity. The magnetocrystalline anisotropy can be understood through the ratios of remanent to saturation magnetization $M_r/M_s$. The ratios are 0.50 and 0.83 for polycrystalline samples with uniaxial and cubic magnetocrystalline anisotropy [44]. Since it is hard to explicitly define the saturation magnetization from the $M-H$ curves due to the moderate slope at high fields, the value corresponding to the end point of the irreversible part is chosen as the saturation magnetization $M_s$. The saturation magnetization (~11 emu cc$^{-1}$ or 0.15 $\mu_B$ f.u.$^{-1}$ at 10 K) is significantly smaller than that of typical magnetic metals like Nd$_2$Fe$_{14}$B (~1280 emu cc$^{-1}$), and typical ferrites like CoFe$_2$O$_4$ (~430 emu cc$^{-1}$), but is comparable with the very recent reported Sr$_2$OsO$_6$ (~49 emu cc$^{-1}$ at 1.9 K) [11]. The temperature dependence of $M_r/M_s$ is displayed in figure 7 at $T = 10$ K, a $M_r/M_s$ value close to 0.64 can be seen, suggesting that the sample tends to be uniaxial anisotropy at low temperatures. With temperature increasing to 50 K, the value increases gradually to 0.77, still less than 0.83 for the cubic anisotropy. Similar results are found in YMn0.5Cr0.5O3 system [44]. The huge coercivity is also related to the magnetization reversal in the ZFC $M-T$ measurement. The magnetization reversal, also called negative magnetization, is termed as a temperature dependent crossover of the dc magnetization from a positive value to a negative one (cooled under a positive applied magnetic field) [45, 46], which is different from a diamagnetic state that occurs in the case of superconducting or diamagnetic materials. The possible explanations for negative magnetization can be classified into different mechanisms, such as negative exchange coupling among ferromagnetic sublattices, among canted antiferromagnetic sublattices and among ferromagnetic/canted-antiferromagnetic and paramagnetic sublattices, etc [45]. The explanation based on the antiferromagnetic coupling between R-site and T-site cations can be excluded first in many ABO$_3$-perovskites with canted AFM sublattices residing at different crystallographic sites [47], since La$^{3+}$ ion is a nonmagnetic cation with fully occupied shells. For the second mechanism resulting from negative exchange coupling among ferromagnetic sublattices, the magnetization reversal always occurs in FC mode, such as Co$_2$VO$_4$ [48]. However, the La$_2$CuIrO$_6$ sample shows magnetization reversal only in the ZFC mode, implying other causes in the present case. Actually, a similar negative magnetization only under ZFC mode in YMn0.5Cr0.5O3 system has been presented very recently [44]. It has been found that the magnetization reversal in ZFC measurements is an artifact caused by negative trapped field of the superconducting magnet of the PPMS in combination with the huge coercivity. Considering that the PPMS superconducting magnet is usually turned off to zero from positive fields, the residual negative trapped field results in negative ZFC magnetization at low temperatures if the applied field is smaller than the coercivity. In fact, the coercivity is as high as 11.96 kOe at 10 K for our La$_2$CuIrO$_6$ sample, much larger than the applied field $H = 500$ Oe (see figure 5). With increasing temperature, the coercivity decreases rapidly to $H_C \sim 580$ Oe at $T = 50$ K (see the inset of figure 7) comparable with the applied field, which results in the negative magnetization approaching to zero. With the further increase of the temperature the coercivity becomes smaller than the applied field, thus the ZFC magnetization becomes positive.

GGA calculations are performed to confirm the FM state in the new structure phase of La$_2$CuIrO$_6$ sample based on the lattice parameters listed in table 1 deduced from the XRD measurements. Apart from the nonmagnetic (NM) state, FM structure with parallel alignment of all Cu and Ir spins is considered since La$_2$CuIrO$_6$ contains two magnetic ions. Three different AFM structures are considered, namely AF1, AF2, and AF3, possible within the unit cell of the new P2$_1$/n structure phase. For AF1, the Ir–Ir spins and Cu–Cu spins are parallel coupling and Ir–Cu spins are antiparallel coupling. AF2 denotes in-plane antiparallel coupling of Ir–Cu spins but parallel coupling of Ir–Cu spins between the layers. While AF3 denotes in-plane parallel coupling of Ir–Cu spins but antiparallel coupling of Ir–Cu spins between the layers. The energetics within GGA scheme of calculation is shown in figure 8. It can be seen that the FM structure is the lowest energetic spin configuration of our new structure phase. The AF1 structure lies 10.3 meV higher than the FM state, resulting in a FM transition temperature of $T_C = 40$ K according to the mean-field estimation of $3/2k_B T_C = \Delta E/N$ with $N = 2$ the number of magnetic ions in the formula unit, which is in reasonable agreement with the value ~62 K determined from $M-T$ experiments. The calculated total magnetic moment is 1.15 $\mu_B$ f.u.$^{-1}$, with 0.69 $\mu_B$ for Ir and 0.46 $\mu_B$ for Cu respectively. Obviously, such value is a bit larger than that of the measured magnetization (0.15 $\mu_B$ f.u.$^{-1}$ at 10 K). In general, DFT calculation would over-estimate the moment because the magnetic moment is defined by the integral inside the linearized augmented plane wave sphere, which is 2.0 a.u. for both Ir and Cu. Moreover, the DFT calculation is performed on a single
AFM: antiferromagnetism and FM: ferromagnetism. Considering different magnetic structures. NM: nonmagnetism, AFM: antiferromagnetism and FM: ferromagnetism.

Coulomb interactions \( U = 2 \) and \( 4 \) eV are adopted on Ir and Cu sites, respectively. The situations: (a) FM GGA calculation, (b) FM GGA + \( U \) calculation. The \( U \) parameter is used in our new P2\( _1/n \) polymorph, which indicates that only in the case of FM GGA + \( U \) calculation. The GGA calculations confirm the observed FM state and suggest that La\(_2\)CuIrO\(_6\) of this polymorph is a weak ferromagnetic insulator assisted by the SOC.

Figure 8. Comparison of GGA total energy of La\(_2\)CuIrO\(_6\) considering different magnetic structures. NM: nonmagnetism, AFM: antiferromagnetism and FM: ferromagnetism.

Figure 9. The total DOS of the La\(_2\)CuIrO\(_6\) system in two different situations: (a) FM GGA calculation, (b) FM GGA + \( U \) + SOC. The Coulomb interactions \( U = 2 \) and \( 4 \) eV are adopted on Ir and Cu sites, respectively.

Crystal, while the magnetic measurements are carried out on polycrystalline samples. Such difference would also lead to the measured magnetization less than that of a full ferromagnetic alignment of the Cu and Ir cations.

The total density of states (DOS) of the La\(_2\)CuIrO\(_6\) system are presented in figure 9 for two different situations, namely the FM GGA and FM GGA + \( U \) + SOC calculation. The Coulomb interactions \( U = 2 \) and \( 4 \) eV are adopted on Ir and Cu sites respectively. A sizeable gap of ~0.2 eV is observed only in the case of FM GGA + \( U \) + SOC + \( U \), which indicates that our new P2\( _1/n \) structure phase of La\(_2\)CuIrO\(_6\) is a Mott insulator assisted by the SOC effect. Note that similar result is reported in other P2\( _1/n \) and P2\( _2/ln \) polymorphs with slightly higher gap of ~0.3 eV [34, 36].

In conclusion, we perform the structural, magnetic, and GGA study of the double perovskite La\(_2\)CuIrO\(_6\). A new P2\( _1/n \) polymorph is found according to the comprehensive analysis of XRD, Raman scattering and phonon spectrum, which is different from the reported triclinic P1 and monoclinic P2\( _1/n \) as well. The magnetization reveals a weak FM transition at \( T_C = 62 \) K and short range FM order in higher temperature range. A Curie–Weiss fit of the inverse susceptibility yields \( \theta_{CW} = +147 \) K and \( \mu_{eff} = 2.54 \) \( \mu_B \) f.u.\(^{-1}\), consistent with the ‘spin only’ model. The magnetic hysteresis loops indicate the magnetocrystalline anisotropy inclines to be uniaxial anisotropy. Particularly, a huge coercivity is found as high as \( H_C \sim 11.96 \) kOe at 10 K, which in combination with the negative trapped field results in the magnetization reversal in the ZFC measurement. The GGA calculations confirm the observed FM state and suggest that La\(_2\)CuIrO\(_6\) of this polymorph is a weak ferromagnetic insulator assisted by the SOC.

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