Two dimensional electron gas in the \(\delta\)-doped iridates with strong spin–orbit coupling: \(\text{La}_\delta\text{Sr}_2\text{IrO}_4\)

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Abstract

Iridates are of considerable current interest because of the strong spin–orbit coupling that leads to a variety of new phenomena. Using density-functional studies, we predict the formation of a spin-orbital entangled two dimensional electron gas (2DEG) in the \(\delta\)-doped iridate \(\text{La}_\delta\text{Sr}_2\text{IrO}_4\), where a single \(\text{SrO}\) layer is replaced by a \(\text{LaO}\) layer. The extra \(\text{La}\) electron resides close to the \(\delta\)-doped layer, partially occupying the \(J_{\text{eff}} = 1/2\) upper Hubbard band and thereby making the interface metallic. The magnetic structure of the bulk is destroyed near the interface, with the \(\text{Ir}_2\) layer closest to the interface becoming non-magnetic, while the next layer (\(\text{Ir}_1\)) continues to maintain the AFM structure of the bulk, but with a reduced magnetic moment. The Fermi surface consists of a hole pocket and an electron pocket, located in two different \(\text{Ir}\) layers (\(\text{Ir}_0\) and \(\text{Ir}_1\)), with both carriers derived from the interface \(\delta\)-doped layer. The presence of both electrons and holes at the \(\delta\)-doped interface suggests unusual transport properties, leading to possible device applications.

Keywords: spin–orbit coupling, delta-doping, 2DEG, Fermi surface, \(\text{Sr}_2\text{IrO}_4\), iridate

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

1. Introduction

The combination of a large spin–orbit coupling (SOC) and a reduced Coulomb interaction in the 4d and 5d transition metal oxides has made these compounds hosts for a number of exotic quantum states, such as the spin–orbit driven Mott insulators [1], Weyl semimetals [2], axion insulators [3, 4], and Kitaev spin liquids [5, 6]. Analogously, one expects any two dimensional electron gas (2DEG) formed in the \(\text{Sr}_2\text{IrO}_4\) (SIO) iridate interface structures [7], similar to the 3d interfaces such as \(\text{LaAlO}_3/\text{SrTiO}_3\) [8], to lead to potentially novel effects due to the spin–orbit entanglement of the electron states. Recently, epitaxial growth of iridate heterostructures and interfaces has been demonstrated by a number of experiments [9–11], which paves the way for the growth of the \(\delta\)-doped iridate structures by substitution of an element with another element having an excess electron or hole. We will show here that such \(\delta\)-doped structures can lead to the formation of novel 2DEG near the \(\delta\)-doped layer.

The characteristic electronic properties of the iridates are controlled by the \(\text{Ir}^{4+}\) ion in the \(d^5\) configuration. A large crystal field splits the \(d\) states into two \(e_g\) and three \(t_{2g}\) states. The sixfold \(t_{2g}\) manifold (including spin) is further split into a fourfold \(J_{\text{eff}} = 3/2\) and a twofold \(J_{\text{eff}} = 1/2\) manifold, with an energy gap of \(\lambda_{\text{SO}} = 3\lambda/2\), \(\lambda \vec{L} \cdot \vec{S}\) being the SOC interaction. Four electrons fill the lower-lying \(J_{\text{eff}} = 3/2\) states, leaving the lone \(d\) electron to occupy the doubly degenerate \(J_{\text{eff}} = 1/2\) state. The wave functions \(|J_{\text{eff}}, m\rangle\) are spin-orbital entangled, viz.,

\[
|e_1\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{2}, -\frac{1}{2} \end{pmatrix} = (|xy \uparrow\rangle + |yz \downarrow\rangle + i|xz \downarrow\rangle)/\sqrt{3},
|e_2\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{2}, \frac{1}{2} \end{pmatrix} = (|yz \uparrow\rangle - i|xz \uparrow\rangle - |xy \downarrow\rangle)/\sqrt{3}.
\]

(1)

The half-filled \(J_{\text{eff}} = 1/2\) band splits further due to the Coulomb interaction into an upper Hubbard band (UHB) and a lower Hubbard band (LHB), producing a Mott insulator. The importance of the spin–orbit coupling on the photoemission spectra has been recently studied [12].
The Mott insulating state can be doped with electrons or holes via impurity substitution. Experimentally, there have been already several studies on the bulk electron doping \cite{10, 13–20} by the substitution of Sr by trivalent metals like La \cite{21, 22}. These bulk doped samples display several interesting features such as the formation of Fermi arcs and pseudogaps by potassium surface doping \cite{18} and a metallic state beyond a critical La dopant concentration $\chi_c$, which is somewhere between 5\% \cite{23} and 15\% \cite{10}. Related to these results, we have shown earlier that indeed the anti-ferromagnetic ground state of the electron-doped SIO becomes unstable beyond a critical doping concentration of about 15\% \cite{24}.

In this paper, we predict the formation of a 2DEG in the $\delta$-doped SIO iridate using density functional methods. The predicted 2DEG is different from a conventional 2DEG obtained at the $\delta$-doped 3d perovskite oxides such as SrTiO$_3$, $\delta$-doped with La \cite{25, 26} in several ways, viz., (i) The 2DEG is spin-orbital entangled, (ii) It is sharply localized on just two Ir (Ir$_0$ and Ir$_1$) planes adjacent to $\delta$-doped LaO layer as opposed to the 3d perovskite systems, where it spreads to several unit-cell layers around LaO, and (iii) As opposed to the multi-band Fermi surface for the 3d structures, the Fermi surface is much simpler in the present case, consisting of just one (nearly circular) hole pocket at $\Gamma$ and an elliptical electron pocket at $M$ point of the 2D interface Brillouin zone. The simultaneous existence of an electron as well as a hole pocket is in contrast with the single square-like Fermi surface of the 2DEG formed in a different system, viz., the polar interface between the LaAlO$_3$/Sr$_2$IrO$_4$, which we have studied elsewhere \cite{7}. The mechanism of the formation of the 2DEG is also quite distinct in the sense that, for the polar interface, it is formed by the diverging electrostatic potential (polar catastrophe), while for the present case, it is formed due to the triangular electrostatic potential of the positively-charged $\delta$-doped LaO layer \cite{25} and the explicit electron doping introduced by the La atoms.

2. Method

In our present study, we used the full-potential linearized muffin-tin orbital (FP-LMTO) method \cite{27, 28} to solve the density functional Kohn–Sham equations in the local spin density approximation \cite{29, 30} including spin–orbit coupling and the Hubbard U term (LSDA+SOC+U). The supercell consisted of 8 SIO layers stacked along the $c$-axis and each layer consisted of two formula units, so as to describe the possible anti-ferromagnetic state in each layer, leading to the unit cell consisting of (Sr$_2$IrO$_4$)$_{16}$. All atom positions were optimized with the lattice constant of the supercell structure fixed at the bulk experimental value. To form the $\delta$-doped structure, we substituted a single layer of SrO by LaO, as indicated in figure 1. We also used the Vienna Ab initio Simulation Package (VASP) \cite{31} within the projector augmented wave (PAW) \cite{32} method including $U$ in the Dubarev scheme \cite{33} and SOC for computing magnetic moments. In the VASP calculations, we used the plane wave cut-off energy of 620 eV and a $6 \times 6 \times 1$ $k$-mesh for Brillouin zone sampling.

1 For details of the methods, see: www.questaal.org

3. V-shaped potential and electron localization at the interface

On general grounds, one expects a $V$-shaped potential at the $\delta$-doped layer. Since La has an extra valence electron as compared to Sr, with the transfer of these electrons to the solid, the La$^{3+}$O$^{-2}$ layer becomes nominally a positively charged layer as compared to the neutral Sr$^{2+}$O$^{-2}$ layer, and thus it produces a uniform electric field on either side of the infinite 2D plane, leading to a $V$-shaped attractive potential, in which the extra valence electron of La becomes bound.

The potential due to a charged sheet is simply $V = (\sigma/\epsilon)|z|$, where $\sigma$ is the surface charge density, $\epsilon$ is the dielectric constant, and $z$ is the distance from the interface. The potential near the $\delta$-doped layer may be examined by studying the core level energy shifts. Using density functional theory (DFT), we have computed the O (1$s$) core energies. The cell averaged core level energies (averaged over the bulk unit cell) are shown in figure 1(b). As one moves away from the interface, the interfacial potential is screened due to the redistribution of electrons around the donor plane. From the DFT calculations, we find a more or less $V$-shaped potential close to the interface. Apart from this, figure 1(b) shows that the Ir layers as close as the second layer to LaO (viz., Ir$_2$ and Ir$_{-1}$) already look like the bulk.

Note that the added extra electron due to $\delta$ doping will be distributed among the Ir atoms depending on the relative potentials of the Ir layers, which can be extracted from the O(1$s$) core level energies in these layers. Even though the oxygen core level in the La layer is below the oxygen core level for the Ir layers in figure 1(b), electrons still will not occupy the La and Sr atoms (as seen from figure 1(c)), because the positions of the unoccupied Sr and La states are far above the Ir states in the band structure.

We find that the interface potential (figure 1(b)) is strong enough to localize the $\delta$-doped electrons in the two Ir layers closest to the interface. This may be seen from the charge density of the electron bands near the Fermi energy ($E_F$). For this purpose, we used the energy range of $E_F$ to 0.15 eV below it. The results shown in figure 1(c) indicate the confinement of the doped electrons to mostly the Ir$_0$ and Ir$_1$ layers. The same conclusion is inferred from the computed charges of the individual atoms shown in table 1, which were estimated by computing the total charges within the muffin-tin spheres and renormalizing them to the total number of electrons in the system.

4. Band structure and the Fermi surface

We now turn to the band structure and the Fermi surface. Figure 2(a) shows the well known \cite{1} spin–orbit assisted Mott insulating state of the bulk SIO, in terms of which the electron states of the $\delta$-doped structure, shown in figure 2(b), may be understood. The individual Ir layers in the structure are separated enough that the electronic structure can be understood in terms of the isolated layers. The upper and the lower Hubbard bands for the interface Ir layers (Ir$_0$ and Ir$_1$) are shifted in
energy due to the V-shaped interface potential and, in addition, they show a layer-dependent splitting $2\Delta = U(n_1 - n_2)$ between the LHB and the UHB, with the respective population being $n_1$ and $n_2$. The LHB is full for each Ir layer ($n_1 = 1$), while the UHB is only partially full, $n_2 < 1$ for Ir0 and Ir1, and 0 for the remaining Ir atoms, which are similar to the SIO bulk. The charges listed in table 1 correspond to the charges $n_2$ in the UHB for the various layers.

Figure 3 shows the density functional band structure, computed using the FP-LMTO method and the LSDA+SOC+U functional ($U = 2.7$ eV was used following earlier works on bulk SIO [34]), as well as the model tight-binding (TB) results. The Ir (d) $J_{\text{eff}} = 1/2$ bands, split into the UHB and LHB, are the ones that occur around the Fermi energy, and the UHB belonging to different Ir layers can be identified in the band structure as marked in figure 3(a). The layer-projected DOS shown in figure 4 indicates the partial occupation of the UHB of the Ir atoms close to the δ-doped layer in order to accommodate the doped electrons, which is consistent with the charge distribution presented in table 1.

In the above calculations, we did not relax the interlayer La–Sr distances, which could conceivably change in the δ-doped structure. Test calculations to optimize these distances showed a small reduction (viz., 0.07 Å for the La–Ir0 distance and 0.10 Å for La–Ir1). This reduction is consistent with the atomic sizes, as for example seen from the atomic core radius values [35]. With these distances, we relaxed all atomic positions, keeping again the bulk lattice constants fixed at the experimental values. The calculated band structure showed very little difference from figure 3; in particular the La-d states are pushed up in energy, while the Irbulk bands come down in energy, but still remaining above the Fermi energy. The new Fermi surfaces show negligible difference from figure 5.

4.1. Tight-Binding model of the interface states

To help in the understanding of the band structure, we have considered the Hubbard model on a square lattice with...
the electron pocket in the UHB for Ir$_1$, while the green region corresponds to the hole pocket in Ir$_0$. Both the UHBs and the LHBs originating from various Ir layers are color coded in the TB results, figure (b), while in the DFT bands, figure (a), only the UHBs can be clearly identified as shown.

Figure 3. Band structure of La$_3$SrIrO$_4$ computed using DFT (a) and the tight-binding model (b). The yellow region represents the electron pocket in the UHB for Ir$_1$, while the green region corresponds to the hole pocket in Ir$_0$. Both the UHBs and the LHBs originating from various Ir layers are color coded in the TB results, figure (b), while in the DFT bands, figure (a), only the UHBs can be clearly identified as shown.

anti-ferromagnetic order as appropriate for a single Ir layer in SIO, keeping the two spin-orbital entangled $J_{\text{eff}} = 1/2$ orbitals ($|e_1\rangle$ and $|e_2\rangle$ in equation (1)). The TB Hubbard Hamiltonian is given by

$$\mathcal{H} = \sum_{\langle ij \rangle \alpha} t_{ij} c_{i \alpha}^\dagger c_{j \alpha} + \text{h.c.} + \frac{U}{2} \sum_{i \alpha} n_{i \alpha} n_{i \alpha},$$

where $c_{i \alpha}^\dagger$ creates an electron at site $i$ (which may be sublattice A or B) and orbital $|e_\alpha\rangle$, $t_{ij}$ is the hopping integral, $U$ is the on-site Coulomb interaction, and the summation $\langle ij \rangle$ is over distinct pairs of neighbors. The same model parameters, which we used earlier [34] to describe the bulk band structure of SIO, were adopted here, viz., $U = 0.65, t_1 = -0.095, t_2 = 0.015, t_3 = 0.035, \text{ and } t_4 = 0.01$, all in units of eV, with $t_n$ being the $n$th nearest neighbor hopping. It is reasonable to consider the square lattice model, which is appropriate for a single Ir layer, since the interactions between the individual Ir layers are weak and the bands corresponding to the individual Ir layers may be identified, e.g. in figure 3. In fact, the bulk band structure of SIO is well described by the square-lattice tight binding model.

In the momentum space, the $4 \times 4$ Hamiltonian (two sublattice sites in the AFM unit cell and two orbitals per site) becomes block diagonal with two identical $2 \times 2$ TB Hamiltonian matrices in the Bloch function basis for $|e_1\rangle$ or $|e_2\rangle$, viz.,

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} -\Delta & h_{11}(\mathbf{k}) \\ h_{12}(\mathbf{k}) & \Delta + h_{11}(\mathbf{k}) \end{pmatrix},$$

where $h_{11}(\mathbf{k}) = 4t_2 \cos k_x \cos k_y + 2t_3 (\cos 2k_x + \cos 2k_y), h_{12}(\mathbf{k}) = 2t_1 (\cos k_x + \cos k_y) + 4t_4 (\cos 2k_x \cos k_y + \cos 2k_y \cos k_x)$, the lattice constant of the square lattice is taken as one, and $\Delta = U/2 \times (n_1 - n_2)$ is the Hartree–Fock staggered field with $n_\alpha$ being the occupancy of the $|e_\alpha\rangle$ orbital. One immediately gets the eigenvalues

$$\varepsilon_{\pm}(\mathbf{k}) = h_{11}(\mathbf{k}) \pm \sqrt{\Delta^2 + h_{12}(\mathbf{k})^2},$$

which are plotted in figure 3(b), where the TB bands for the individual Ir layers are shifted somewhat to fit with the DFT bands.

The bands originating from the various Ir layers are shown in figure 3(b), and the UHBs can be clearly identified in the DFT bands, figure 3(a), as well. Note that the staggered field $\Delta = U(n_1 - n_2)/2$ that characterizes the band splitting between the UHB and the LHB, following equation (4), is layer dependent, which leads to different shapes of the bands for different Ir layers, as clearly seen in the TB band structure.

The band structure clearly indicates that the $\delta$-doped electrons occupy the UHB of the Ir$_0$ and Ir$_1$ layers. In addition, the layer resolved Ir densities-of-states (DOS) shown in figure 4 confirms the same picture. We estimated the amount of $\delta$-doped charge in each layer by integrating the layer projected DOS, which yields 64% for Ir$_0$, 18% for Ir$_1$, and the remaining 18% shared among other atoms. These are the charge density values listed in table 1.
4.2. Fermi surface: electron and hole pockets

The Fermi surface, shown in figure 5, consists of a hole pocket at \( \Gamma \) and an electron pocket at \( M \). An interesting point is that the electrons and holes are spatially separated, with the electron pocket occurring in the Ir\(_1\) layer, while the hole pocket occurs in Ir\(_0\). The presence of both an electron and a hole pocket is quite unusual and it happens because of the presence of multiple bands in the electronic structure, with the nearly empty bands behaving as electrons, while the nearly filled bands behaving like holes. We note that this feature is not always found, e.g. in the La\(\delta\)-doped perovskite La\(_{5}\)Sr\(_{1−δ}\)TiO\(_3\), where also a 2DEG is found along with multiple bands, there is only electron-like behavior [25]. Transport measurements should show the presence of these two different types of carriers, unraveling this unusual behavior.

4.3. Magnetic moments

The 2DEG alters the magnetic moments of the Ir atoms near the \( \delta \)-doped layer. The computed spin and orbital magnetic moments given in table 1 shows that both the spin and orbital magnetic moments, \( \mu_s \) and \( \mu_l \), are zero for Ir\(_0\) making it non-magnetic, while for Ir\(_1\) they are roughly half of the bulk moments given in table 1 shows that both the spin and orbital magnetic moments are zero for Ir\(_0\) making it non-magnetic and Ir\(_2\) and Ir\(_{-1}\) layers. For these layers, the calculated net magnetic moment is 0.39 \( \mu_B \) compared to the calculated \( \approx 0.36 \mu_B \) for the bulk [34]. The experimental magnetic moment in the bulk has been estimated to be 0.5\( \mu_B \) from magnetic susceptibility measurements [36]. We note that while the Ir\(_0\) layer is non-magnetic and Ir\(_2\) and Ir\(_{-1}\) are already bulk like as seen from table 1, interestingly, Ir\(_{1}\) has an electron dopant concentration of \( x_c = 0.18 \) electrons, which is close to the predicted concentration of \( x_c \sim 0.15 \), beyond which the anti-ferromagnetic state becomes unstable [24]. Thus, even though we obtain the Ir\(_1\) layer to be AFM from the DFT calculations, the state could be close in energy to a paramagnetic state or a spiral state (the FM state is a special case of the spiral state).

5. Summary

In summary, we predicted the formation of a spin-orbital entangled 2DEG in the \( \delta \)-doped iridate La\(_{5}\)Sr\(_2\)IrO\(_4\), where a single layer of SrO is replaced by LaO in the Sr\(_2\)IrO\(_4\) crystal. The doped electron remains close to the interface, which becomes metallic, with an electron and a hole pocket forming the Fermi surface, while the bulk, away from the interface is insulating. Experimental observation of the 2DEG would be quite interesting as it would result in a novel, spin-orbital entangled electron gas, with properties quite different from the 2DEG in the 3d oxide structures such as the well-studied LaAlO\(_3\)/SrTiO\(_3\) interface.

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