Recent ARPES Results from 4d & 5d TMOs (Sr$_2$RhO$_4$, Sr$_2$IrO$_4$)

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Effect of the Octahedra Rotation on the Electronic Structure of $\text{Sr}_2\text{RhO}_4$

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Outline

- Background - (Sr,Ca)$_2$RuO$_4$
- ARPES data from Sr$_2$RhO$_4$ – Missing $d_{xy}$ Fermi Surface
- Comparison with Band Calculation
- Summary – Octahedra Rotation Effect on the Electronic Structure
Phase diagram of $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$


Mott transition

Orbital Selective Mott Transition (OSMT)
Various ground states are realized by structural distortions.
4d transition-metal oxide

• Large spatial extent of 4d orbitals
  → large bandwidth, large $10Dq$.
  → tends to be weakly-correlated.
• Low-spin configuration is expected.

$\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$
$\text{Sr}_2\text{RhO}_4$

$10Dq$
$t_{2g}$
$xy$
$yz, zx$
Rotation brings about:

- Doubling of the unit cell
- Decrease of M-O-M bond angle

which cause:

- Band folding
- Bandwidth narrowing

Fig. 1. Structure diagram of the Sr$_2$RhO$_4$ with I4$_1$/acd space group showing the RhO$_6$ octahedra rotation at $z = 1/8$ and $z = 3/8$ in ref. 4. The dotted lines show the structure of Sr$_2$Ru with I4/mmm space group.
Unit cell doubling and band folding

1D

\[ a \]

\[ 2a \]

2D

\[ (\pi,\pi) \]

\[ \Gamma \]
**Band width narrowing**

- **Octahedra rotation**
- Decrease of M-O-M bond angle
- Decrease in hopping energy $t$
- Increase in $U/t$

Metal, small $U/W$

Insulator, large $U/W$
ARPES data on Ca-doped SRO

S.-C. Wang et al. PRL 93,177007 (2004)

ARPES signal is generally broad and weak.
• Share same crystal structure with Sr$_2$RuO$_4$.
• 5 electrons in 4$d$ orbitals.
• Rotation angle $\sim 10^\circ$.
• No superconductivity.

Sr$_2$RhO$_4$ presents an opportunity to study the effect of rotation without “disorder”.
Similar to $\rho(T)$ in $\text{Sr}_2\text{RuO}_4$

- Large anisotropy
  \[ \frac{\rho_c}{\rho_{ab}} (3K) = 2400 \]
- $T^2$-dependence
  Fitting with $\rho = \rho_0 + AT^2$
  \[ \rho_{ab} (T) \quad A_{ab} = 6.26 \times 10^{-3} \, \mu\Omega \text{cm/K}^2 \]
  \[ \rho_c (T) \quad \rho_0 = 20.1 \, \text{m}\Omega \text{cm} \quad A_c = 10.55 \, \mu\Omega \text{cm/K}^2 \]
- Below $\sim 250$ K, $\rho_c$ decreases with lowering temperature.
- No superconducting transition was observed down to 36 mK.

$\text{Sr}_2\text{RhO}_4$ is a two-dimensional Fermi liquid.
Expected FS of $\text{Sr}_2\text{RhO}_4$

By doping one electron: (rigid-band model)

$\alpha$

$\beta$

$\gamma$

Hase et al. J. of solid state chemistry 123,186 (1996)

We expect basically similar FS topology in $\text{Sr}_2\text{RhO}_4$
**ARPES measurements**

High energy ARPES
- ALS BL 7
  - Analyzer: Scienta 100
  - Temperature: 40K
  - Total Energy Resolution: 40 meV
  - Angular Resolution: 0.25°
  - Photon energy: 85 eV
  - Sample cleaved *in situ*

Low energy ARPES
- SSRL BL
  - Analyzer: Scienta 2002
  - Temperature: 20K
  - Total Energy Resolution: 40 meV
  - Angular Resolution: 0.25°
  - Photon energy: 20 eV
  - Sample cleaved *in situ*
FS of $\text{Sr}_2\text{RhO}_4$

Fermi Surface Mapping

Missing $xy$-band (g)
FS in $\text{Sr}_2\text{RhO}_4$!

B.J. Kim et al.
a hole pocket formed by $xz/yz$ orbital band. ($\alpha$)

an electron pocket formed by $x^2-y^2$ orbital band. ($\delta$)

two electron pockets formed by $xy$ ($\gamma$) and $yz,zx$ band ($\beta$)

**LDA calculation**

**WITHOUT** distortion (rotation of octahedra)

<table>
<thead>
<tr>
<th>Occupation</th>
<th>Value</th>
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<tr>
<td>$\alpha$</td>
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<tr>
<td>$\beta$</td>
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<tr>
<td>$\gamma$</td>
<td>72.5%</td>
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<tr>
<td>$\delta$</td>
<td>7.1%</td>
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</tbody>
</table>
Effects of the rotational distortion

LDA calculation shows disappearance of $\gamma$-FS and $x^2-y^2$ FS.

Other’s result

F. Baumberger et al., PRL 96, 246402 (2006)
Effects of the rotational distortion

Effects of the rotational distortion

Observation of $xy$-band sunken under $E_r$
What about $(\text{Ca,Sr})_2\text{RuO}_4$? - LDA

E. Ko, et al., to appear in PRL
Rotation of the octahedra leads to hybridization of $xy$ and $x^2-y^2$ bands.

Hybridization of $xy$ and $x^2-y^2$ bands results in:
1. transfer of electrons from $yz/zx$ to $xy$ band and
2. disappearance of the $xy$ Fermi surface.

$e_g$ states play vital role in determining electronic structures near $E_f$, and therefore should be included in the theoretical models that deals with 4$d$ TMOs.