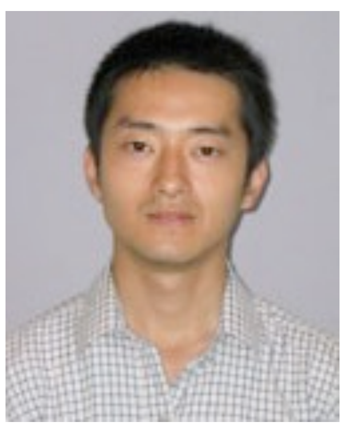
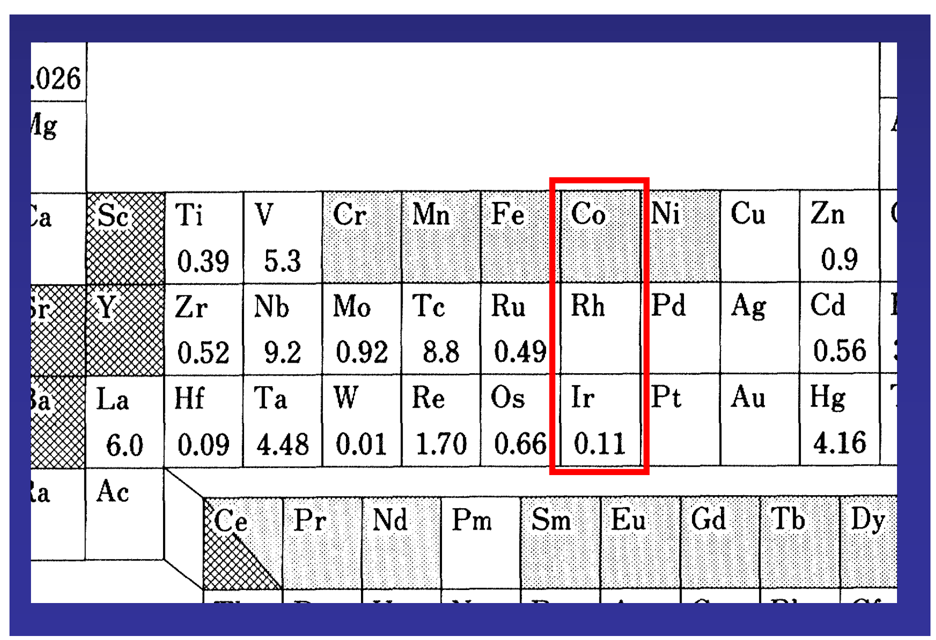


Superconductivity in iridates?
Remarks on (un)doped Sr2IrO4

Fa Wang and T. Senthil, to appear.



Iridium oxide materials: various kinds of exotic physics

$Na_4Ir_3O_8$: insulating quantum spin liquid (Okamoto, Takagi et al, 2007)

Sr_2IrO_4: $J_{eff} = 1/2$ spin-orbit entangled Mott insulator (B.J. Kim et al, 2008)

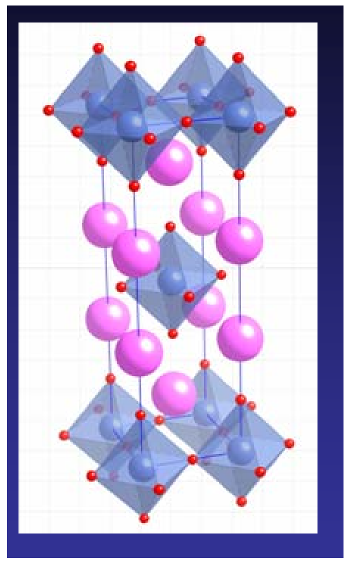
Other interesting proposals:

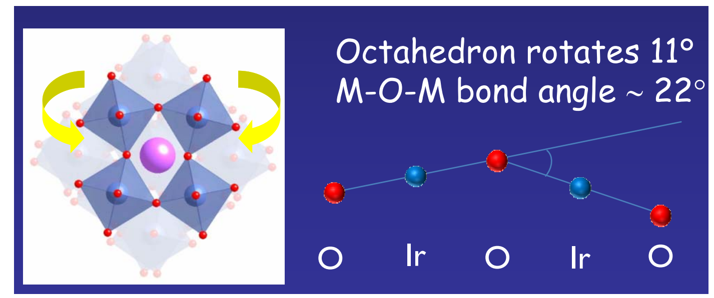
A_2IrO_3: quantum spin Hall effect? (Shitade, Nagaosa et al, PRL 2009), realization of Kitaev spin liquid? (Jackeli, Khaliullin, PRL 2009)

$Ln_2Ir_2O_7$ pyrochlore iridates: 3d correlated topological insulator? (Pesin, Balents, Nat Phys 2010).

Sr2IrO4: prelimaries

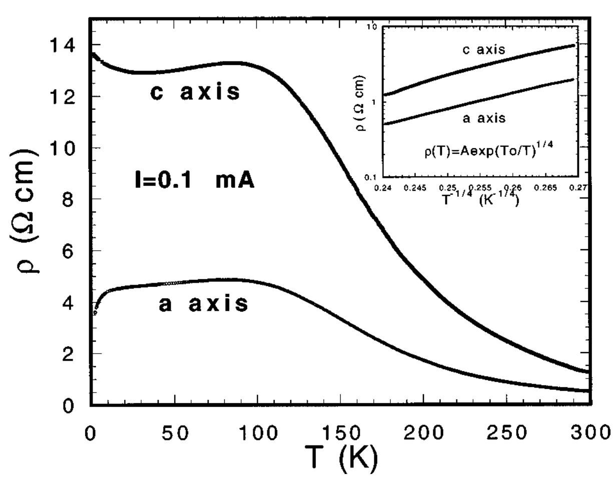
K_2NiF_4 structure similar to La_2CuO_4



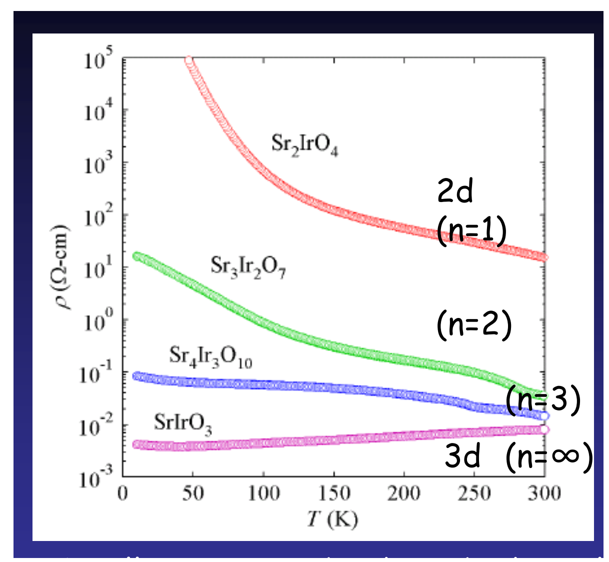


Layers of IrO2 ;
Ir4+ ions on a 2d square lattice.
Each Ir surrounded by O octahedra.

Mott insulator



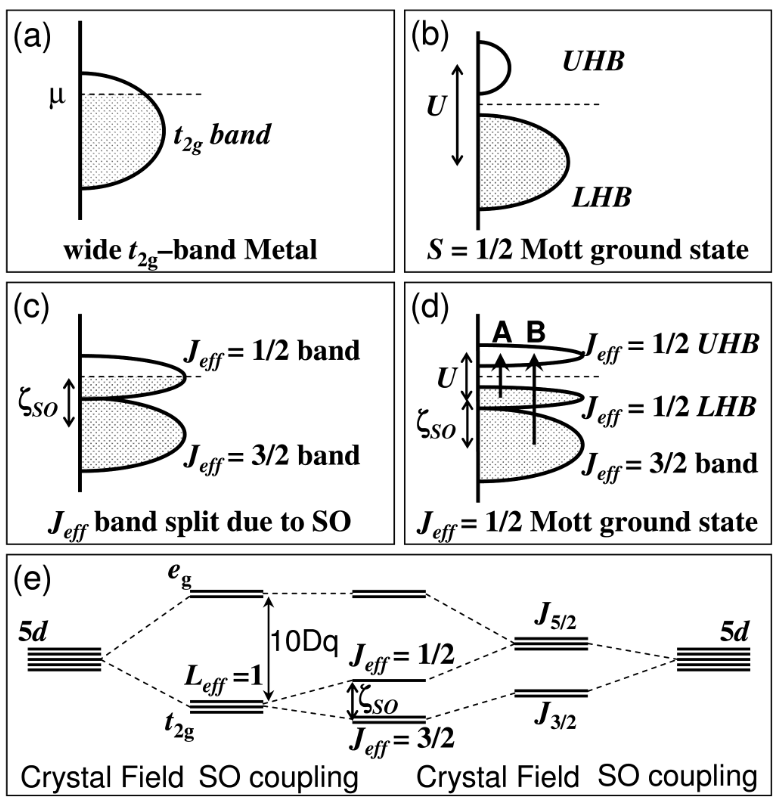
Cao et al, PR B 1998



H. Takagi et al, 2008

Why a Mott insulator?

Ir 4+ is in a $5d^5$ configuration.



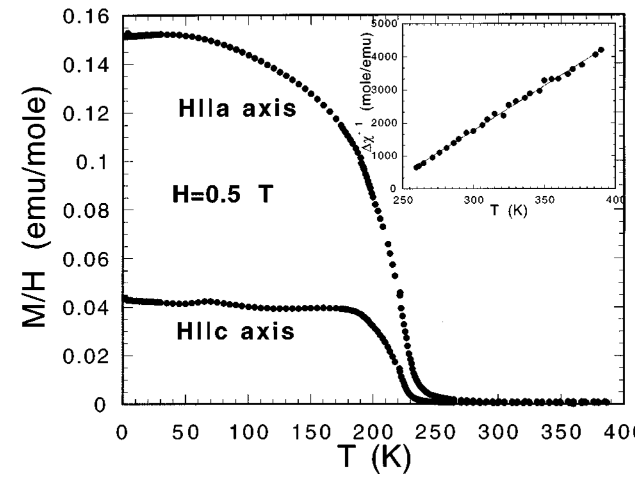
B. J. Kim et al, PRL 08

SO coupling splits t_{2g} level into J_{eff} = 1/2 and J_{eff} = 3/2 bands.

J_{eff} = 1/2 band is half-filled and narrow
=> moderate U can drive it into a Mott insulator

Spin-orbit entangled Mott insulating magnet

$$J_{eff\,1/2} = \frac{1}{\sqrt{3}}\left(|xy, \pm 1/2\rangle \pm |yz, \mp 1/2\rangle + i|zx, \mp 1/2\rangle \right)$$



J_{eff} moments order into a magnetic state below 240 K.
Weak ferromagnetism (from canting of AF moments): 0.14 μ_B

Spin-orbital content confirmed by resonant magnetic X-ray diffraction
(Takagi et al, Science 2009)

A microscopic model

Jin, Jaejun Yu, et al, PR B 2009

Tightbinding model for spin-orbit coupled t_{2g} orbitals projected to $J_{eff} = \frac{1}{2}$ subspace

Spin dependent nearest neighbor hopping between local $J_z = \pm\frac{1}{2}$ states.

$t_0 + i\sigma^z t_1$

$t_0 \approx 0.2eV, t_1 \approx -.04eV$

Further neighbors $t' \approx .05eV, t'' \approx -.02eV$.

On-site Hubbard $U \sim 2eV$

Spin model at half-filling:

$$\mathcal{H}_{\text{spin}} = \sum_{\langle ij \rangle} \left[I_0 \mathbf{J}_i \cdot \mathbf{J}_j + I_1 J_{zi} J_{zj} + \mathbf{D}_{ij} \cdot \mathbf{J}_i \times \mathbf{J}_j \right]$$

Spin canting explained by Dzyaloshinski-Moriya term

Mapping to isotropic model

Sublattice dependent $SU(2)$ spin rotation

$$d_{r\alpha} = \left(e^{i\phi\epsilon_r\sigma^z}\right)_{\alpha\beta} c_{r\beta} \tag{1}$$

gets rid of complex spin dependent hopping.
Rotated basis: Map to isotropic Hubbard model

Wang, TS, 2010

Spin model limit: staggered spin rotation removes anisotropic exchange (Jackeli, Khaliullin, PRL 2009, also Shektman et al, PR L 1992 for cuprates)

Explains success of recent fits of high-T spin correlation length to isotropic Heisenberg AF (Fujiyama, Takagi et al, talk at Highly Frustrated Magnetism conference, 2010) with $J \sim 1000K$.

Compare to cuprate

Effective isotropic Hubbard model parameters:
$t \approx 0.2eV$, $t' \approx \frac{t}{4}$, $t" \approx -\frac{t}{10}$, $U \approx 10t$.

Similar to cuprate?

1. Roughly same parameter range as cuprate Hubbard model except overall energy scale smaller by ≈ 2.
2. t'/t positive for iridate - opposite to cuprate

Doped system - superconductivity?

If the doped square lattice 2d Hubbard model is superconducting, can we expect doping the iridate will give a `high temperature' superconductor?

From comparison to cuprate
(i) $t'/t > 0$ => Electron doping better than hole doping for iridate
(Example: Replace Sr by La)

(ii) Overall energy scale smaller by 2 => Tc in range of 50 K???

Pairing symmetry

In **rotated** basis, expect $d_{x^2-y^2}$ pairs

$$\Delta \sim \sum_r (d_{r\uparrow}d_{r+x\downarrow} - d_{r\downarrow}d_{r+x\uparrow}) - (x \to y) \tag{1}$$

In **lab** basis (i.e undo staggered spin rotation)

$$\Delta = \sum_r cos(\phi)\,(d_{r\uparrow}d_{r+x\downarrow} - d_{r\downarrow}d_{r+x\uparrow}) - (x \to y) - i\sum_r \epsilon_r sin(\phi)\,(d_{r\uparrow}d_{r+x\downarrow} + d_{r\downarrow}d_{r+x\uparrow}) - (x \to y) \tag{2}$$

i.e, a mixture of 'conventional' d-wave singlet pairing and a d-wave 'triplet' centered at (π, π).

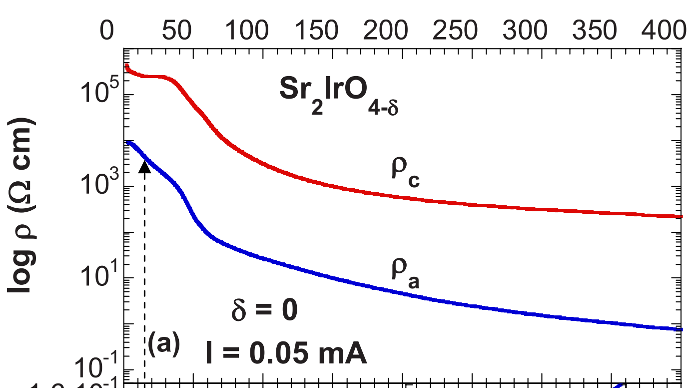
Note: despite apparent complex pair wavefunction, T-reversal preserved.

Differences with cuprates: more coherent c-axis transport?

Interlayer tunneling matrix element in cuprate:
$(cosk_x - cosk_y)^2$ factor which blocks c-axis transport of nodal states.

Iridate: different orbital content implies no suppression of nodal c-axis hopping.

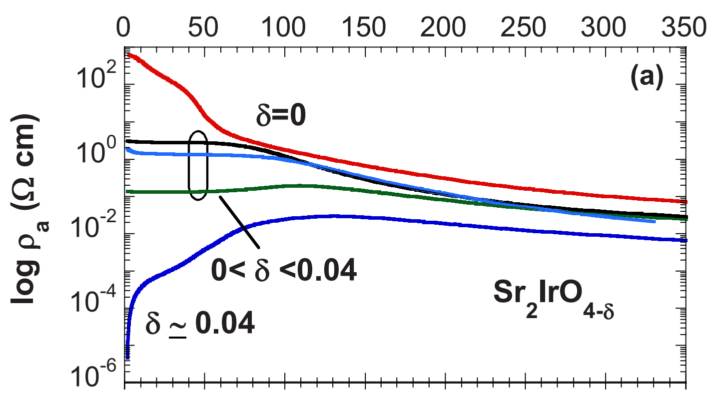
Better c-axis coherence?

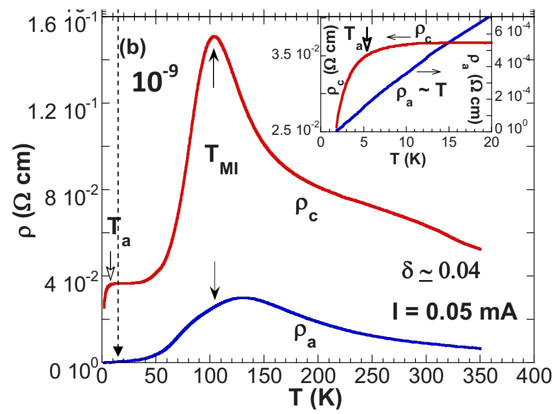


Overall resistivity anisotropy of about 100 in undoped insulator

Experimental prospects?

Recent report: Metal-insulator transition with Oxygen doping





Cornetta, Cao et al, PR B 2010

Will it be possible to dope Sr2IrO4
to higher doping levels?

Summary

Iridium oxides: spin-orbit coupling enhances importance of correlation effects even with moderate U.

Sr2IrO4: spin-orbit entangled moments in a Mott insulator Hubbard model similar to cuprates but smaller overall energy scale.

Doping: Possible high-Tc superconductor, interesting lessons by comparing with cuprates.

Other interesting iridate:
Na2IrO3 - J_{eff} = 1/2 frustrated AF Mott insulator on honeycomb lattice (Singh, Gegenwart, PR B 2010)
Nature yet to be clarified? effects of doping?