Superconductivity in iridates?
Remarks on (un)doped Sr2IrO4
Iridium oxide materials: various kinds of exotic physics

Na4Ir3O8: insulating quantum spin liquid (Okamoto, Takagi et al, 2007)

Sr2IrO4: $J_{\text{eff}} = 1/2$ spin-orbit entangled Mott insulator (B.J. Kim et al, 2008)

Other interesting proposals:


Ln2Ir2O7 pyrochlore iridates: 3d correlated topological insulator? (Pesin, Balents, Nat Phys 2010).
Sr$_2$IrO$_4$: preliminaries

K$_2$NiF$_4$ structure similar to La$_2$CuO$_4$

Layers of IrO$_2$; Ir$^{4+}$ 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.

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

B. J. Kim et al, PRL 08
Spin-orbit entangled Mott insulating magnet

\[ J_{\text{eff}} = \sqrt[3]{\frac{1}{3} \left( \langle xy, \pm 1/2 \rangle \pm \langle yz, \mp 1/2 \rangle \pm i \langle zx, \mp 1/2 \rangle \right)} \]

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

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.

$t_0 + i \sigma^z t_1$

$t_0 \approx 0.2 eV, t_1 \approx -0.04 eV$

Further neighbors $t' \approx 0.05 eV, t'' \approx -0.02 eV$.

On-site Hubbard $U \sim 2eV$

Spin model at half-filling:

$$\mathcal{H}_{spin} = \sum_{\langle ij \rangle} [I_0 \mathbf{J}_i \cdot \mathbf{J}_j + I_1 J_{z i} J_{z j} + \mathbf{D}_{ij} \cdot \mathbf{J}_i \times \mathbf{J}_j]$$

Spin canting explained by Dzyaloshinski-Moriya term
Mapping to isotropic model

Sublattice dependent $SU(2)$ spin rotation

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

(1)

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

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 $J \sim 1000K$. 

Wang, TS, 2010
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 \( \approx 2 \).
2. \( \frac{t'}{t} \) 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) $t’/t > 0 \Rightarrow$ Electron doping better than hole doping for iridate
(Example: Replace Sr by La)

(ii) Overall energy scale smaller by 2 $\Rightarrow$ $T_c$ in range of 50 K???
Pairing symmetry

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

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

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

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

i.e, a mixture of ‘conventional’ d-wave singlet pairing and a d-wave ‘triplet’ centered at $(\pi, \pi)$.

Note: despite apparent complex pair wavefunction, T-reversal preserved.
Differences with cuprates: more coherent c-axis transport?

Interlayer tunneling matrix element in cuprate: 
\((\cos k_x - \cos k_y)^2\) 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?
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.

Sr$_2$IrO$_4$: 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:
Na$_2$IrO$_3$ - $J_{\text{eff}} = 1/2$ frustrated AF Mott insulator on honeycomb lattice (Singh, Gegenwart, PR B 2010)
Nature yet to be clarified? effects of doping?