More or different?
Exploring analogs of the cuprates in other oxides

1. *Pseudogap of metallic layered nickelate $R_{2-x}Sr_xNiO_4$ (R=Nd, Eu) crystals measured using angle-resolved photoemission spectroscopy*
Authors: M. Uchida, K. Ishizaka, P. Hansmann, Y. Kaneko, Y. Ishida, X. Yang, R. Kumai, A. Toschi, Y. Onose, R. Arita, K. Hel, O. K. Andersen, S. Shin, Y. Tokura
arXiv:1012.5516

2. *Phase-Sensitive Observation of a Spin-Orbital Mott State in Sr_2IrO_4*
Authors: B. J Kim, H. Ohsumi, T. Komesu, S. Sakai, T. Morita, H. Takagi, T. Arima
ArXiv:0907.0956 Science, **323** 1329, 2009.

3. *Twisted Hubbard Model for Sr_2IrO_4: Magnetism and Possible High Temperature Superconductivity*
Authors: Fa Wang and T. Senthil
ArXiv:1011.3500

Recommendation and Commentary by Leon Balents, KITP, UCSB

The cuprate family of high temperature superconductors have fascinated condensed matter physicists for about 25 years. A consensus explanation for the many intriguing phenomena (not just superconductivity!) in these materials continues to elude us. An important question is whether there are other materials with properties similar to the cuprates which might shed light upon on the essential microscopic physics. Two recent investigations exploring this question are discussed here.

Paper 1 above describes very recent angle-resolved photoemission studies which reveal strikingly "cuprate-like" behavior in *nickelates*, $R_{2-x}Sr_xNiO_4$. The idea that nickelates might behave similarly to cuprates is not new. Nickelates form the same perovskite-type layered structures, with an underlying square lattice, as do the cuprates. Formally, the Ni^{3+} ionization state is analogous to that of the Cu^{2+} ion in the cuprates, with one unpaired electron in the so-called e_g orbital manifold. However, there are important differences (for example the absence of any binary compounds with Ni^{3+}), so that the idea died out for some time.[1] Recently, it has revived in the context of artificial oxide heterostructures grown as thin films,[2] but this proposal too has so far not been successful.

The material studied in Paper 1 is not a heterostructure but a bulk single crystal of the "214" material, which is the single-layer perovskite structure, where the most two-dimensional behavior would be expected. The paper focuses on the sample with $x = 1.1$, which is analogous to an underdoped cuprate. Several features observed are strikingly similar to the cuprates. The energy integrated spectrum displays a large, hole-like Fermi surface, which seems to fade on approaching the "anti-nodal" points, very reminiscent of the Fermi arcs seen in the cuprates. This picture is reinforced by the energy distribution curves in the anti-nodal region, which shows a broad pseudogap feature over about 0.1eV. Some evidence for kinks in the hole dispersion is also reported, another prominent cuprate feature.

These observations raise many questions. LDA predicts an additional small electron Fermi surface in this material, associated with the two-fold degeneracy of the e_g orbitals. Its absence in the experiment may indicate an unexpectedly large e_g splitting, or simply that the electron pocket is "hiding" at a different k_z not accessible at this photon energy. The mechanism for the pseudogap and arcs is another key issue. Given the predominance of stripe physics in the nickelates, charge ordering or fluctuations may play an important role. Note that superconductivity has *not* been observed here or anywhere else in this material. Why?

Papers 2 and 3 address a much more unlikely candidate for an ersatz cuprate. While Sr_2IrO_4 also has the single-layer cuprate structure, one usually expects very different physics from 5d transition metals like iridium. As a rule, the size of the d orbitals increases on progressing downward in the transition metals, consequently increasing the bandwidth and decreasing the on-site Coulomb repulsion U. Thus Mott insulators and strong correlations are primarily the domain of the 3d's. However, because of its large atomic number ($Z = 77$), iridium also has very strong spin-orbit coupling, of the order of half an electron volt. The spin-orbit coupling in this case splits the orbital degeneracy present in its absence, creating a $j = 1/2$ ionic ground state Kramer's doublet. In the band picture, the usual spaghetti of states near the Fermi level is largely split. The spin-orbit split bands are much narrower than the "bare" 5d bands, and indeed narrow enough in Sr_2IrO_4 that the weak U is sufficient to stabilize a Mott insulator.

Paper 2 directly verifies this picture of a Sr_2IrO_4 as a spin-orbit assisted Mott insulator using resonant x-ray scattering. Based on the selection rules associated with the 2p to 5d transition being probed, B. J. Kim *et al* were directly able to verify the $j = 1/2$ nature of the Ir^{4+} state. Moreover, because

the wavelength of light at this energy in iridium is of order $1\mathring{A}$, spatial information can be obtained. In this way, Sr_2IrO_4 was found to be essentially a Néel ordered two-sublattice antiferromagnet as in the undoped cuprates such as La_2CuO_4, but with a large canting angle of about 10°. This work has shown that iridium oxides are nearly ideal systems for study with resonant x-ray scattering, and further elastic and inelastic studies of these materials are proceeding rapidly in several labs worldwide.

From the above discussion, it is apparent that Sr_2IrO_4 has a single $j = 1/2$ band near the Fermi energy, and has predominantly antiferromagnetic interactions like the cuprates. The authors of Paper 3 push this argument further, and construct a one-band Hubbard model for the $j = 1/2$ states. The most interesting question is the remaining role of the large spin orbit interaction. Wang and Senthil argue that the spin orbit effects appear in the Hubbard model in a form that is "pure gauge", so that the model can be transformed back into the "usual" Hubbard model without spin-orbit coupling. In this way they conclude that electron doped Sr_2IrO_4 should should display high-T_c superconductivity.

Predicting superconductivity is a bold and often frustrating game. Very recent experiments reported in Ref.[3] do *not* find superconductivity in hole-doped $Sr_2IrO_{4-\delta}$, but this could perhaps be blamed on oxygen deficiency in the IrO_2 planes. Alternatively, perhaps the "pure gauge" terms in the Wang-Senthil Hubbard model do not capture all the spin-orbit effects, leading to essential differences between the physics of the cuprates and this iridate.

The experiments and theory described here are just a small part of growing efforts to explore novel correlated oxides, especially off the beaten track. Comparing and contrasting the behaviors of *more* materials that are like the cuprates but *different* will surely lead to a better understanding of the physics of strong correlations and superconductivity.

References

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[2] Jiri Chaloupka and Giniyat Khaliullin. Orbital Order and Possible Superconductivity in $LaNiO_3/LaMO_3$ Superlattices. *Phys. Rev. Lett.*,

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[3] O. B. Korneta, Tongfei Qi, S. Chikara, S. Parkin, L. E. De Long, P. Schlottmann, and G. Cao. Electron-doped $Sr_2IrO_{4-\delta}$ $(0 \leq \delta \leq 0.04)$: Evolution of a disordered $J_{eff} = \frac{1}{2}$ Mott insulator into an exotic metallic state. *Phys. Rev. B*, 82(11):115117, Sep 2010.