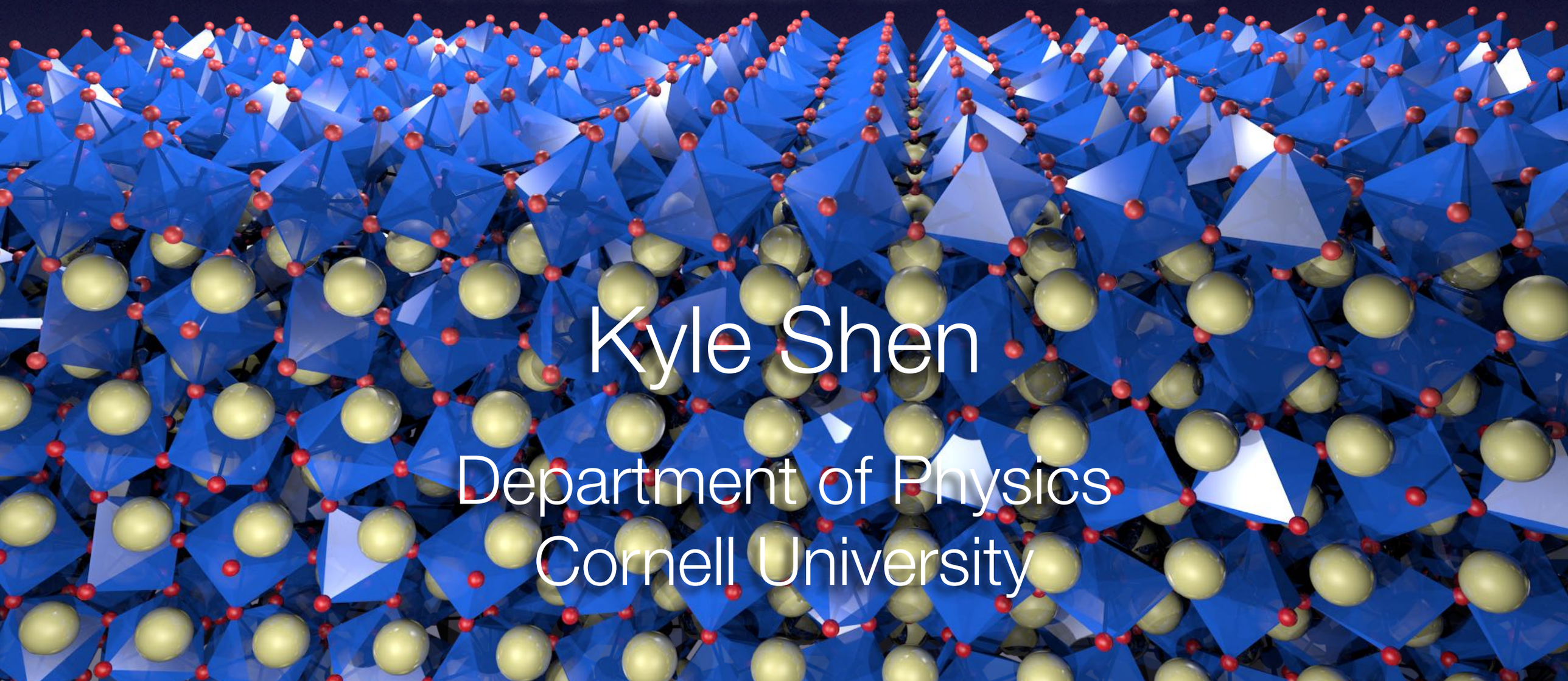
KITP LS Matter Workshop July 2015

Interplay of Spin-Orbit Coupling, Dimensionality, and Coulomb Interactions in Iridate Thin Films & Artificial Quantum Wells



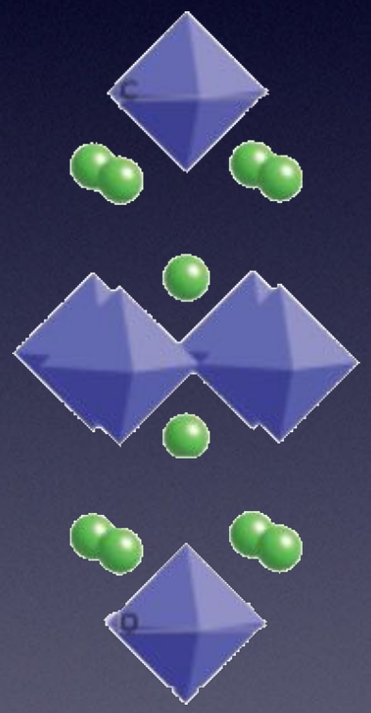
Kyle Shen

Department of Physics
Cornell University

Ruddlesden-Popper series of iridates : $Sr_{n+1}Ir_nO_{2n+1}$

2D → **3D**

Sr_2IrO_4
Ba_2IrO_4



J_{eff} = 1/2
AF insulator

$Sr_3Ir_2O_7$

J_{eff} = 1/2
AF semiconductor

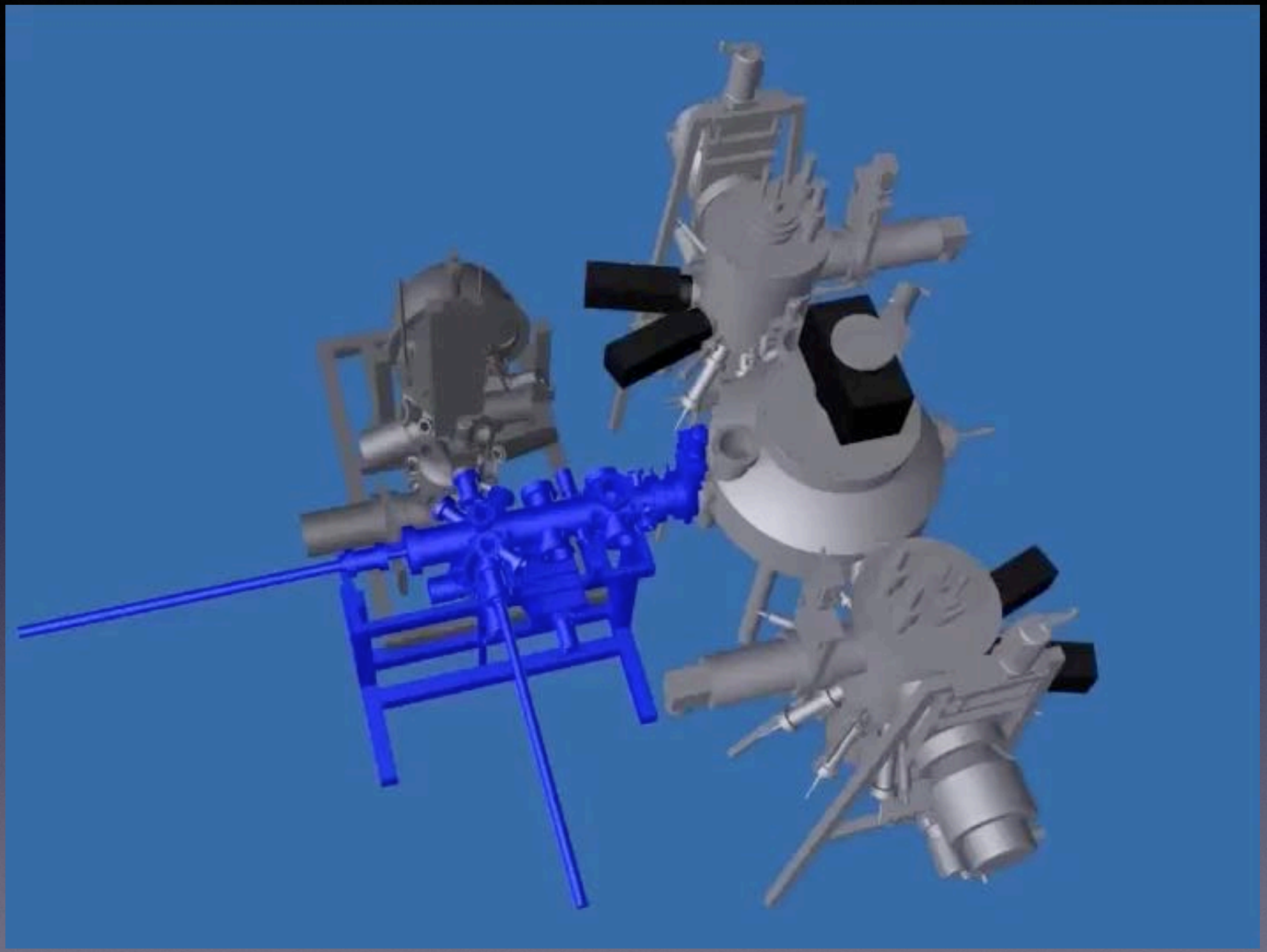
$SrIrO_3$

semimetallic

integrated ARPES & oxide MBE system

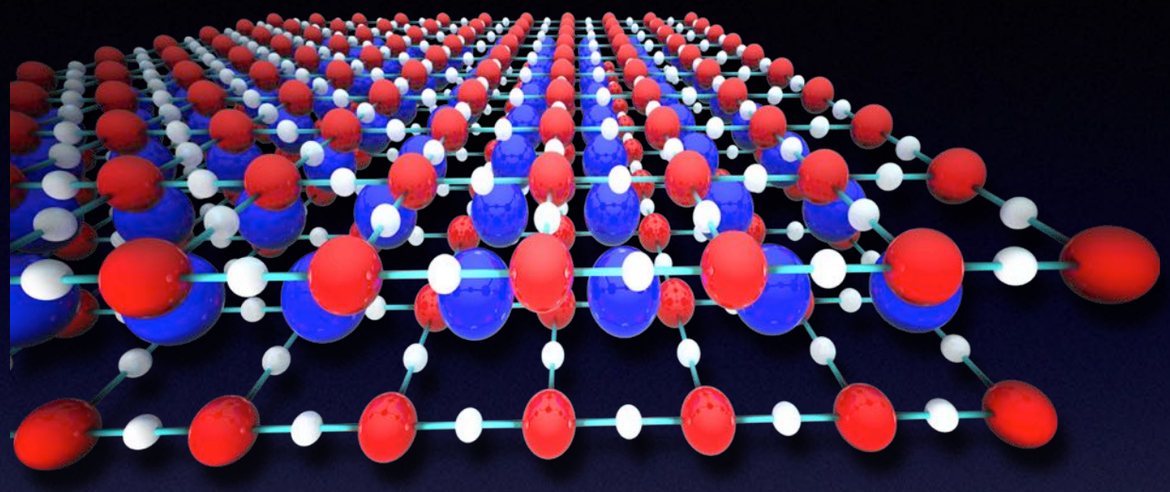
Darrell Schlom

integrated ARPES & oxide MBE system



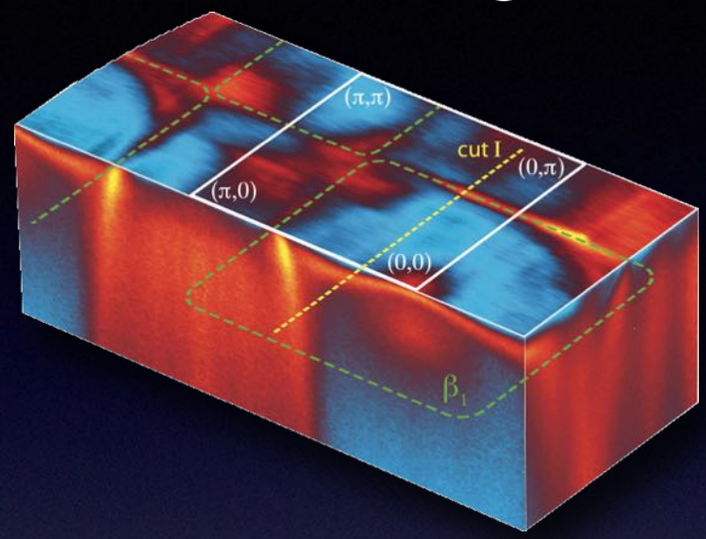
some recent work involving this system

archetypal cuprate : $SrCuO_2$



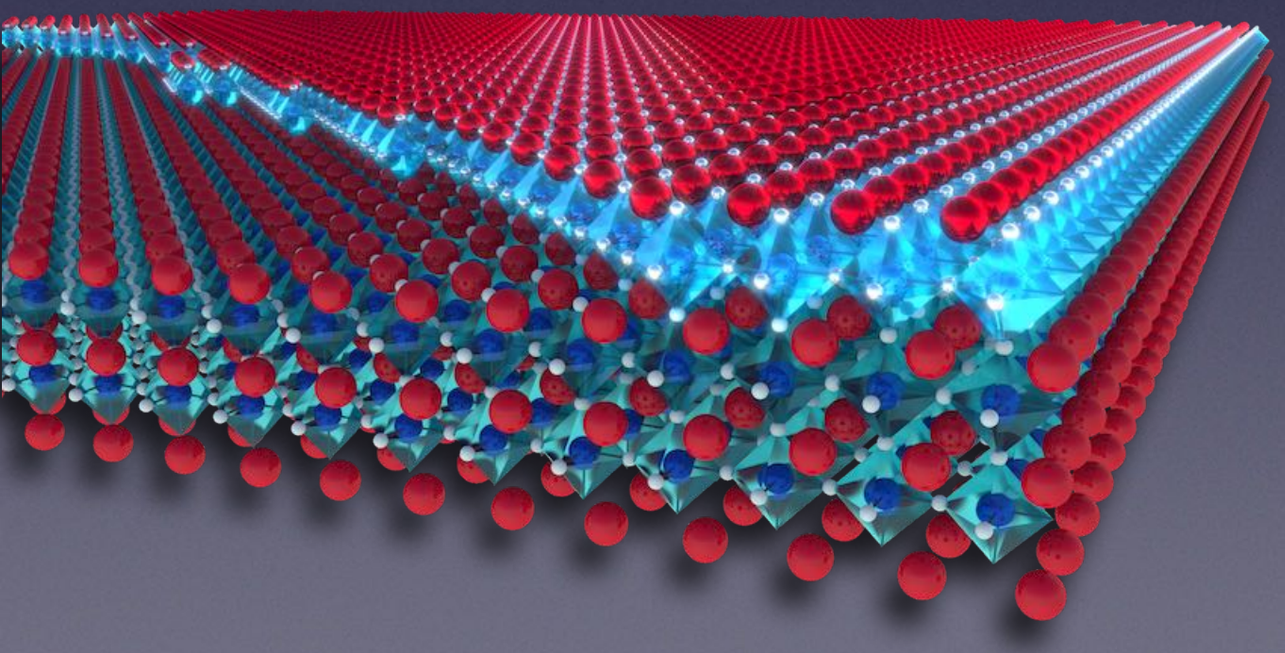
J.W. Harter et al., *Phys. Rev. Lett.* **109**, 267001

correlated ferromagnet : $SrRuO_3$



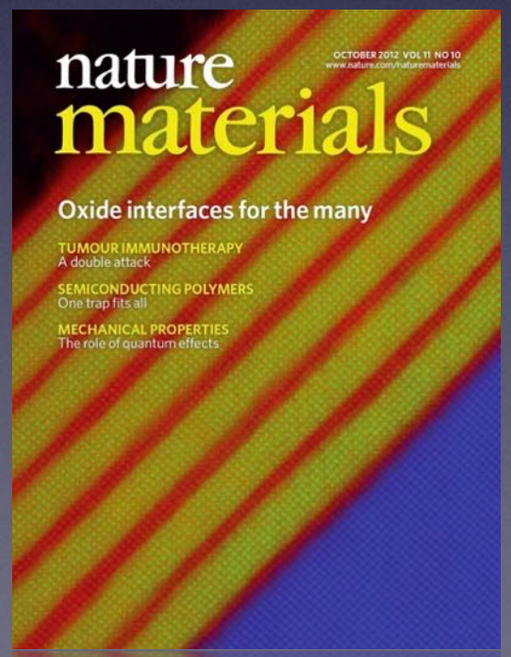
D.E. Shai et al., *Phys. Rev. Lett.* **110**, 087004

atomically thin nickelates : $LaNiO_3$



P.D.C. King et al., *Nature Nanotechnology* **9**, 443

oxide interfaces : $LaMnO_3$ / $SrMnO_3$



E.J. Monkman et al., *Nature Materials* **11**, 855

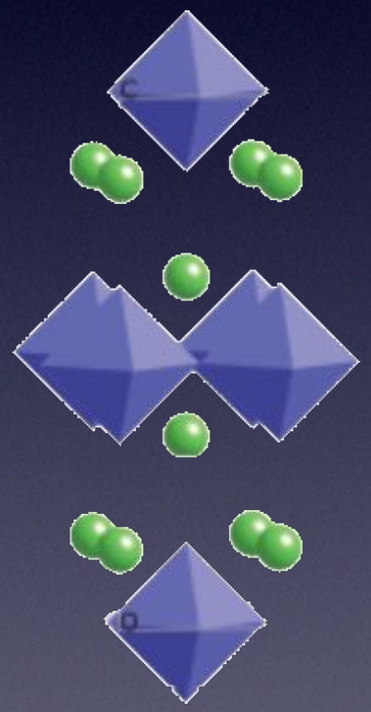
Ruddlesden-Popper series of iridates : $Sr_{n+1}Ir_nO_{2n+1}$

2D → **3D**

Sr_2IrO_4
Ba_2IrO_4

$Sr_3Ir_2O_7$

$SrIrO_3$



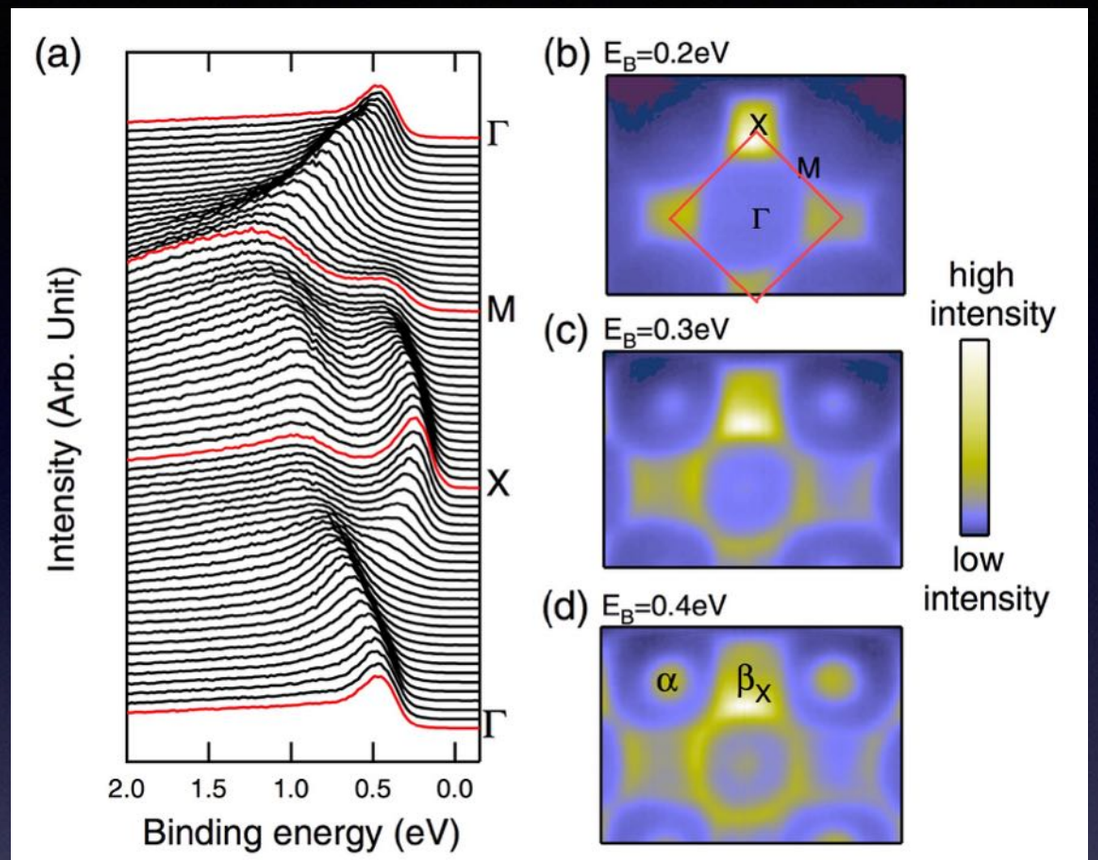
- what are the many-body interactions for a single hole in the undoped insulator?
- generic behavior for different parent insulating iridates?
- similarities / differences with undoped parent cuprates?

J_{eff} = 1/2
AF insulator

J_{eff} = 1/2
AF semiconductor

semimetallic

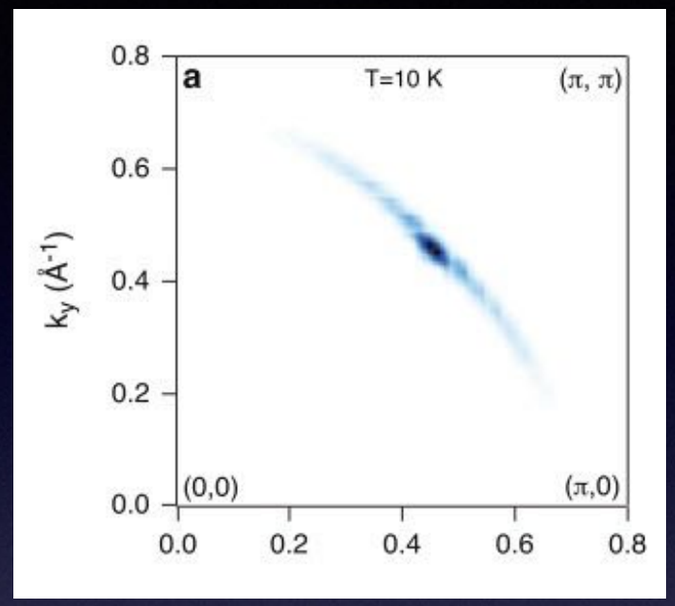
electronic structure of Sr_2IrO_4 : J_{eff} = 1/2 insulator



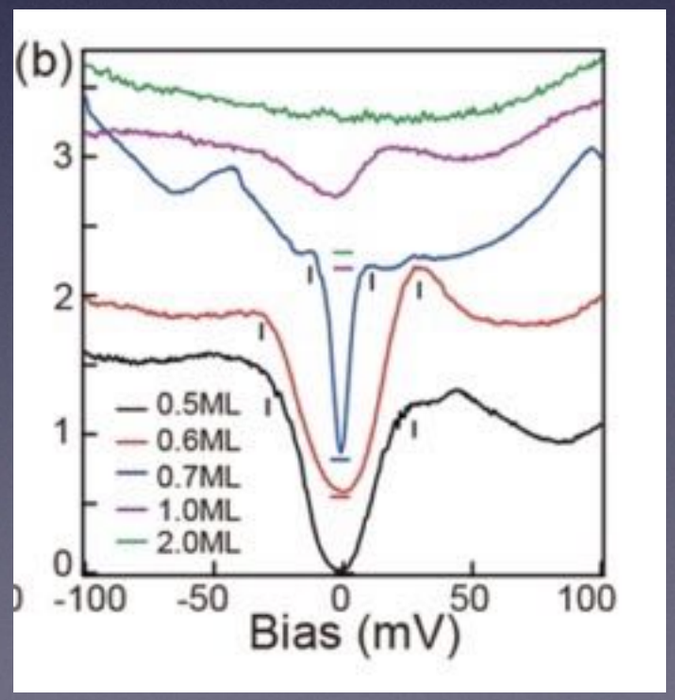
G. Cao et al., *Phys. Rev. B* **57**, 11039 (1998)

B.J. Kim et al., *Phys. Rev. Lett.* **101**, 076402 (2008)

high-T_c superconductivity?



Y.K. Kim et al., *arXiv* 1506.06639



Y.J. Yan et al., *arXiv* 1506.06557

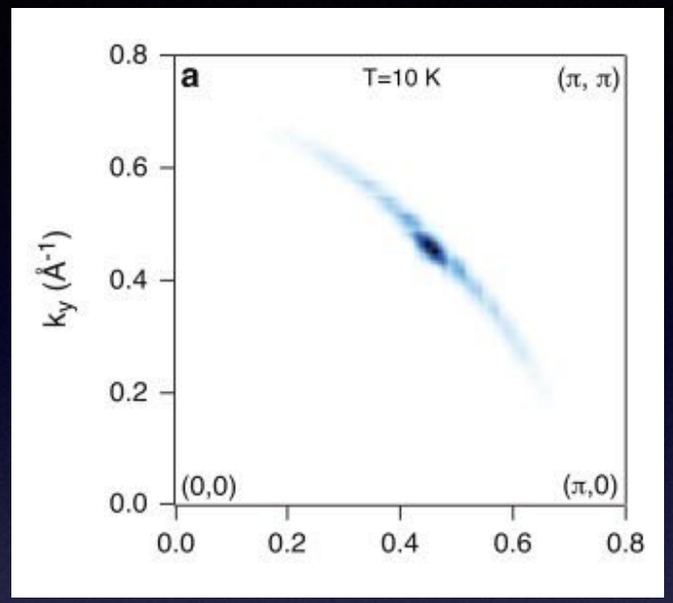
electronic structure of Sr_2IrO_4 : J_{eff} = 1/2 insulator

high-T_c superconductivity?

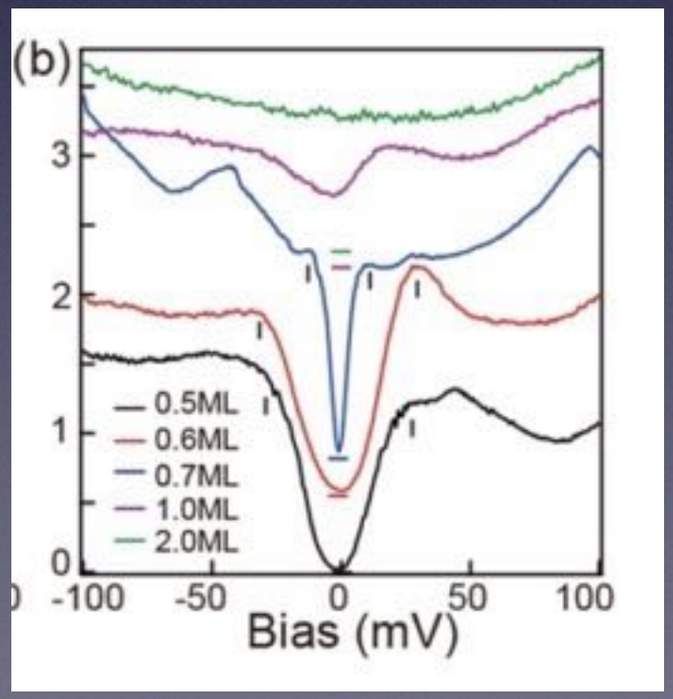
Similarities between Undoped Cuprates & Iridates

- *S* or *J* = 1/2 Heisenberg antiferromagnet
- Comparable values of exchange *J* ~ 100 meV
- Correlated insulator with ~ 1-2 eV charge gap
- Hopping integrals are similar (scaled within factor of 2) by particle-hole transformation

any other similarities between parent cuprates & iridates?



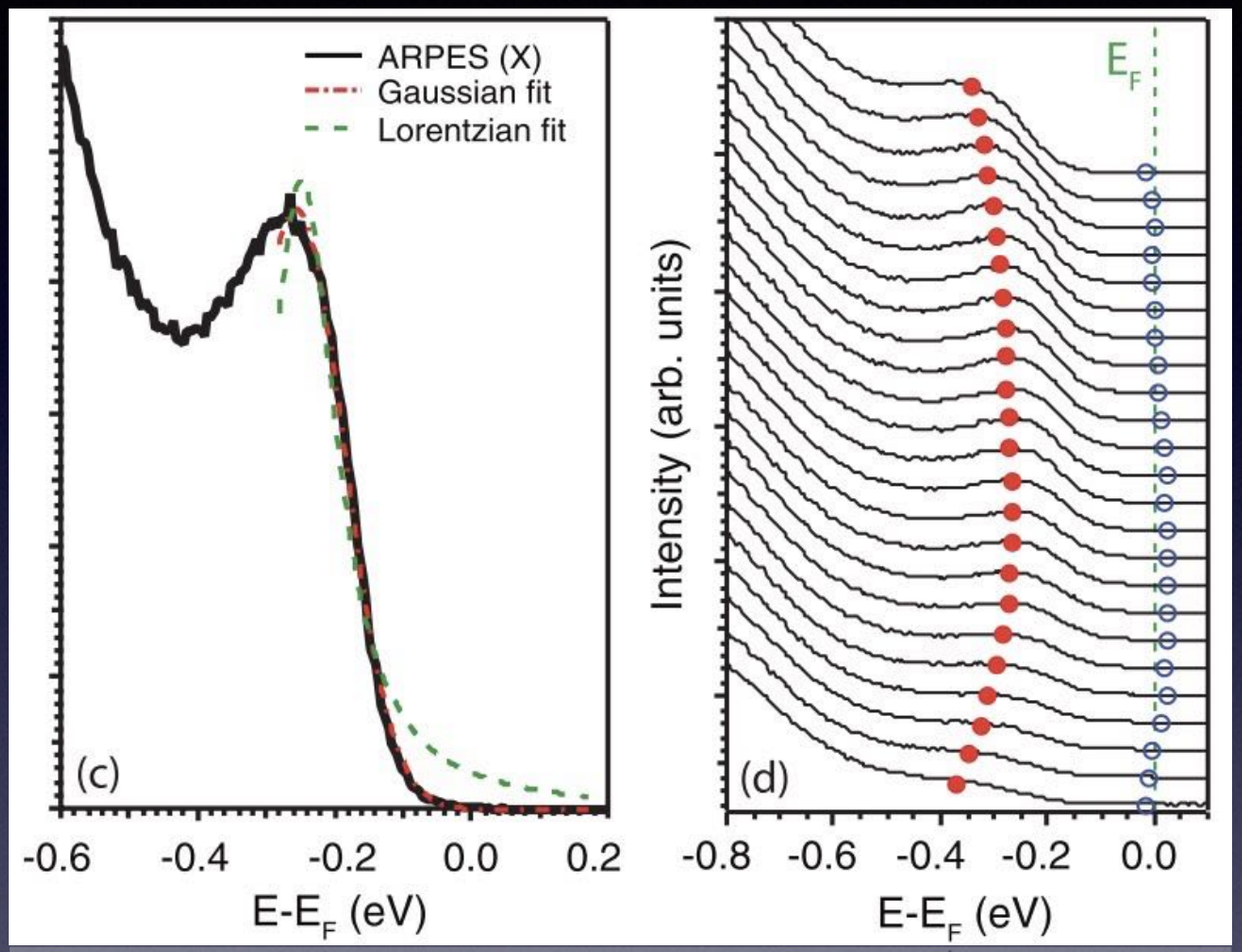
Y.K. Kim et al., *arXiv* 1506.06639



Y.J. Yan et al., *arXiv* 1506.06557

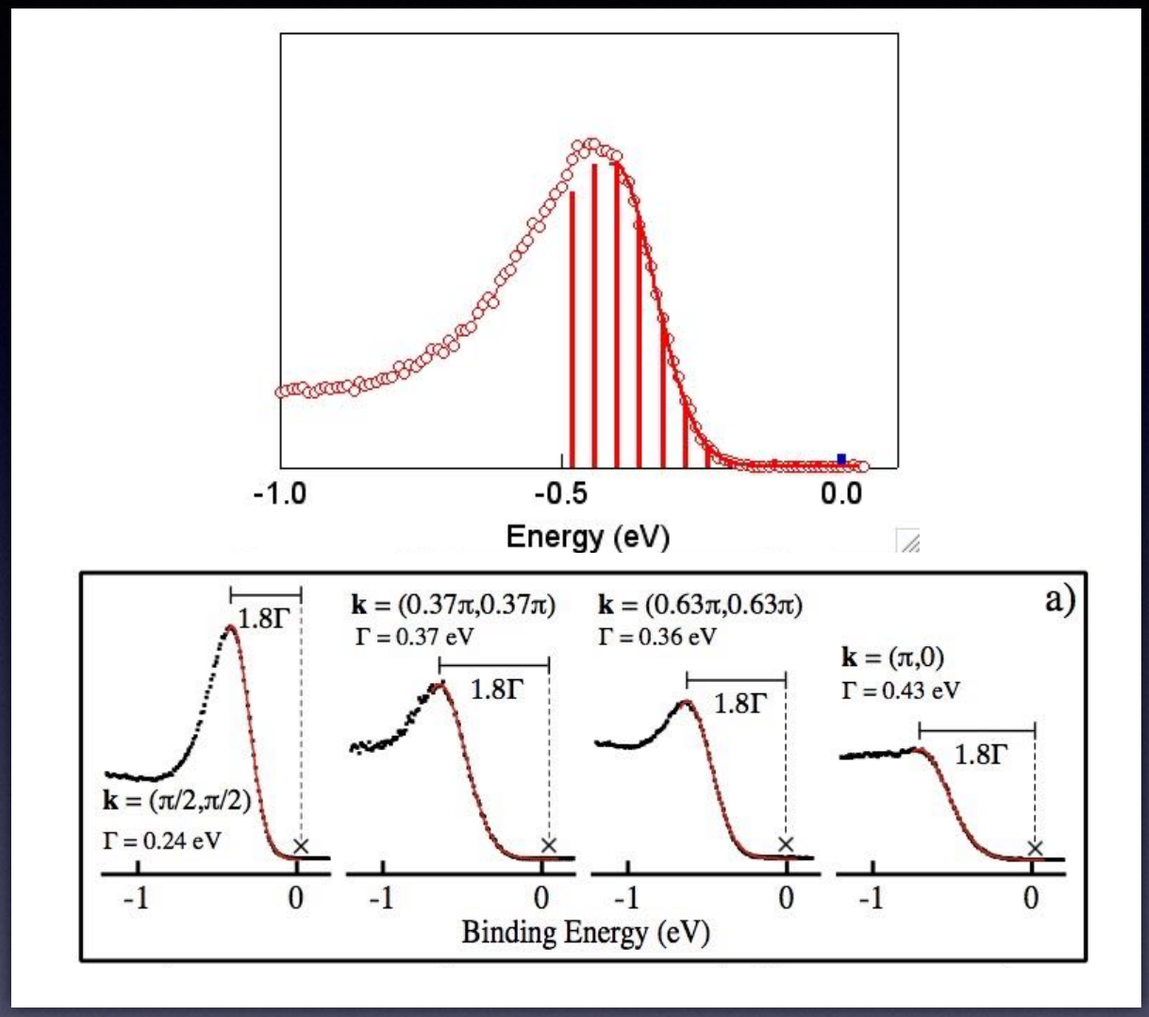
a single hole in Sr_2IrO_4 & $Ca_2CuO_2Cl_2$: polaron formation

Sr_2IrO_4



Phys. Rev. B **87** 241106R (2013)

$Ca_2CuO_2Cl_2$



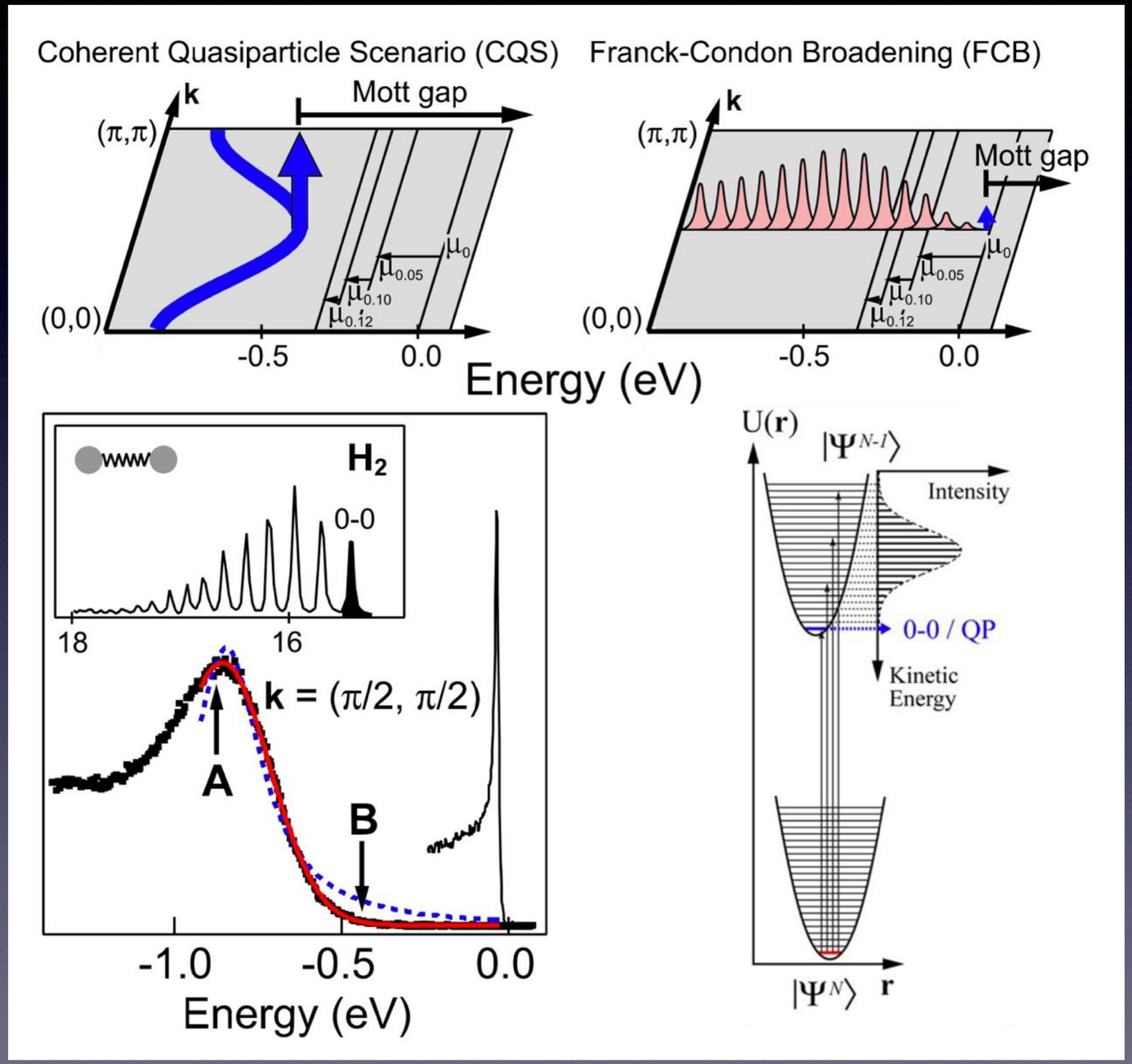
KMS et al. *Phys. Rev. Lett.* **87**, 267002
KMS et al. *Phys. Rev. B* **75**, 075115

- very broad, non-Fermi liquid lineshapes (Gaussian vs. Lorentzian)
- chemical potential pinned well above the peak location
- strong temperature & momentum dependent broadening


P.D.C. King, K.M.S, H. Takagi, F. Baumberger

Franck-Condon broadening for small polarons

Parent cuprate $Ca_2CuO_2Cl_2$

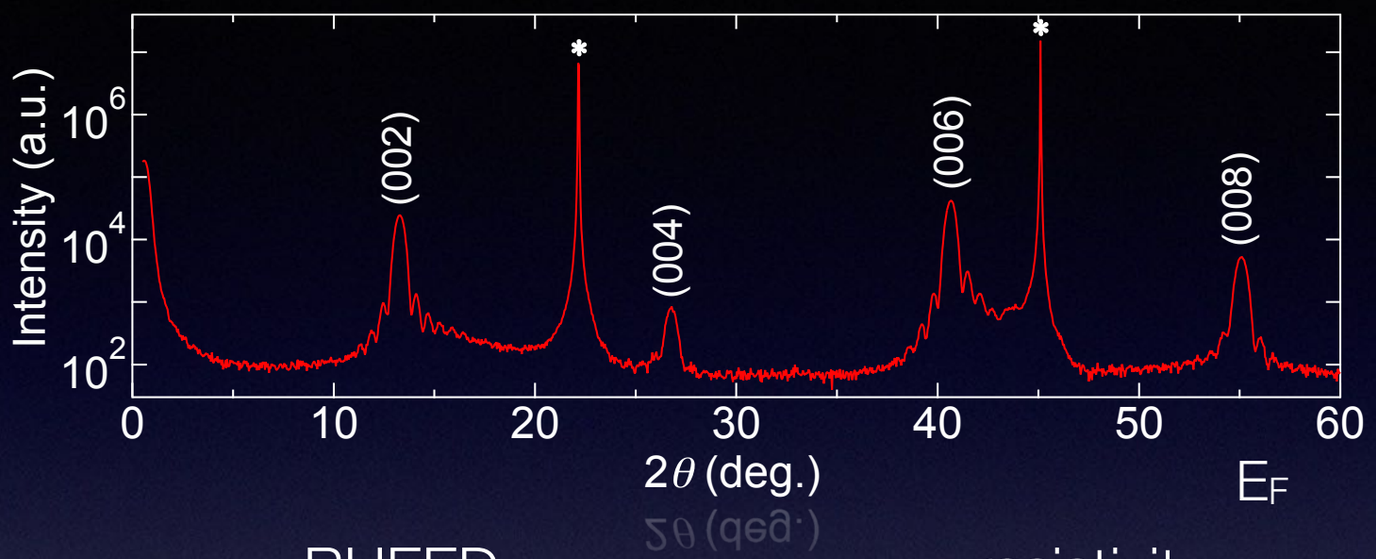


K.M.S. *et al.*, *Phys. Rev. Lett.* **93**, 267002

K.M.S. *et al.*, *Phys. Rev. B* **75**, 075115

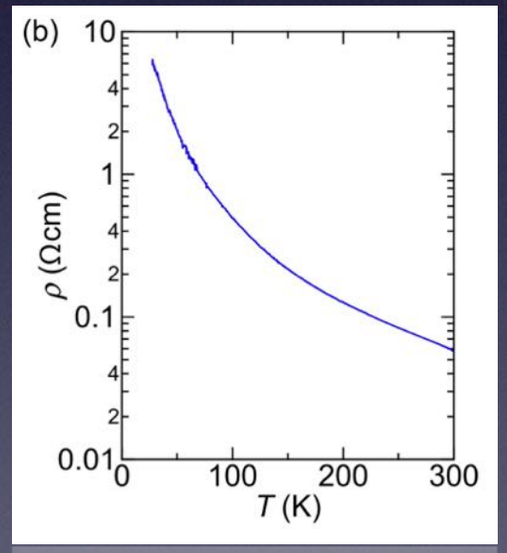
structure & properties of Ba_2IrO_4 thin films

x-ray diffraction



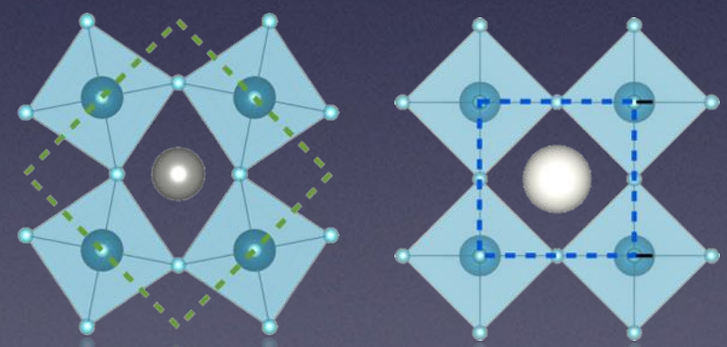
RHEED

resistivity



- MBE-grown epitaxial thin films grown on $PrScO_3$ at 800° C at 10^{-6} torr of 100% O_3 (adsorption controlled)
- films typically ~ 10-20 nm; a = 4.021 A; c = 13.34 A

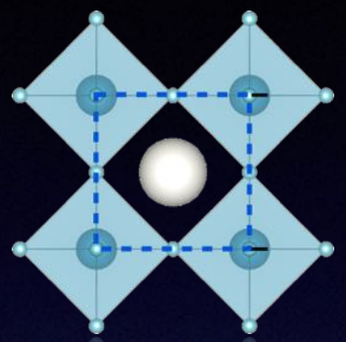
Sr_2IrO_4 Ba_2IrO_4

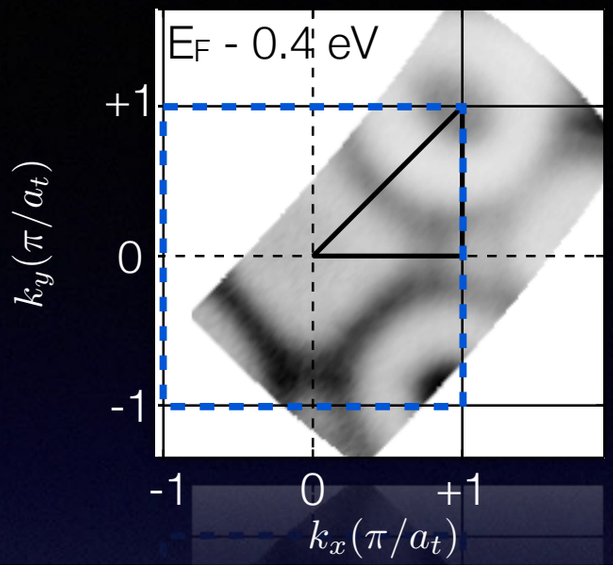


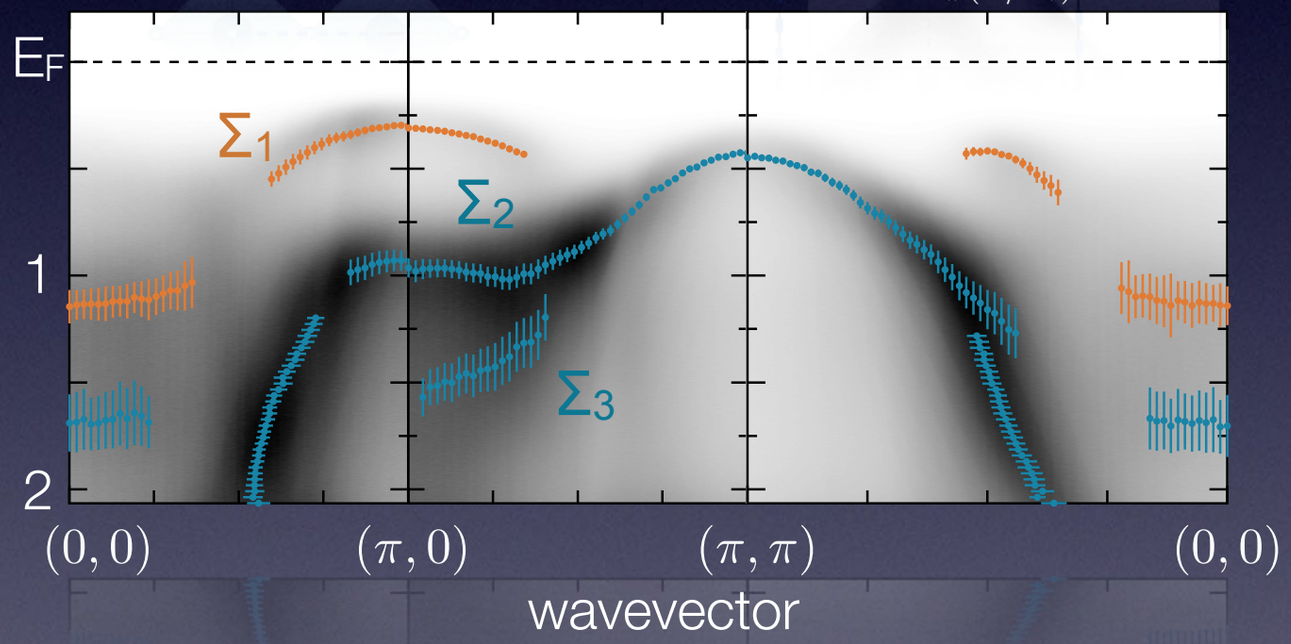
M. Uchida et al., *Phys. Rev. B* **90**, 075142 (2014)

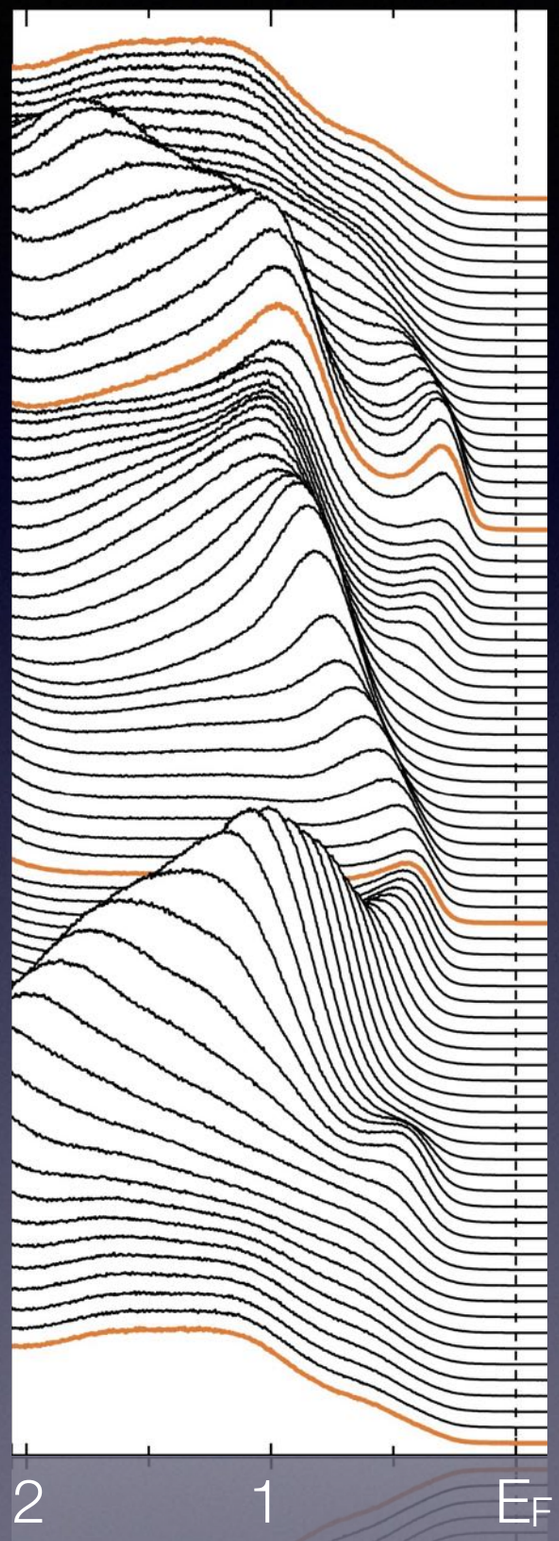
comparison of electronic structure of Sr_2IrO_4 vs Ba_2IrO_4

Ba_2IrO_4







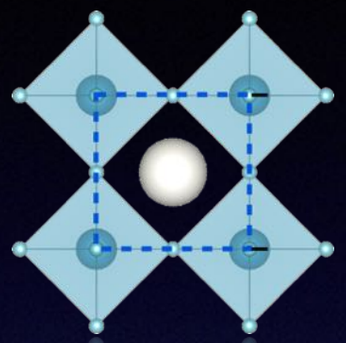


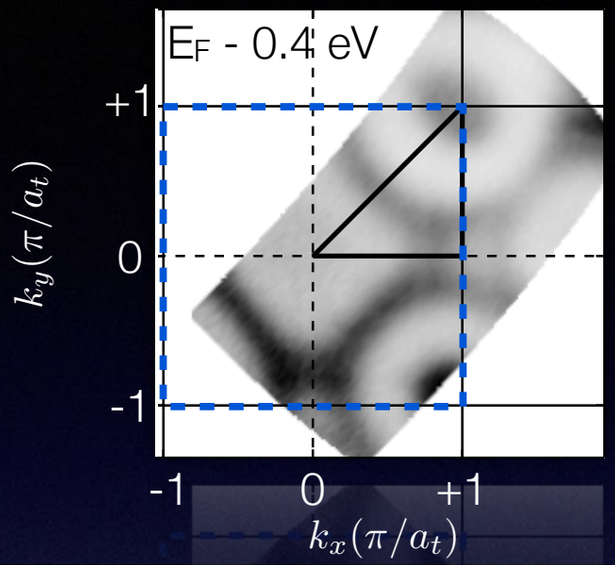
M. Uchida et al., *Phys. Rev. B* **90**, 075142 (2014)

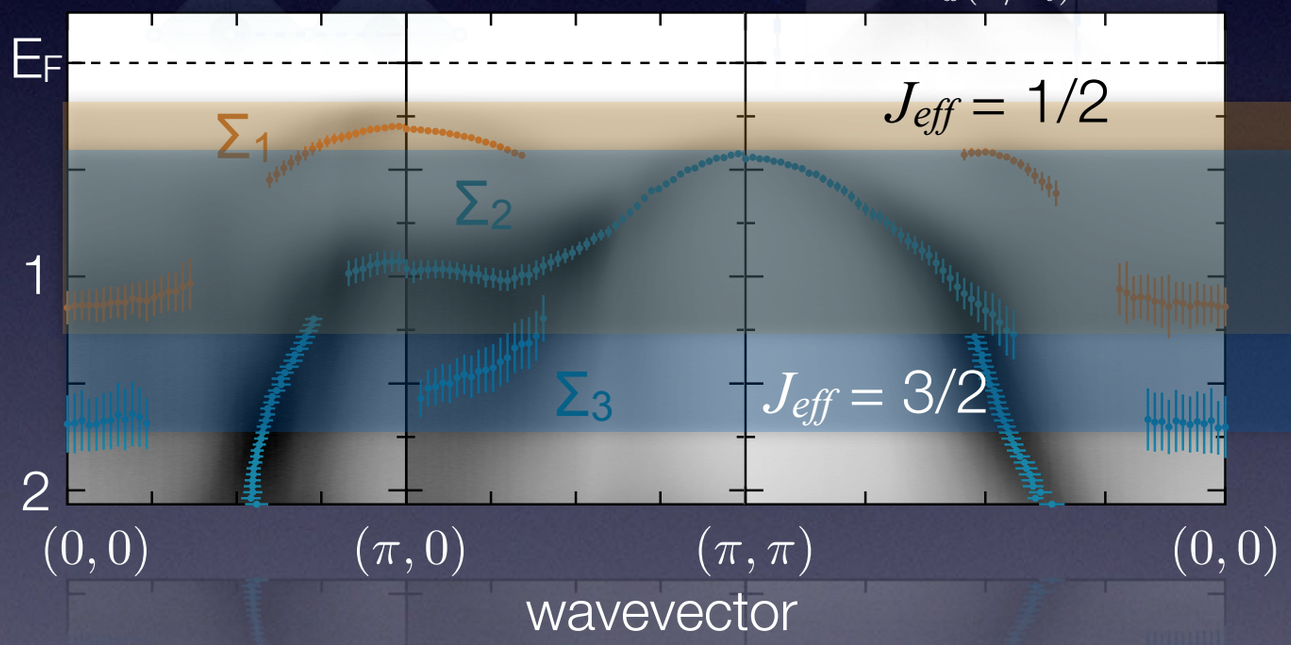
*see also S. Moser, M. Grioni et al., *N.J. Phys* **16**, 013008 (2014)

comparison of electronic structure of Sr_2IrO_4 vs Ba_2IrO_4

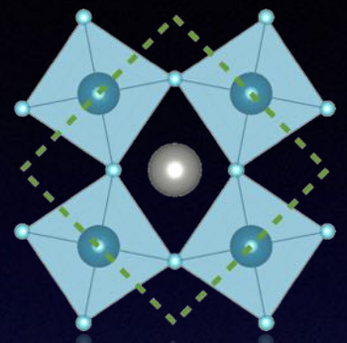
Ba_2IrO_4

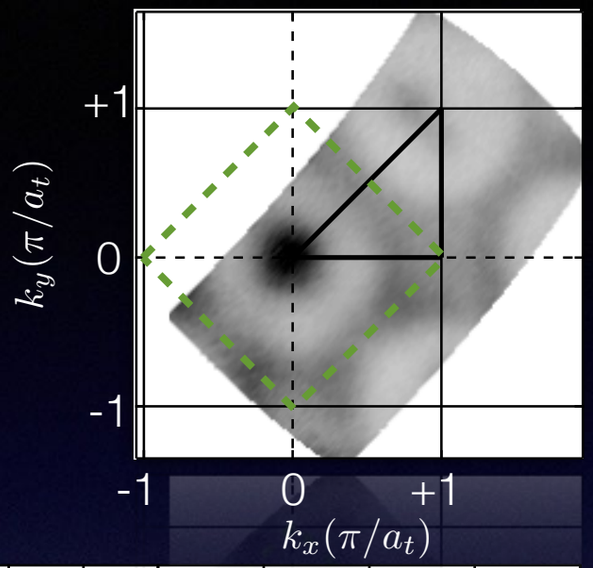


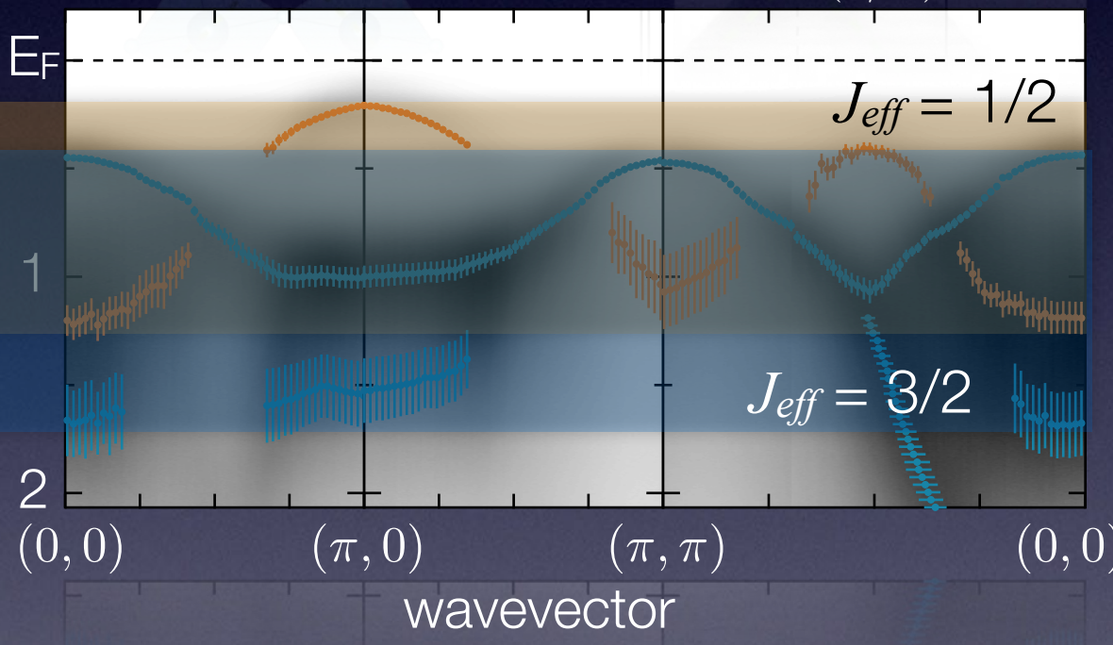




Sr_2IrO_4







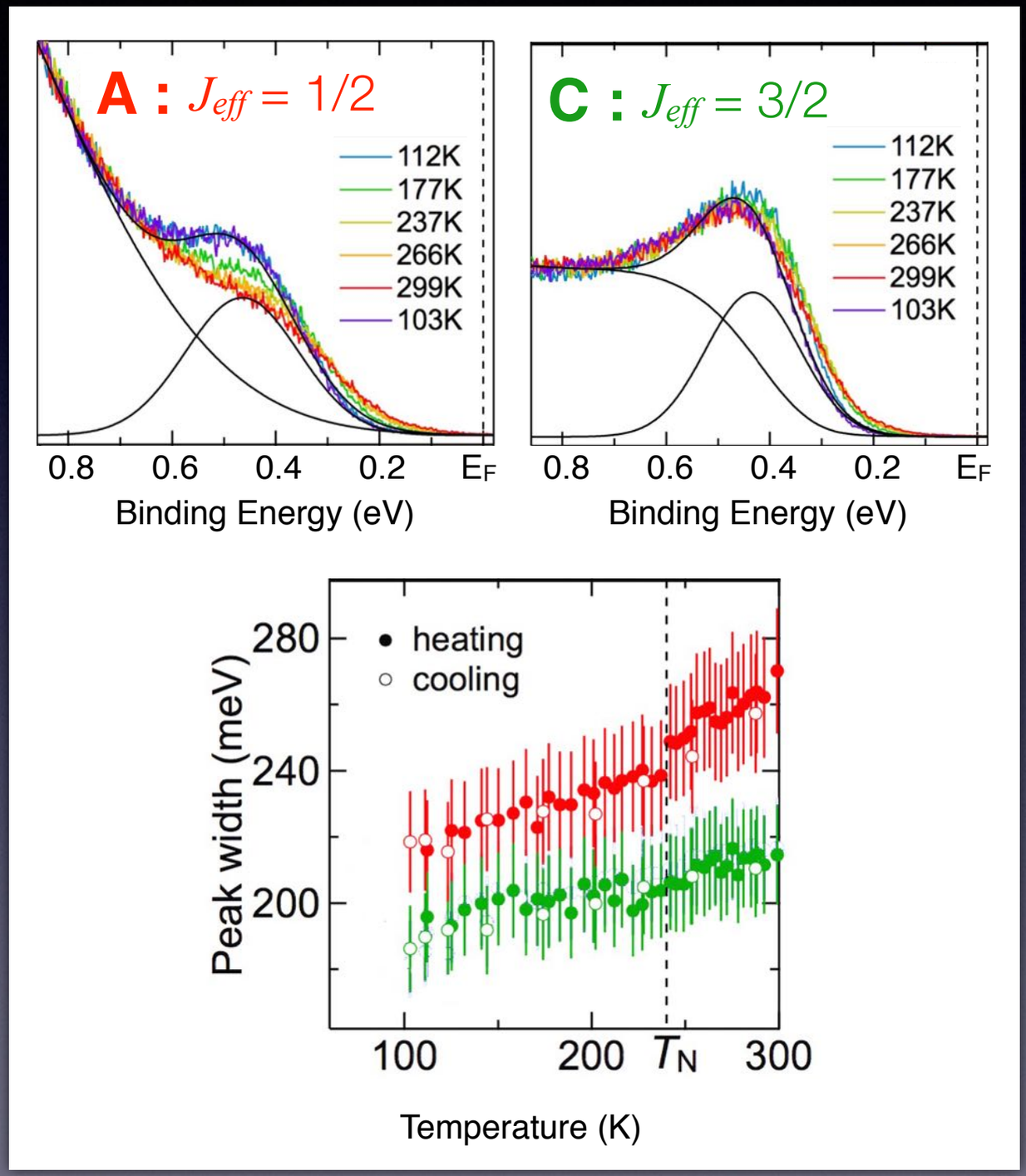
- Sr_2IrO_4 & Ba_2IrO_4 show quantitatively similar bandwidths and band positions (to within 10% for the lowest energy states)

M. Uchida et al., *Phys. Rev. B* **90**, 075142 (2014)

*see also S. Moser, M. Grioni et al., *N.J. Phys* **16**, 013008 (2014)

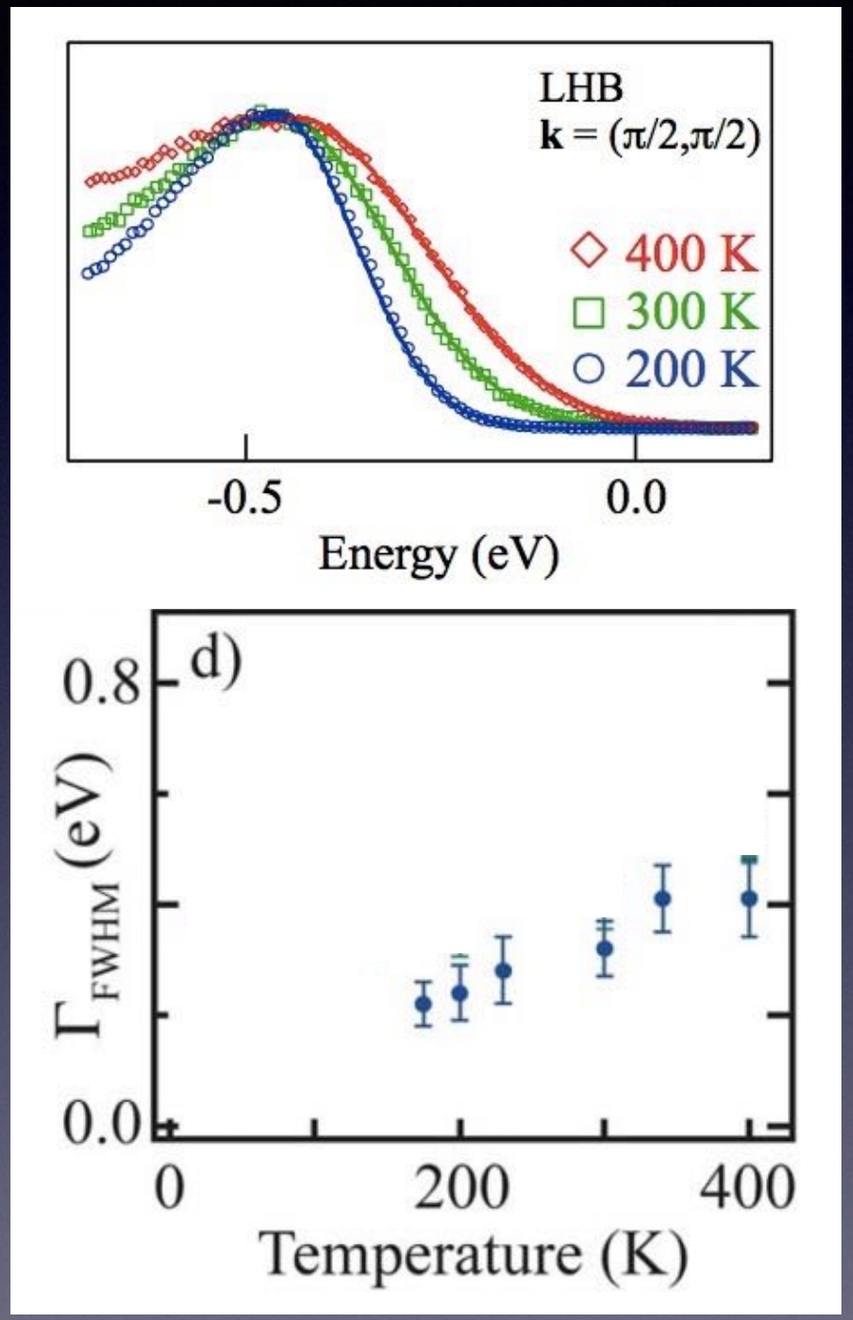
temperature dependence of Franck-Condon broadening

Ba_2IrO_4



M. Uchida et al., *Phys. Rev. B* **90**, 075142 (2014)

$Ca_2CuO_2Cl_2$



KMS et al., *Phys. Rev. B* **75**, 075115

Ruddlesden-Popper series of iridates : $Sr_{n+1}Ir_nO_{2n+1}$

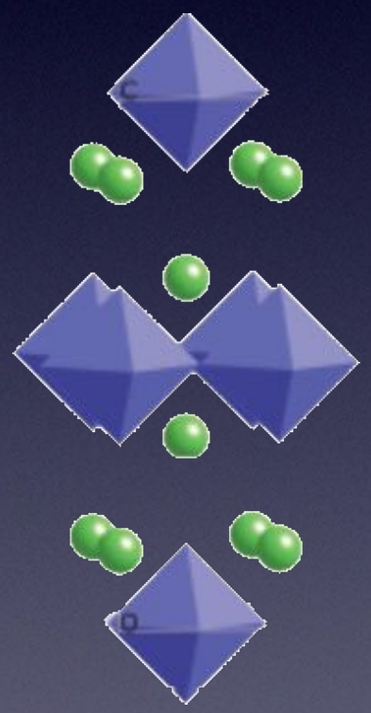
2D → **3D**

Sr_2IrO_4
Ba_2IrO_4

$Sr_3Ir_2O_7$

$SrIrO_3$

- how does the electronic structure of $Sr_3Ir_2O_7$ (bilayer) compare to Sr_2IrO_4?
- does polaron formation persist in $Sr_3Ir_2O_7$?



J_{eff} = 1/2
AF insulator

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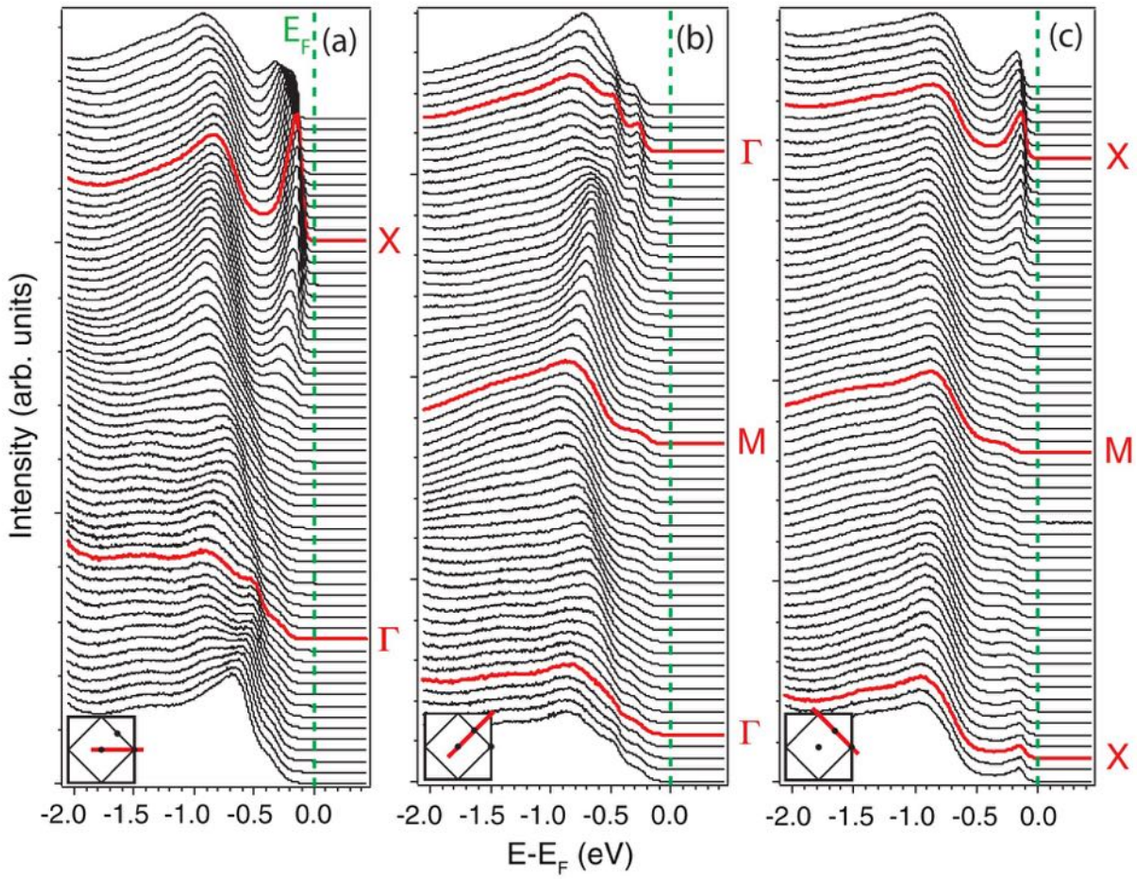
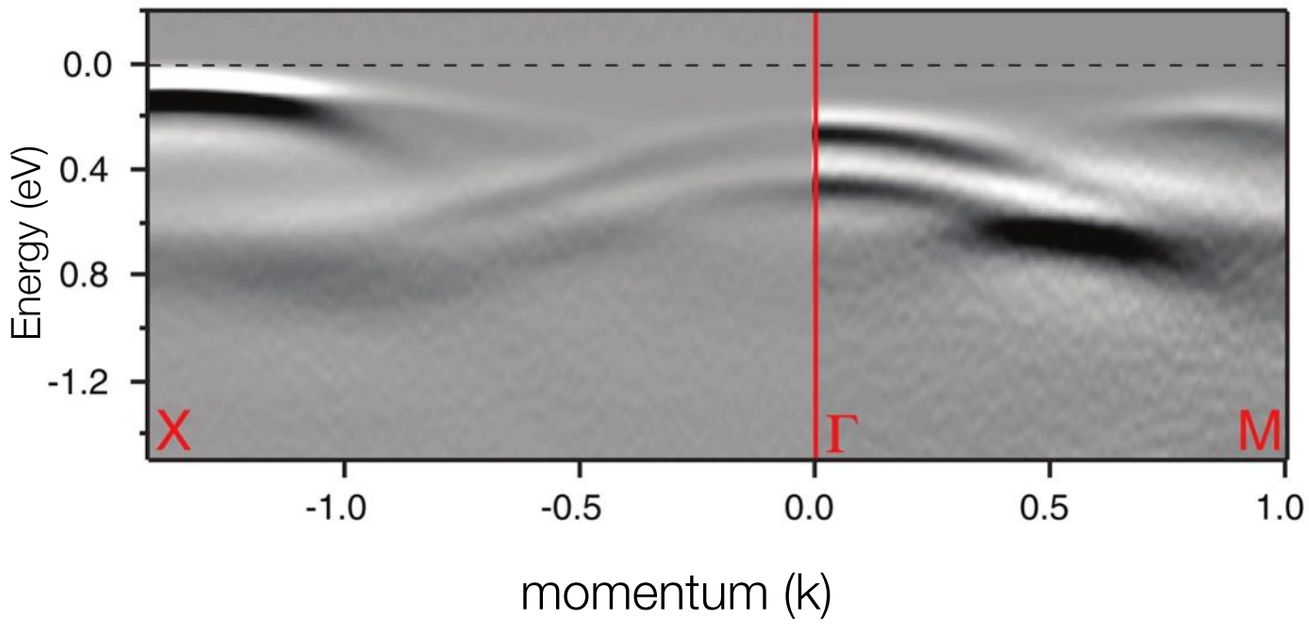
electronic structure of $Sr_3Ir_2O_7$





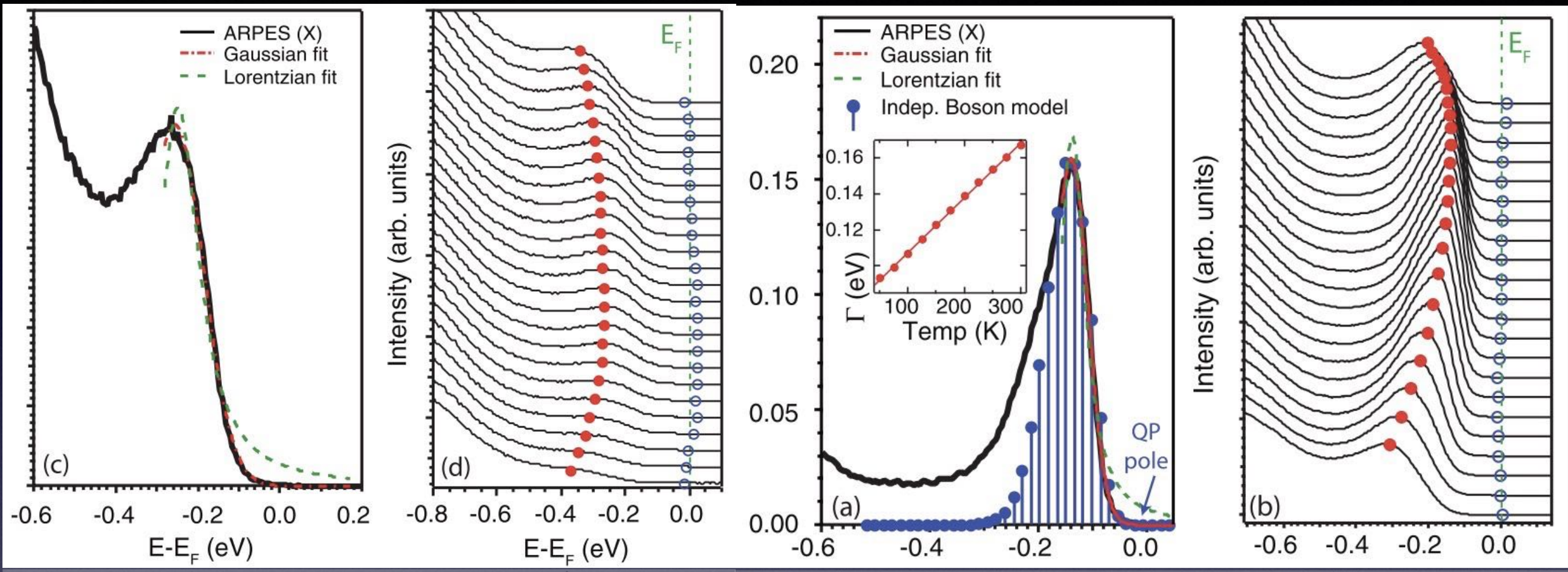
- bandwidths similar to Sr_2IrO_4, but with bilayer splitting, qualitatively consistent with LDA +SO+U (band maximums incorrect)
- LHB maximum pinned close to E_F (consistent with optical measurements)


P.D.C. King, K.M.S, H. Takagi, F. Baumberger
Phys. Rev. B **87** 241106R (2013)

*see also : L. Moreschini, M. Grioni et al., *PRB* **89**, 201114R (2014)
Q. Wang, D.S. Dessau et al., *PRB* **87**, 245109 (2013)
B.M. Wojek, O. Tjernberg et al., *J.Phys.C* **24**, 415602 (2012)

polaron formation also exists in $Sr_3Ir_2O_7$

Sr_2IrO_4 $Sr_3Ir_2O_7$

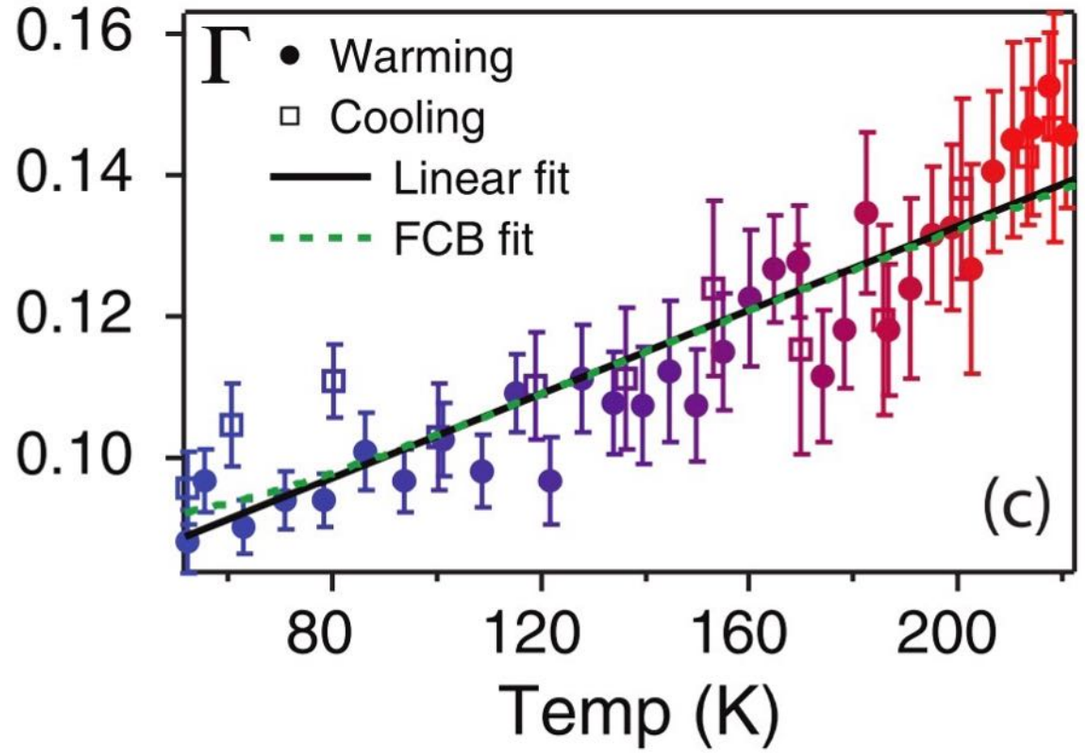


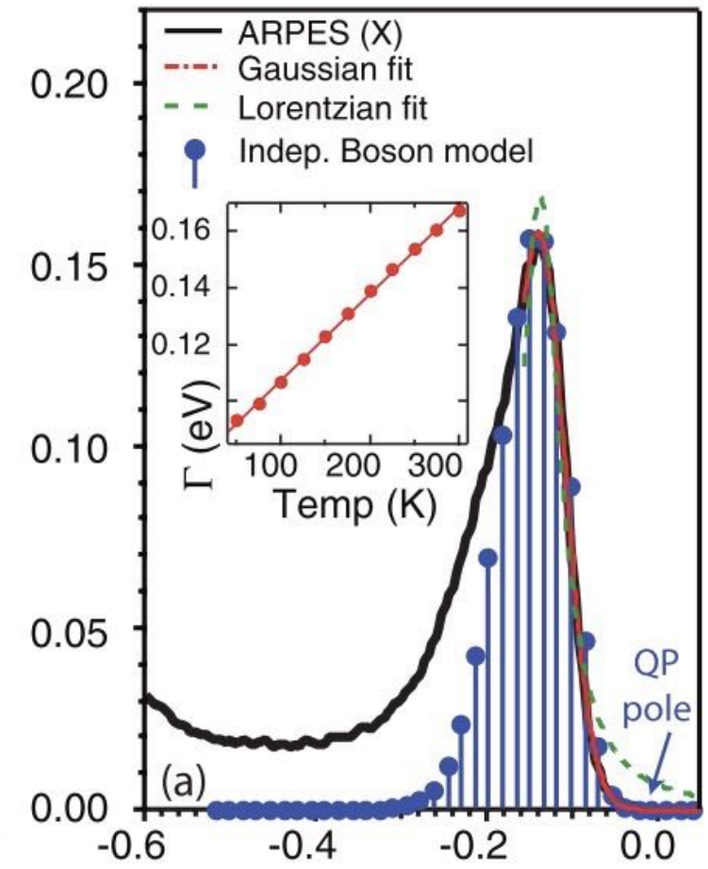
- LHB maximum pinned close to E_F (consistent with optical measurements of a smaller gap than Sr_2IrO_4)
- fitted boson energy : ω_0 = 15 meV; coupling constant $g \sim 6$

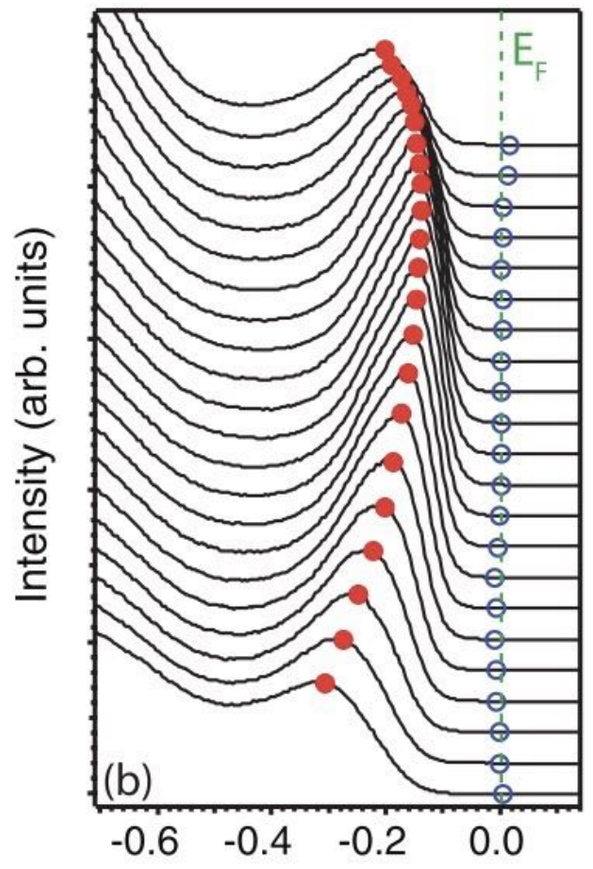
P.D.C. King, K.M.S, H. Takagi, F. Baumberger, *Phys. Rev. B* **87** 241106R (2013)

temperature dependence of broadening in $Sr_3Ir_2O_7$

$Sr_3Ir_2O_7$







- temperature-dependent broadening consistent with boson energy of ~ 15 meV and coupling constant of g ~ 6
- large spin gap in $Sr_3Ir_2O_7$ (~ 90 meV) suggests that this is due to low-energy phonons

P.D.C. King, K.M.S, H. Takagi, F. Baumberger, *Phys. Rev. B* **87** 241106R (2013)

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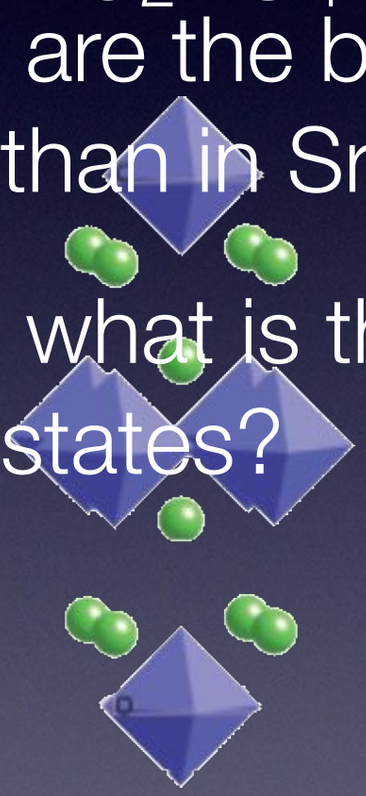
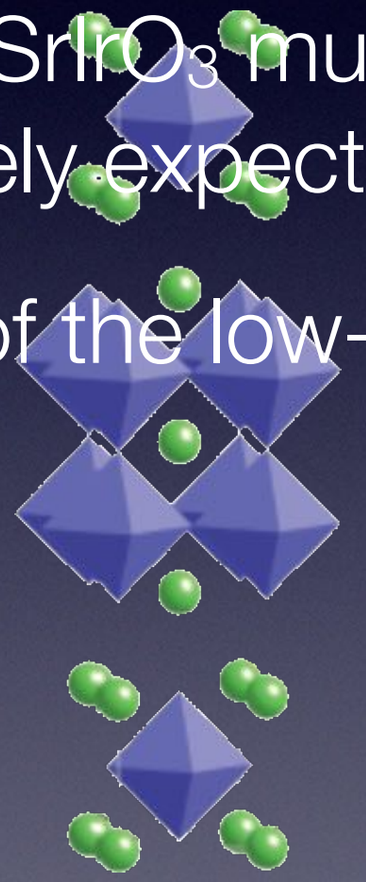
Sr_2IrO_4
Ba_2IrO_4

$Sr_3Ir_2O_7$

$SrIrO_3$

- are the bandwidths in $SrIrO_3$ much wider than in Sr_2IrO_4, as naively expected?
- what is the character of the low-energy states?





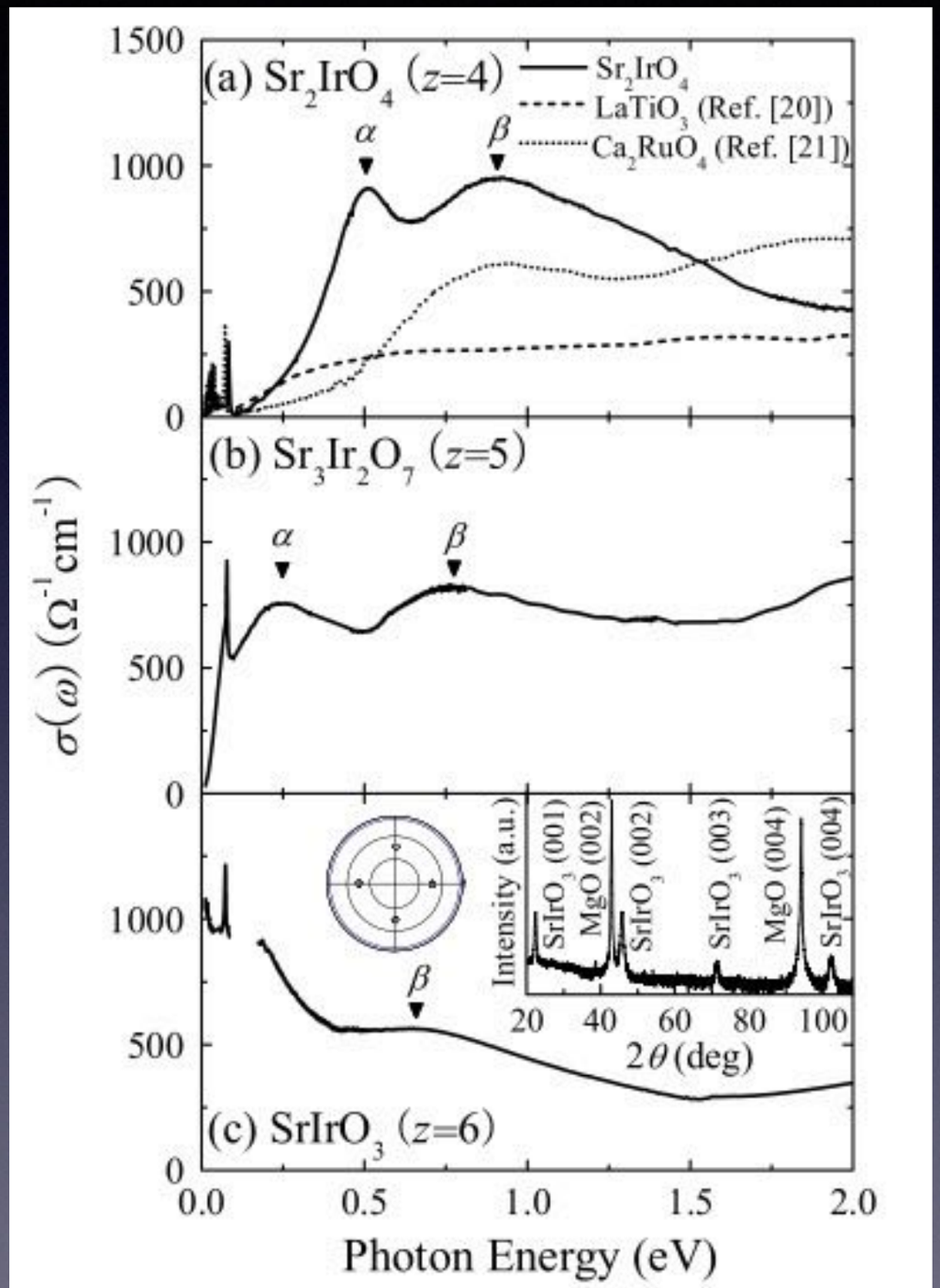
J_{eff} = 1/2
AF insulator

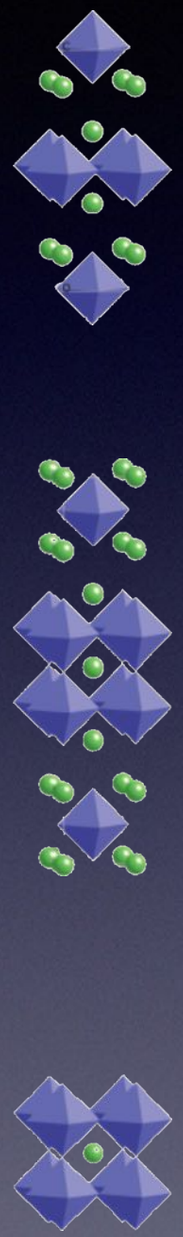
J_{eff} = 1/2
AF semiconductor

semimetallic

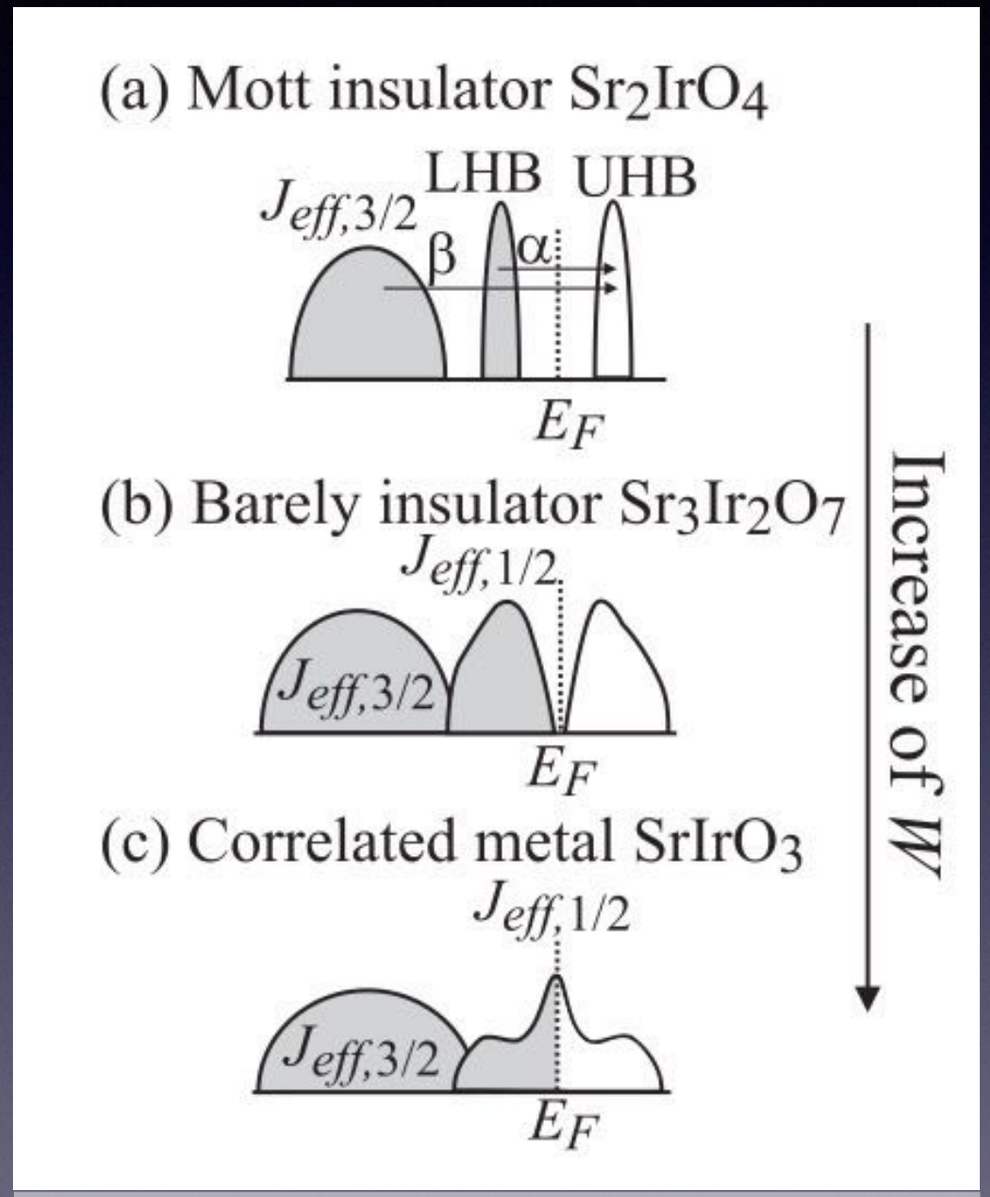
evolution from insulator to metal with increasing dimensionality

optical conductivity





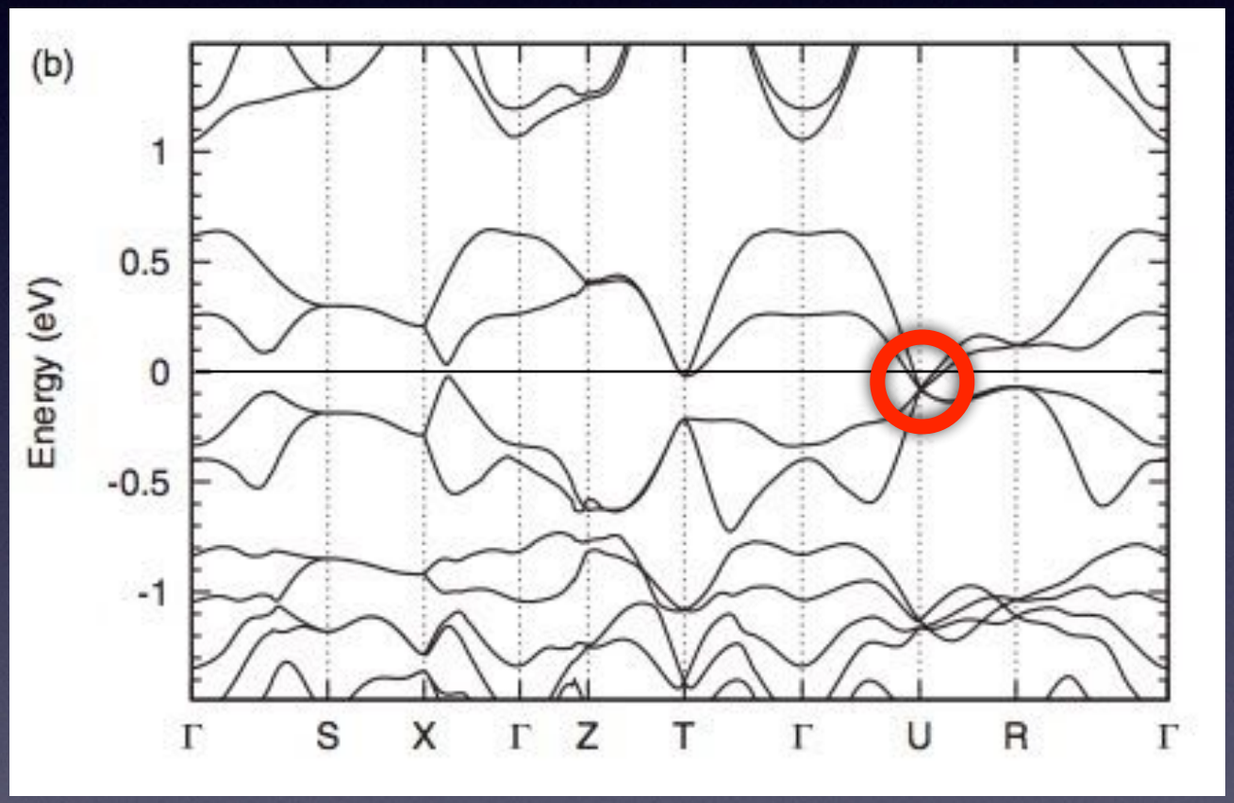
increasing bandwidth
with dimensionality?

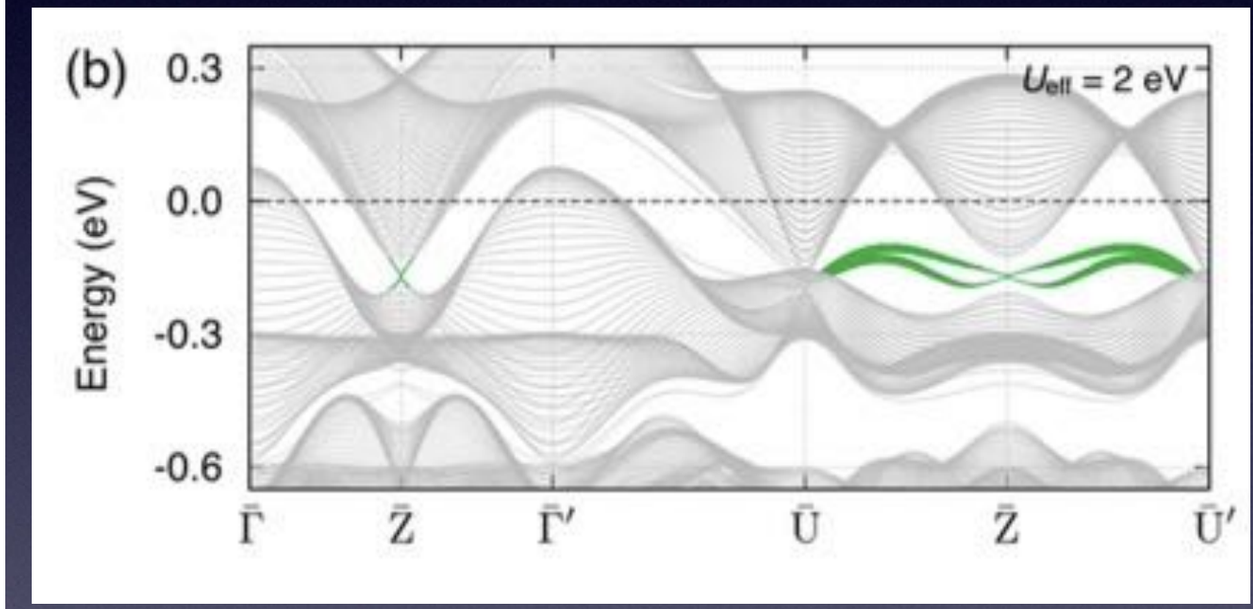


S.J. Moon, T.W. Noh *et al. Phys. Rev. Lett.* **101**, 226402 (2008)

electronic properties of $SrIrO_3$

- possibility of line nodes in the bulk, or topological surface states

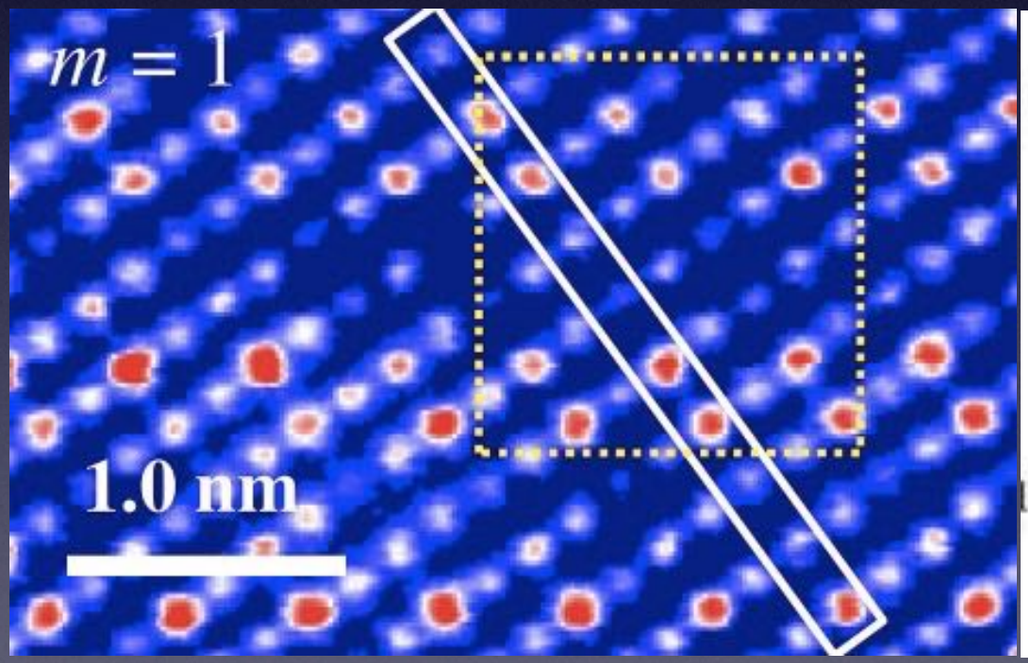


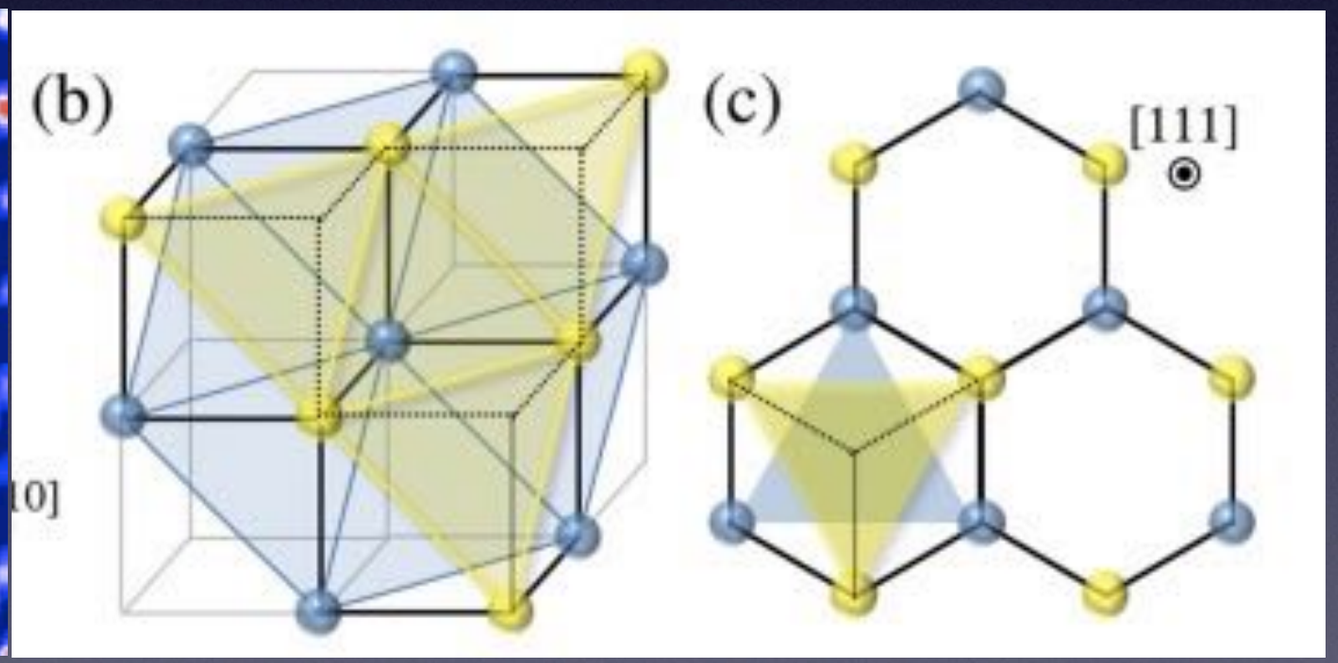


H. Kim, Y. Chen, H.Y. Kee, arXiv:1411.1406 (2014)
J.M. Carter, H.Y. Kee et al., *Phys. Rev. B* **85**, 115105 (2012)

electronic properties of $SrIrO_3$

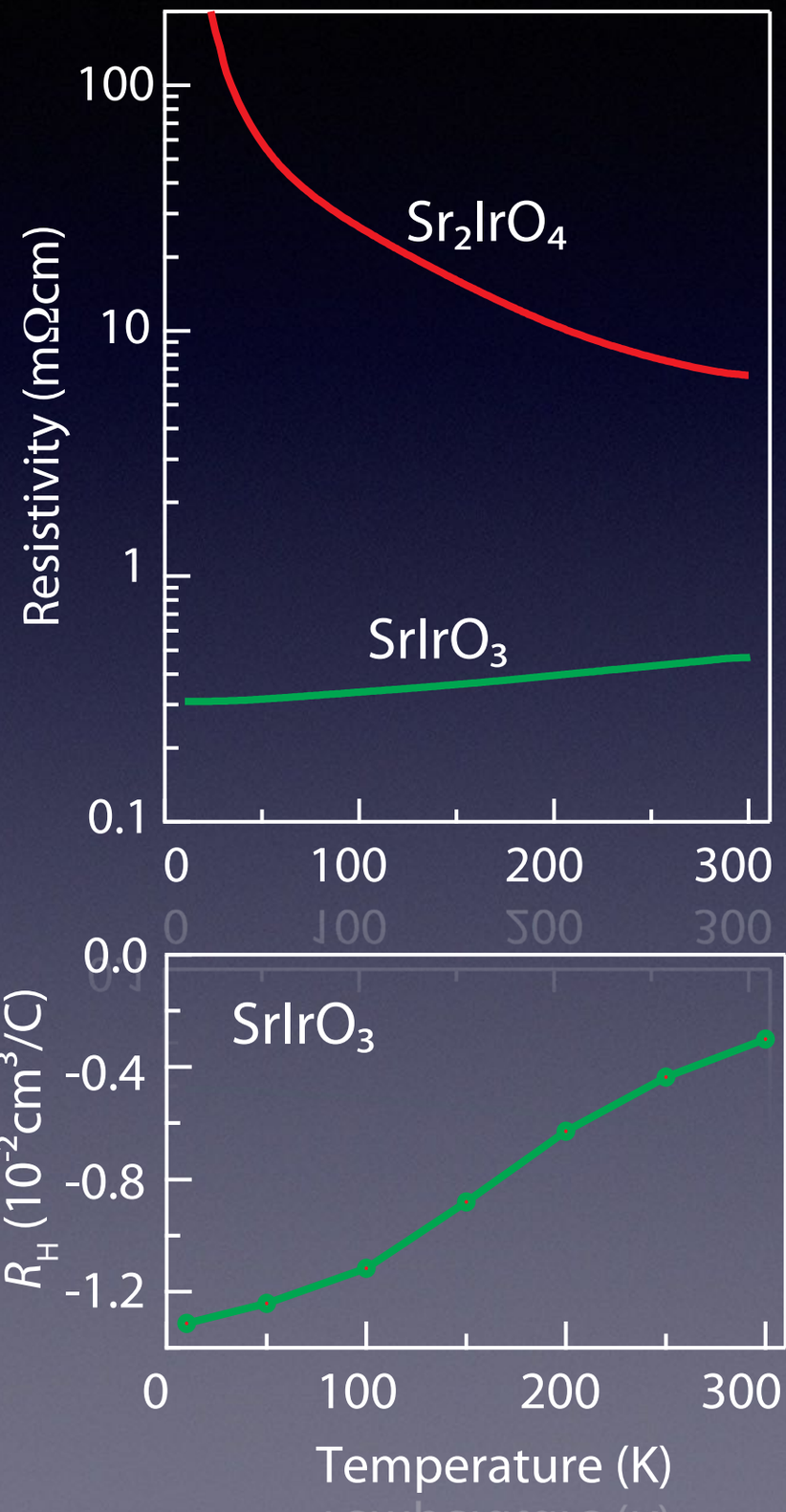
- possibility of line nodes in the bulk, or topological crystalline metallic surface states
- realization of exotic electronic, magnetic, or topological phases in $SrIrO_3$-based superlattices or bilayers

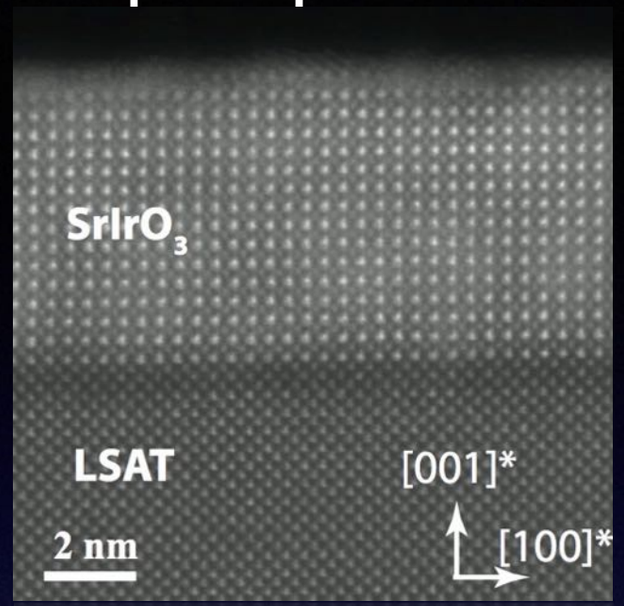


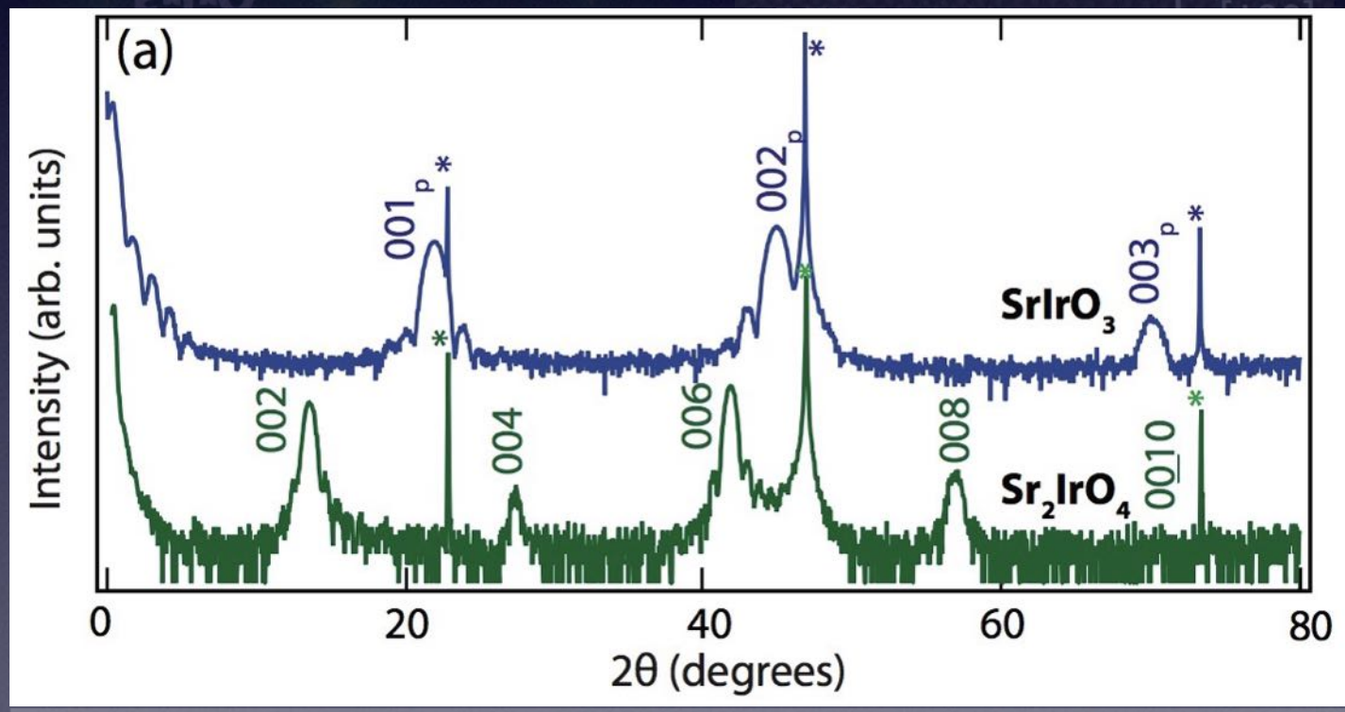


D. Hirai, J. Matsuno, H. Takagi, *APL Materials* **3**, 041508 (2012)
H. Kim, Y. Chen, H.Y. Kee, arXiv:1411.1406 (2014)
J.M. Carter, H.Y. Kee et al., *Phys. Rev. B* **85**, 115105 (2012)
D. Xiao et al., *Nature Comm.* **2**, 596 (2011)

$SrIrO_3$ epitaxial thin films : structure & properties



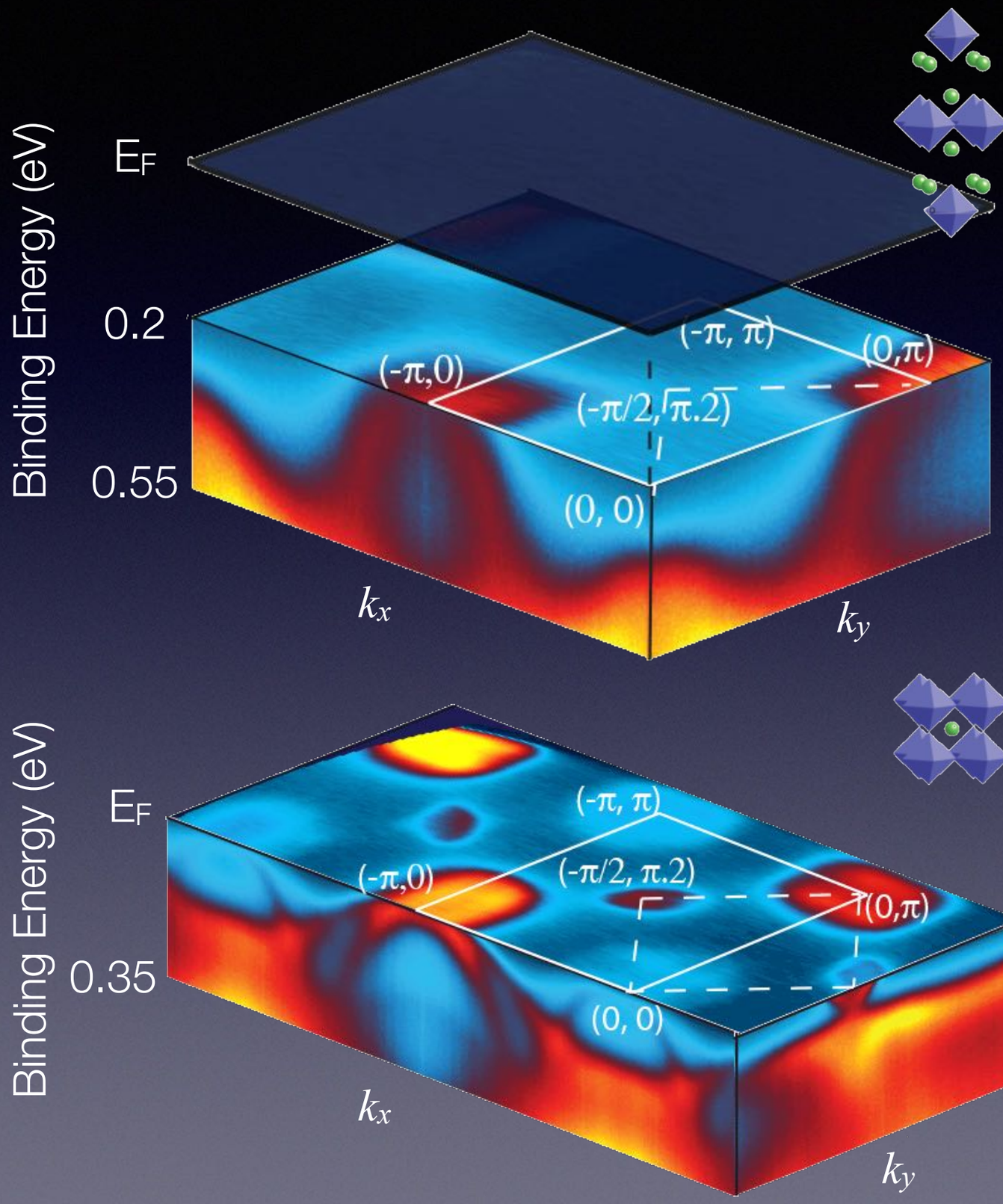


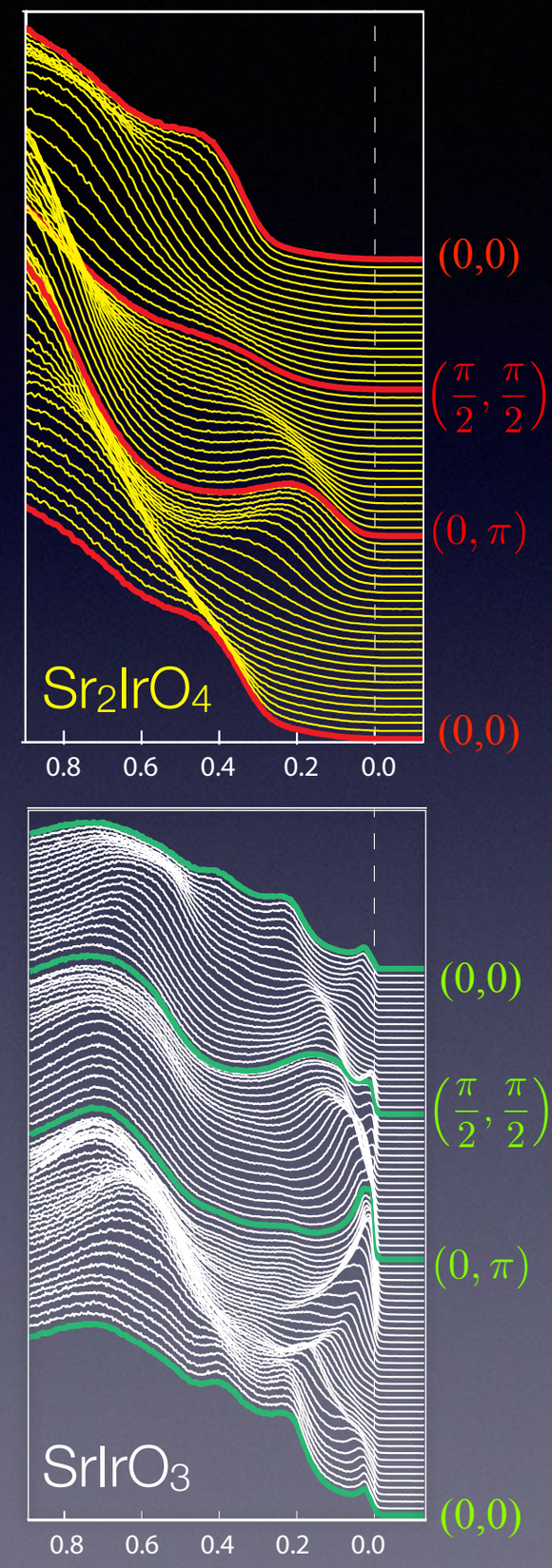


- bulk single crystals not available
- MBE-grown epitaxial thin films grown on LSAT at 700° C at 10^{-6} torr of 100% O_3

Yuefeng Nie

ARPES shows a complex Fermiology

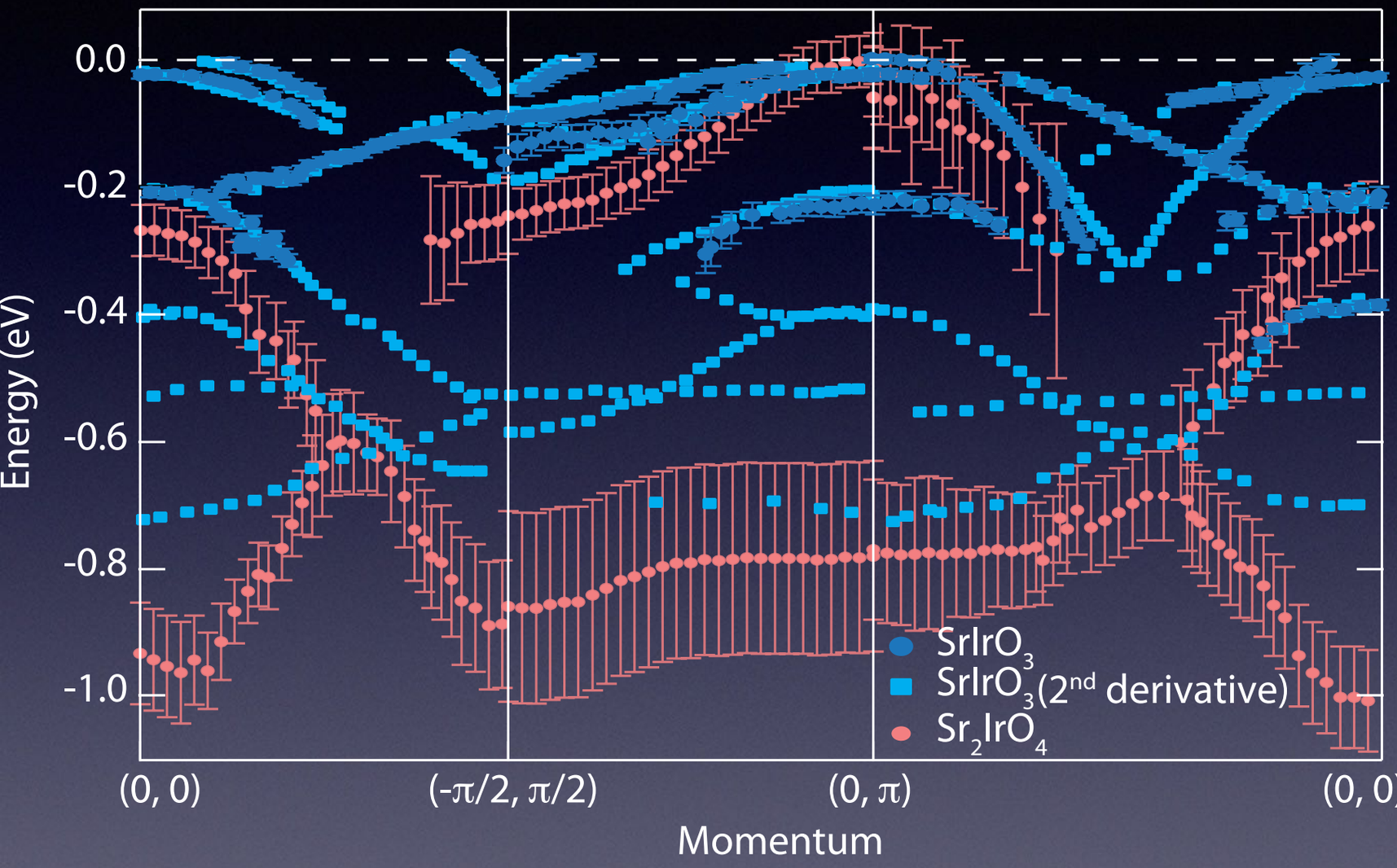


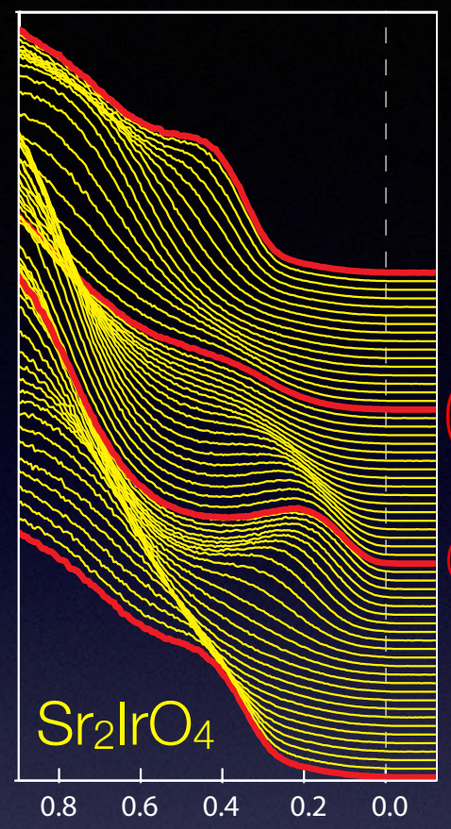


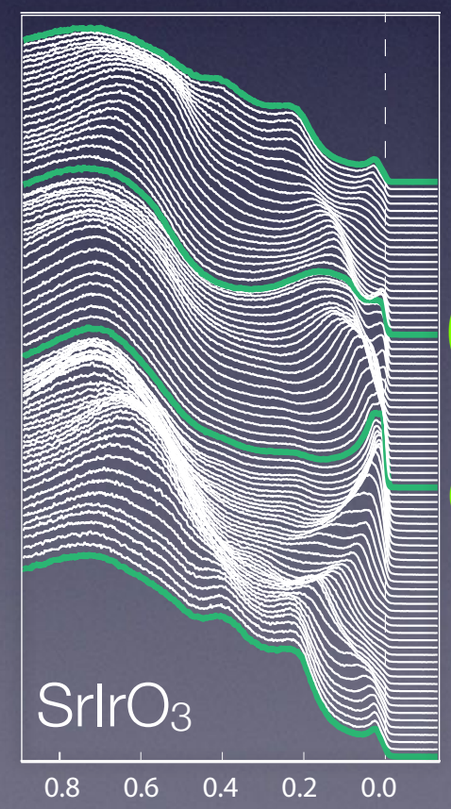
Y.F. Nie et al., *Phys. Rev Lett* **114** 016401 (2015)

individual bands of $SrIrO_3$ are narrower than Sr_2IrO_4

dispersions of $SrIrO_3$ and Sr_2IrO_4





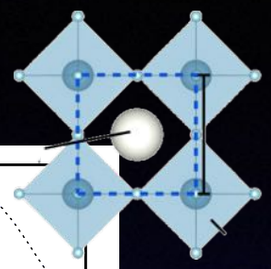


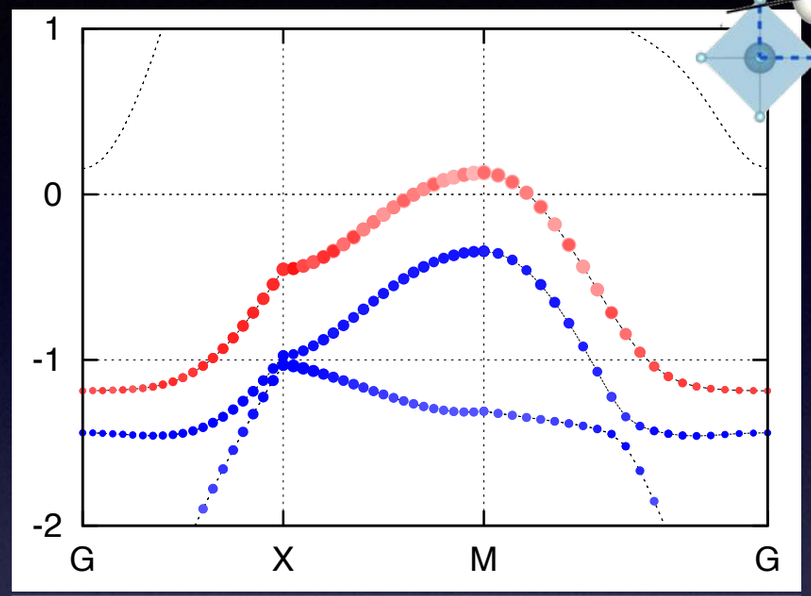
Y.F. Nie et al., *Phys. Rev Lett* **114** 016401 (2015)

effects of octahedral rotations on band structure

Sr_2IrO_4

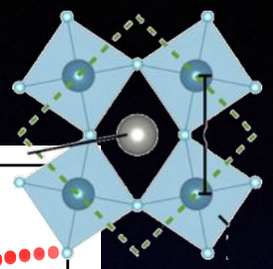
no rotations

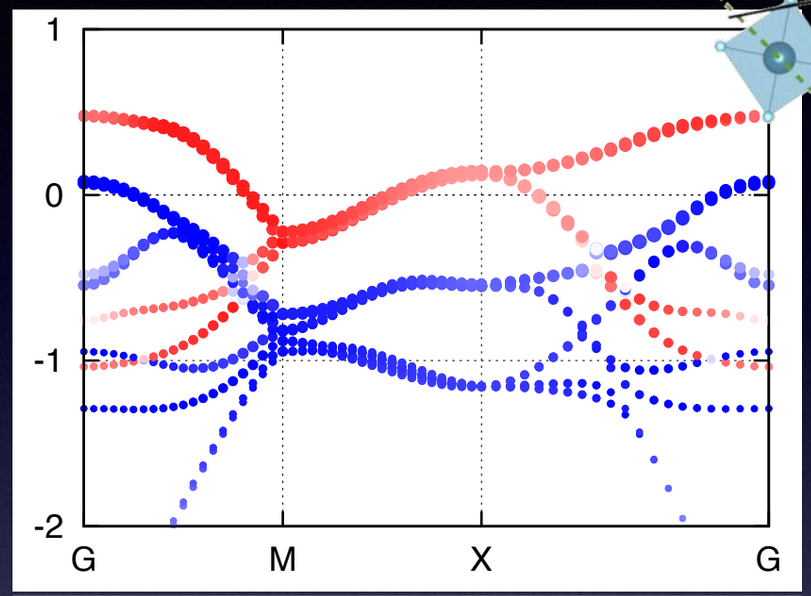




with rotations

[001]



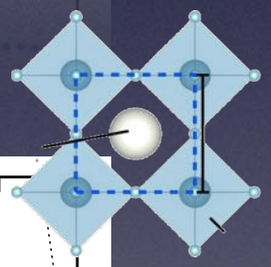


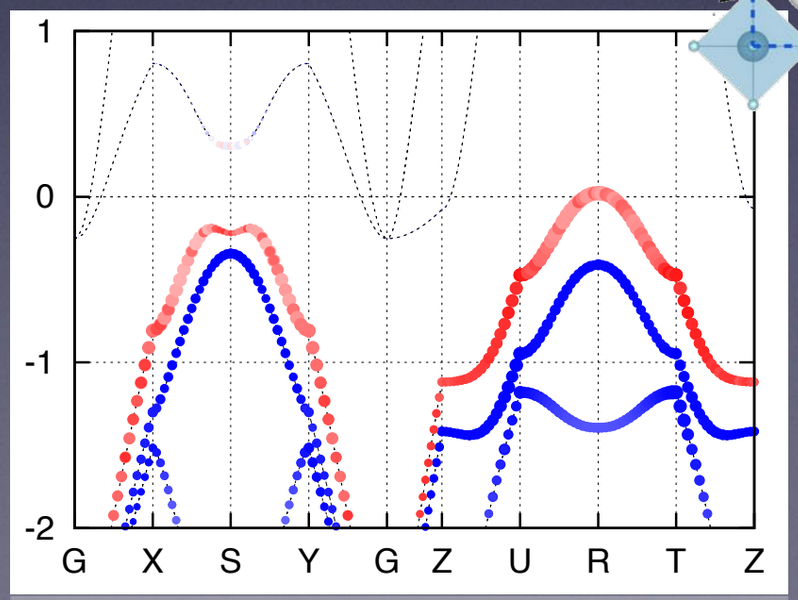
OpenMX,
U = 0

$J_{eff} = 1/2$

$J_{eff} = 3/2$

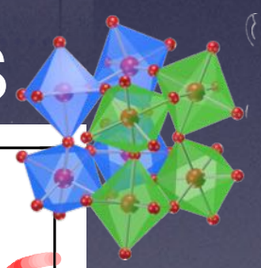
$SrIrO_3$ cubic

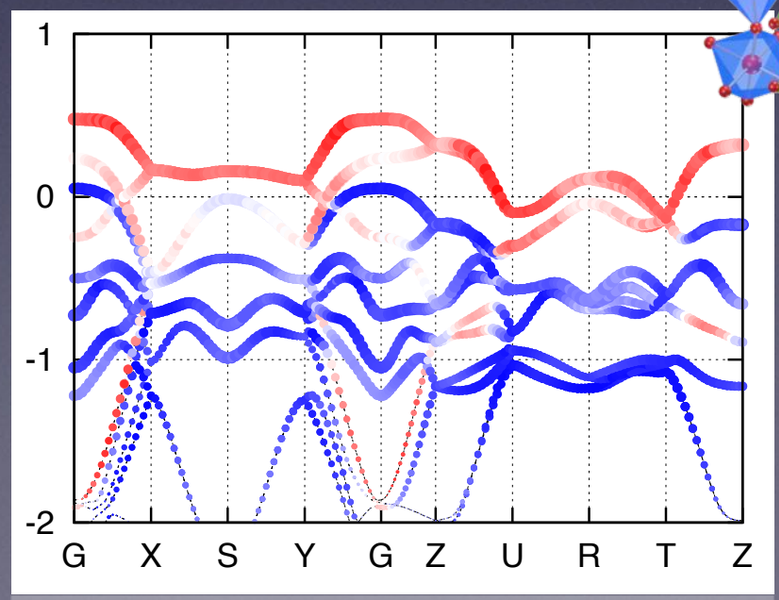




with rotations

[001] + [110]

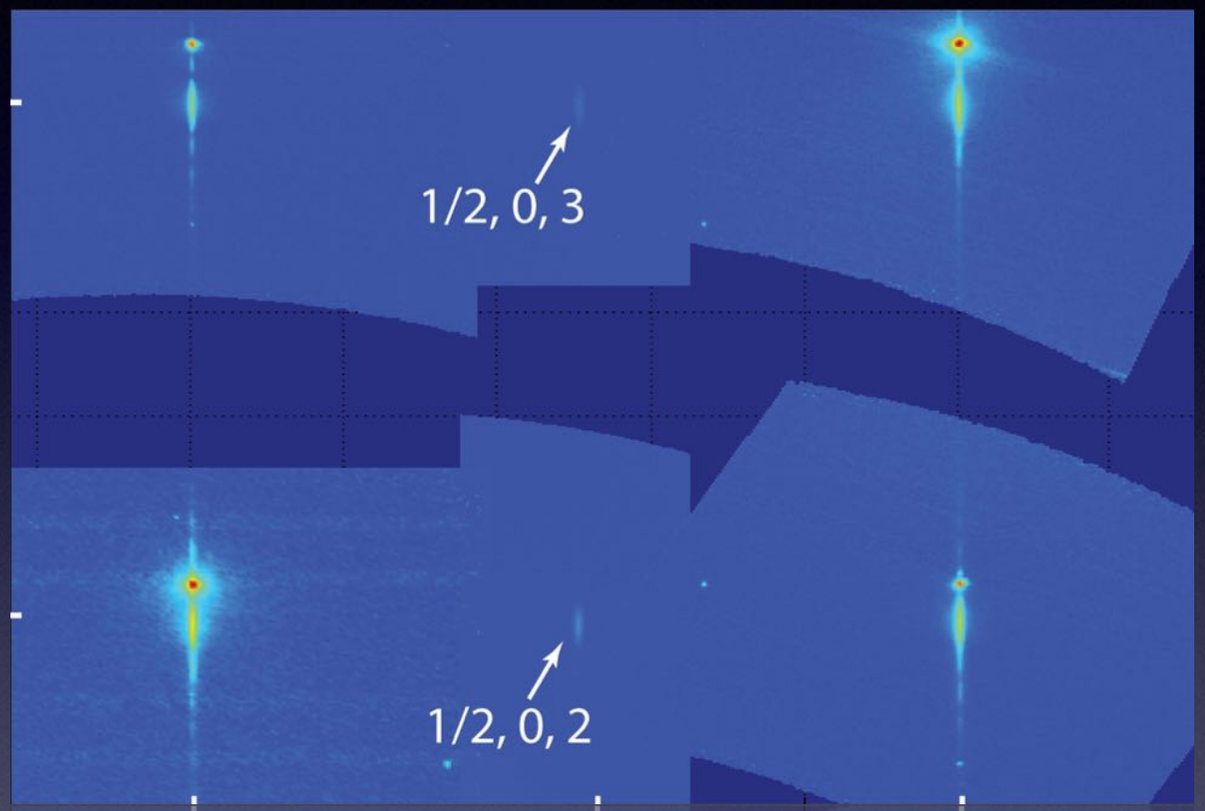


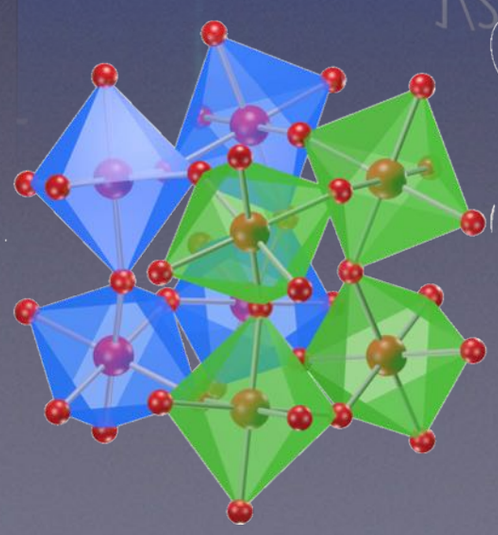


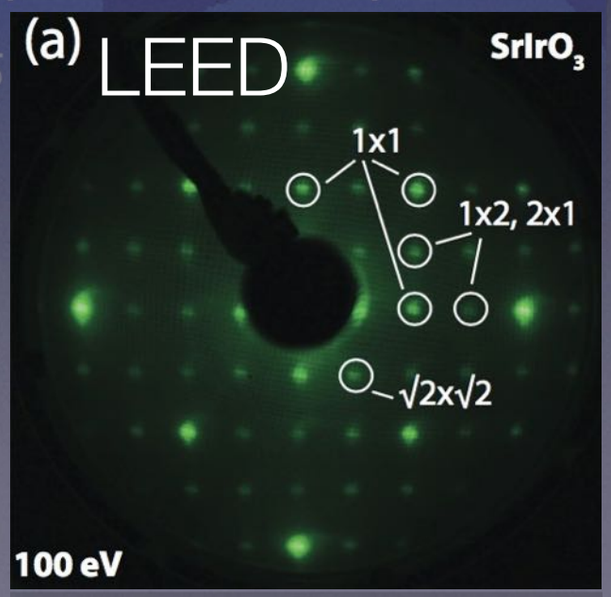
Choong
Hyun
Kim

octahedral rotations in $SrIrO_3$ thin films

synchrotron x-ray diffraction
of half-order peaks



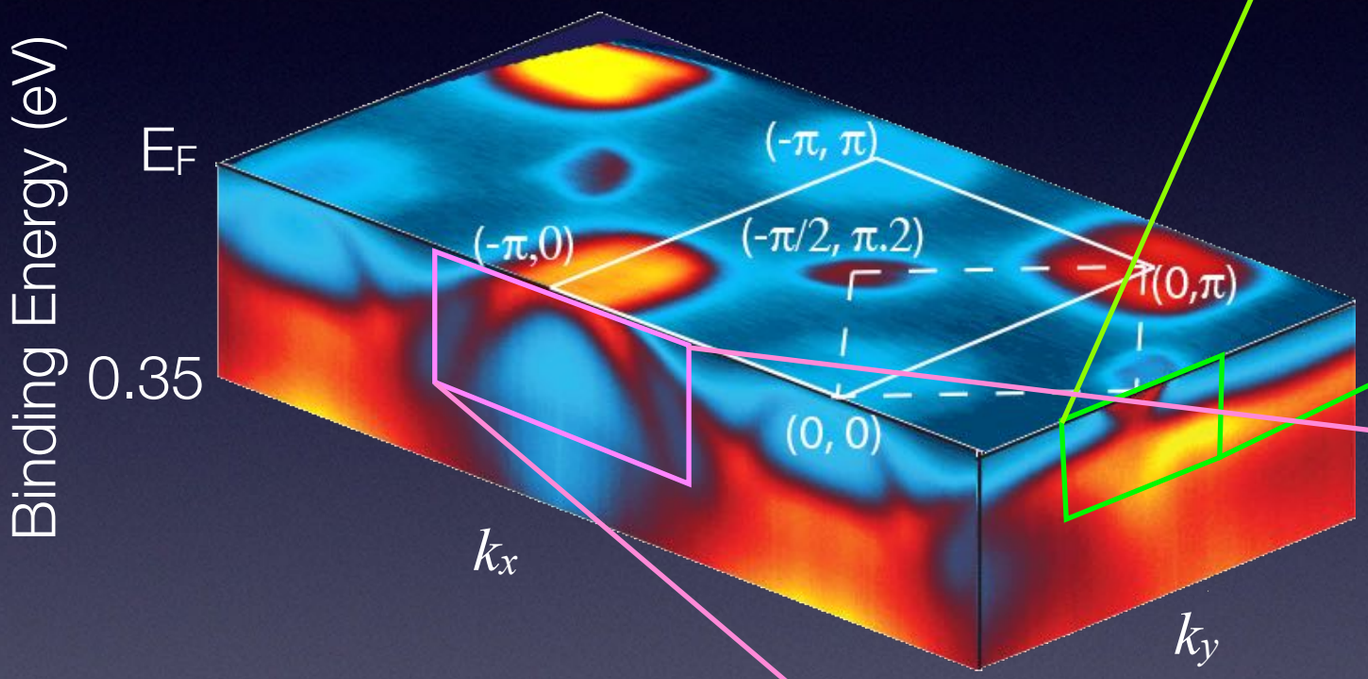


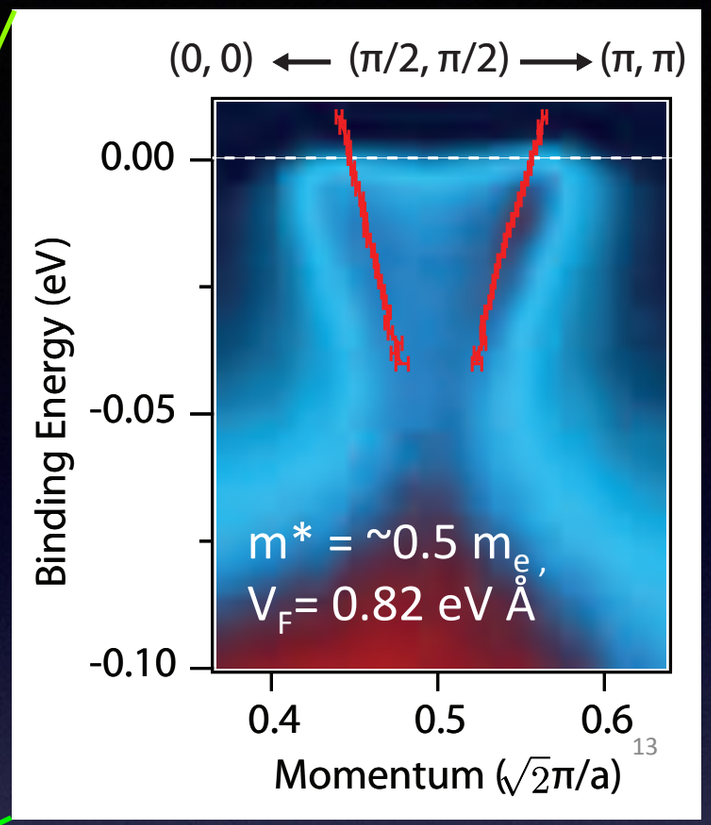


TEM measurements
of half-order peaks

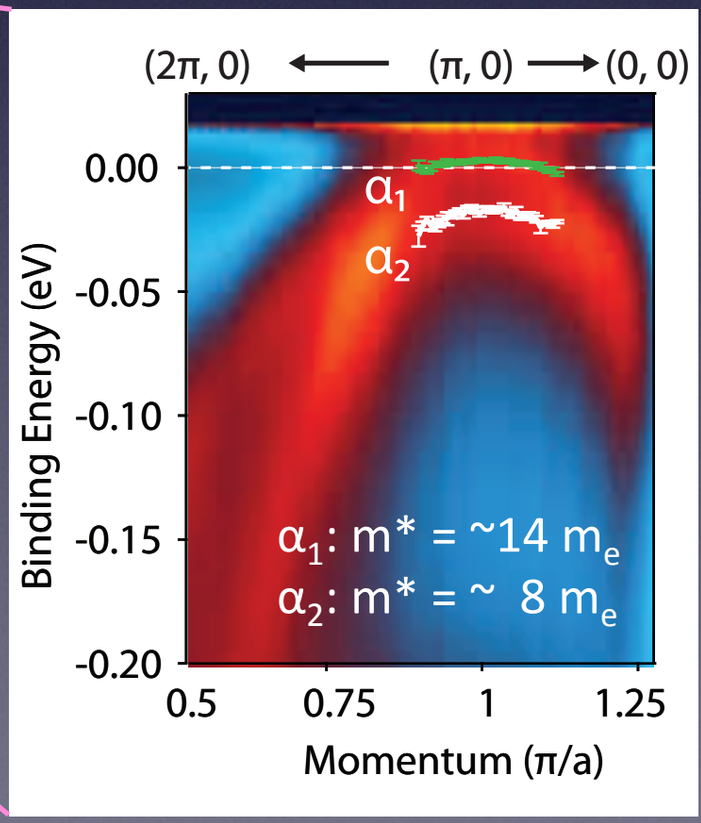
- synchrotron x-ray, TEM, and LEED measurements show out-of-plane [110] and in-plane [001] octahedral rotations

intriguing features in electronic structure of $SrIrO_3$





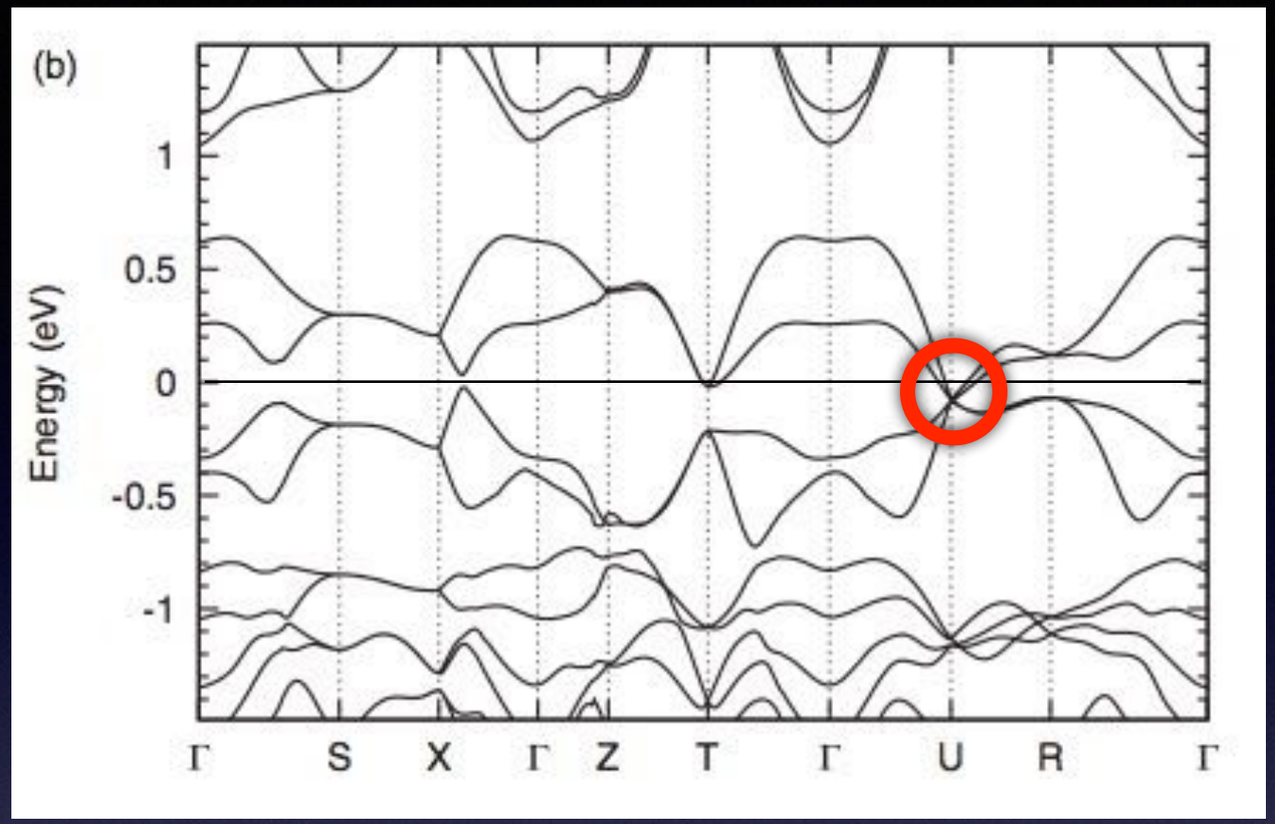
- light (Dirac-like), small electron pockets
- symmetry-protected 3D Dirac points?

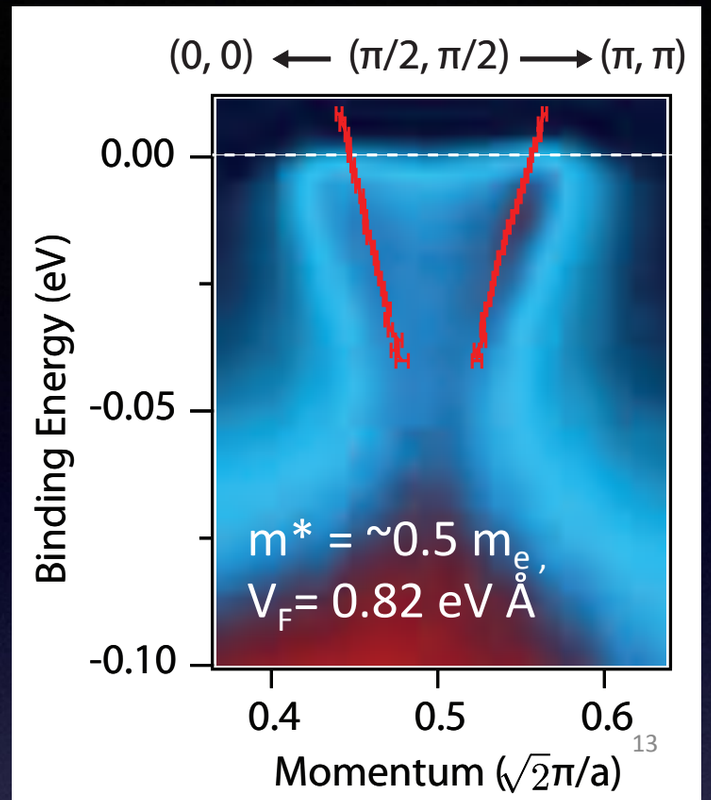


- massive hole bands with van Hove singularity close to E_F

Y.F. Nie et al., *Phys. Rev Lett* **114** 016401 (2015)

intriguing features in electronic structure of $SrIrO_3$





- light (Dirac-like), small electron pockets
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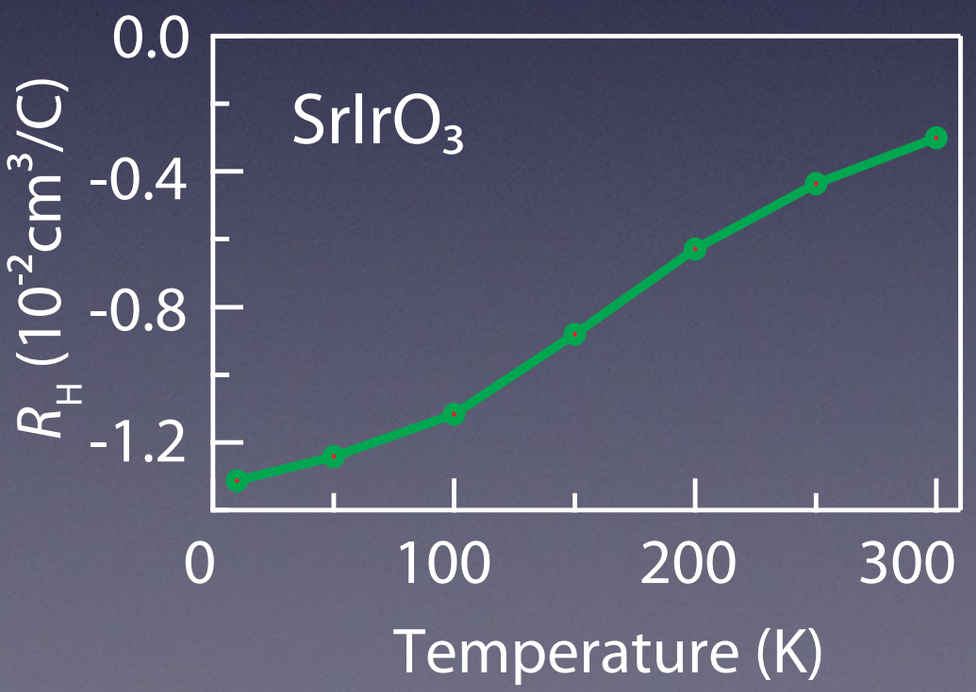
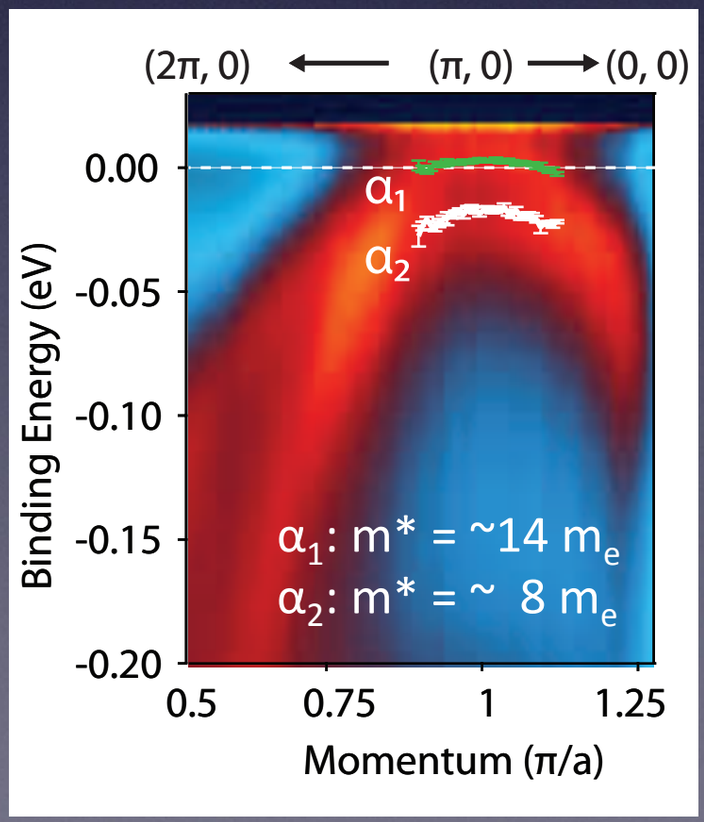
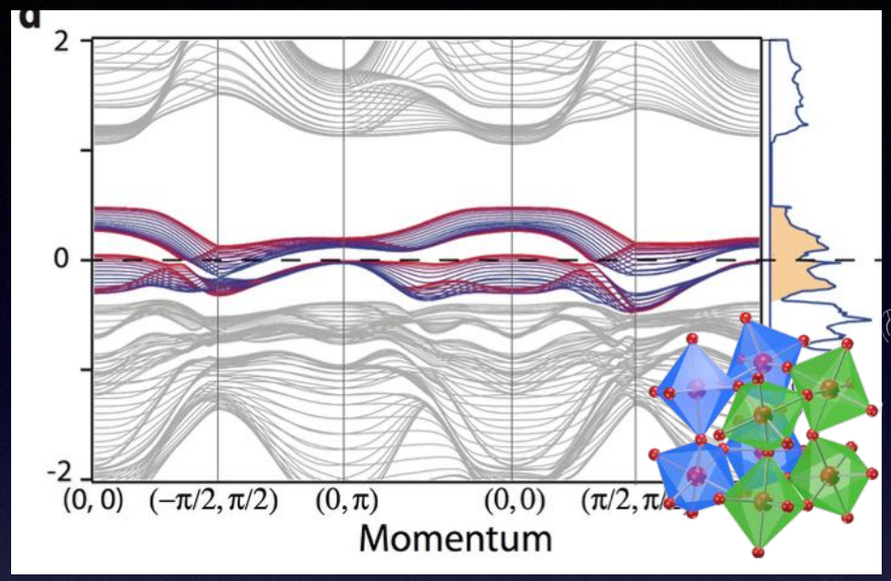




- massive hole bands with van Hove singularity close to E_F

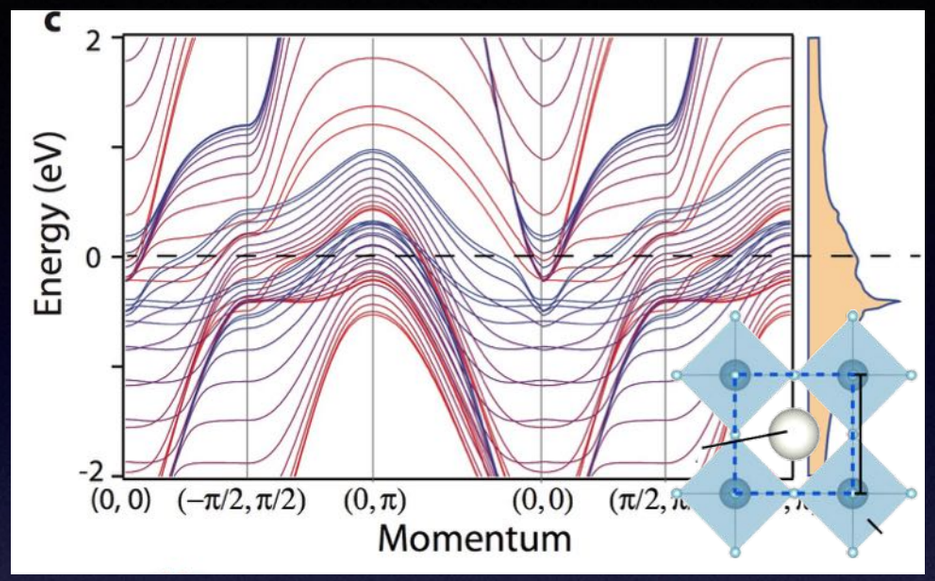
Y.F. Nie et al., *Phys. Rev Lett* **114** 016401 (2015)

future directions : strain control of properties



tensile strain?

$BaIrO_3$



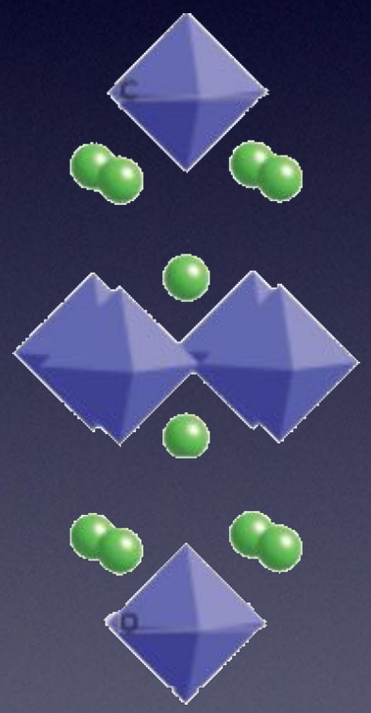
- large enhancement of bandwidths and mobilities in $AIrO_3$ by “unrotating” octahedra, e.g. through tensile strain?
- $BaIrO_3$ in perovskite structure (larger cation) has 180^o Ir-O-Ir bonds, and exhibits more metallic behavior (high pressure growth of polycrystalline)

J.G. Cheng et al., *Phys. Rev B* **88** 205114 (2013)

Ruddlesden-Popper series of iridates : $Sr_{n+1}Ir_nO_{2n+1}$

2D → **3D**

Sr_2IrO_4
Ba_2IrO_4



J_{eff} = 1/2
AF insulator

$Sr_3Ir_2O_7$

J_{eff} = 1/2
AF semiconductor

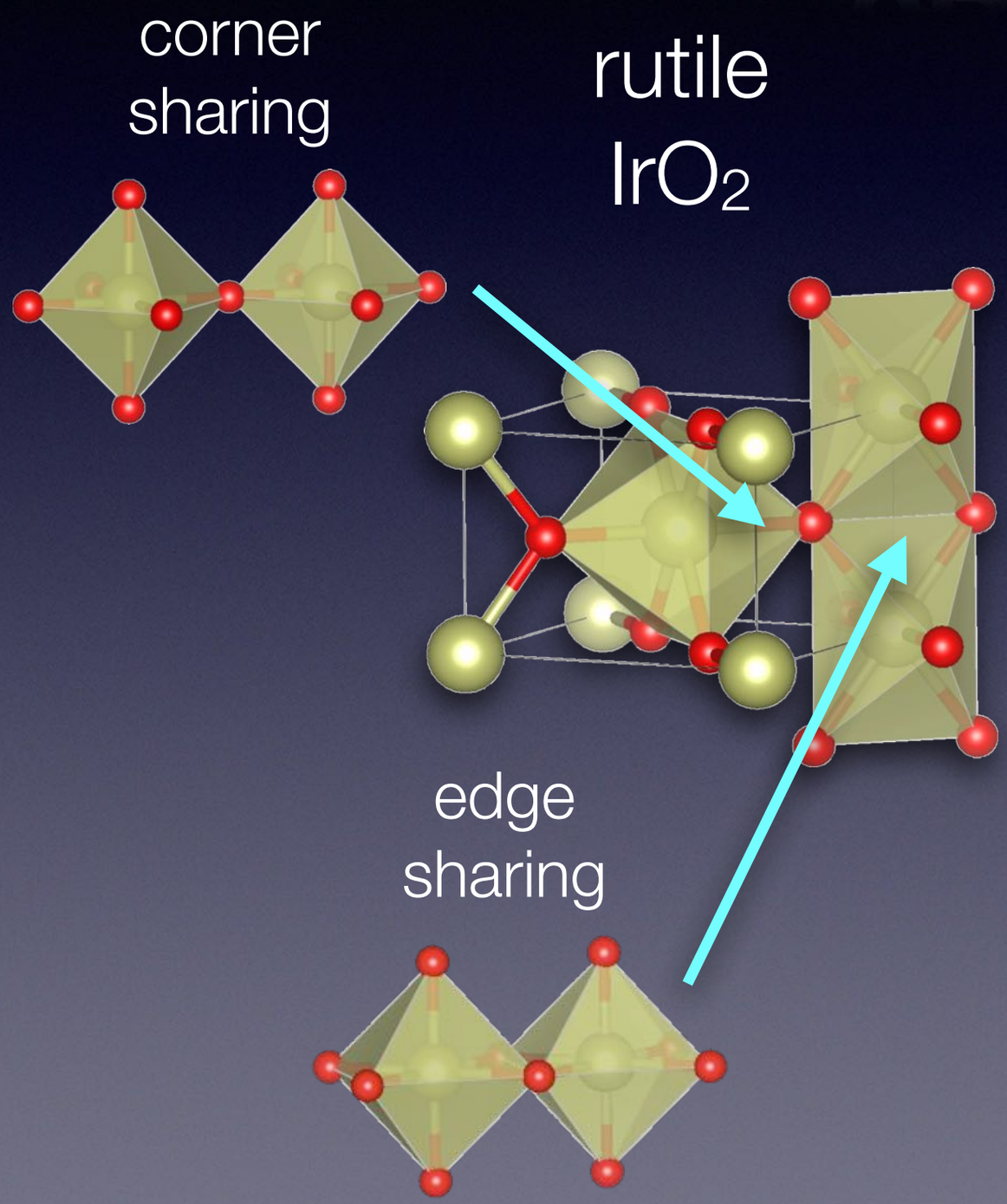
$SrIrO_3$

semimetallic

Beyond the Ruddlesden-Popper iridates : Rutile IrO_2

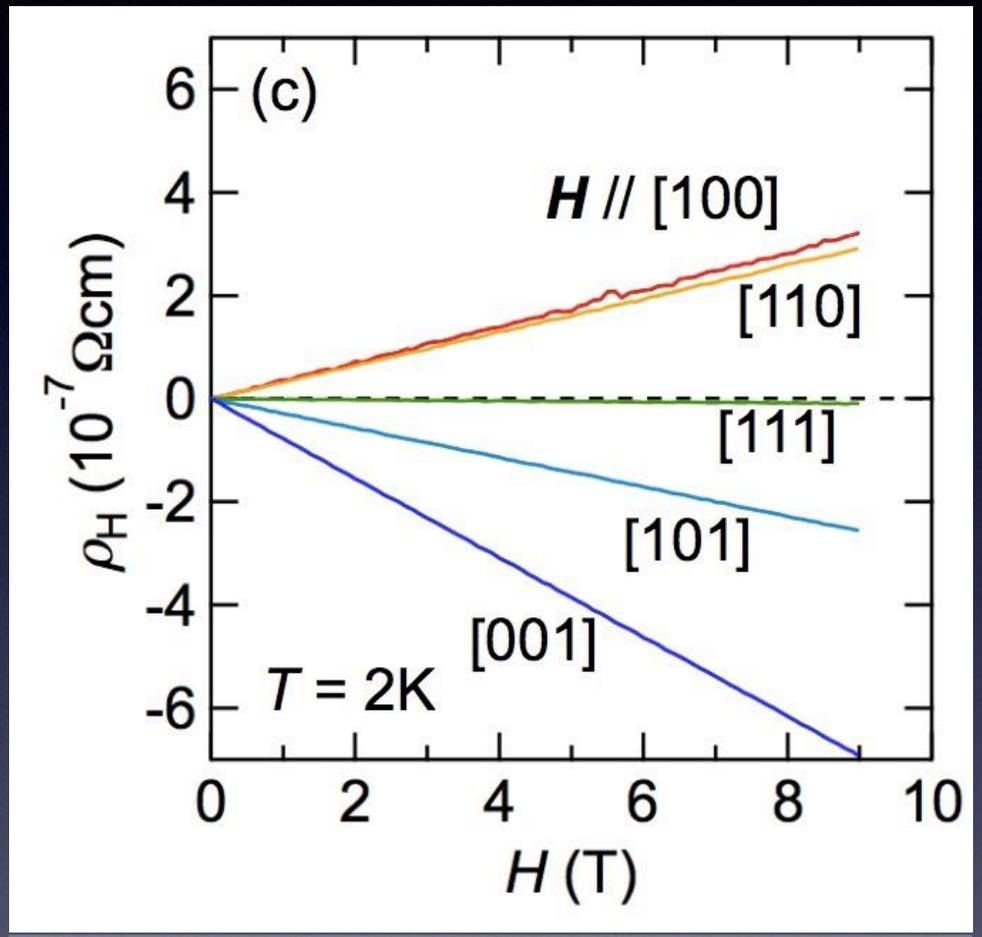
2D → **3D**

- does additional connectivity beyond perovskite lead to further metallicity?
- how do the edge & corner-shared octahedra change the electronic structure?
- how do SOC and Coulomb U affect electronic structure?



exotic magnetotransport in IrO_2

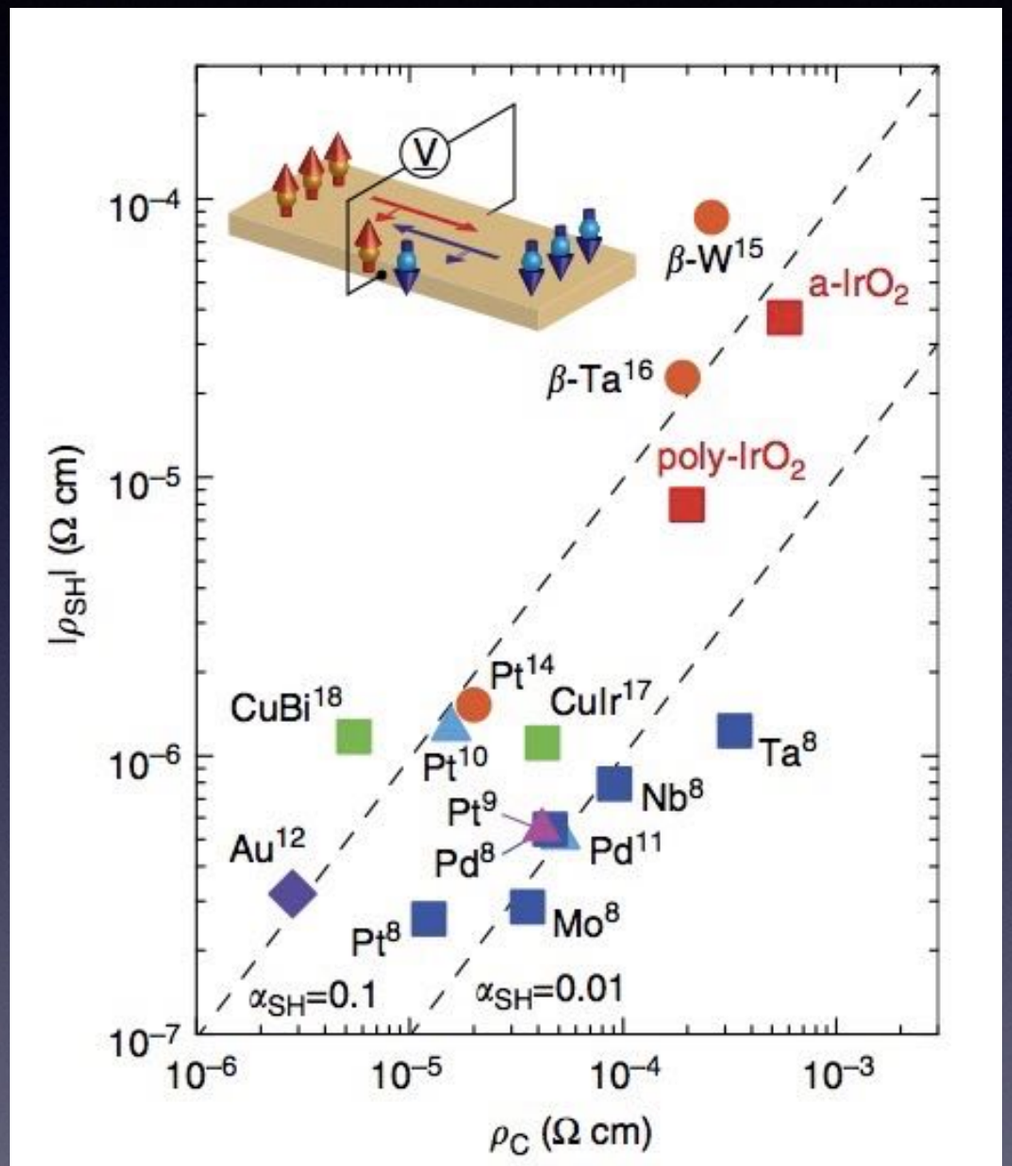
hole or electron transport can be switched with field direction



M. Uchida, R. Arita, Y. Tokura, M. Kawasaki, et al. *Phys. Rev. Lett.* (submitted)

Masaki Uchida

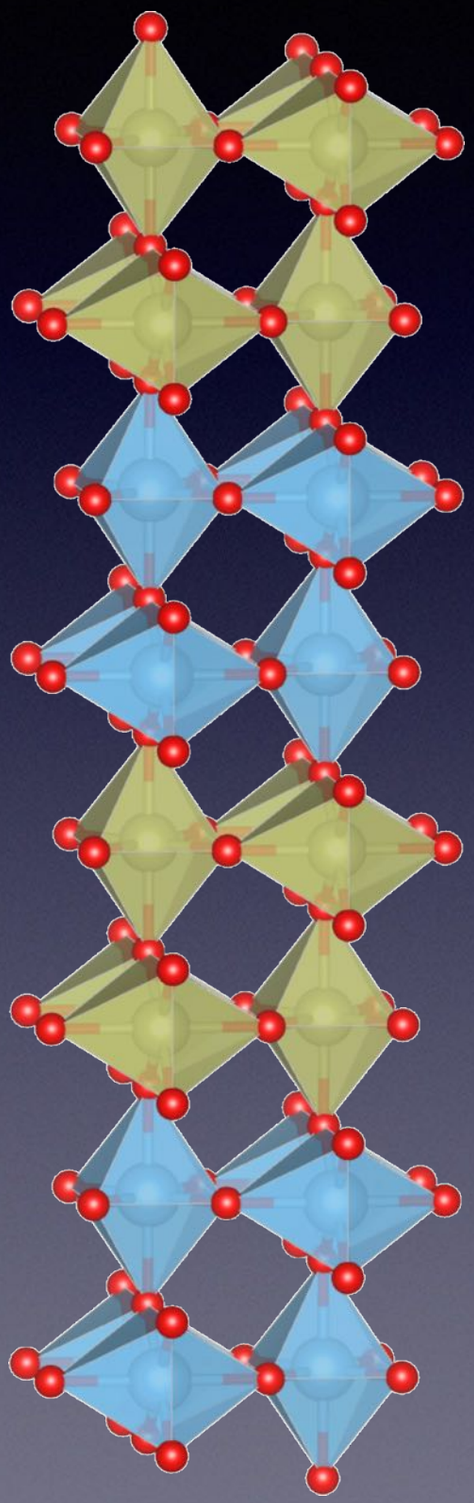
large spin Hall resistivity



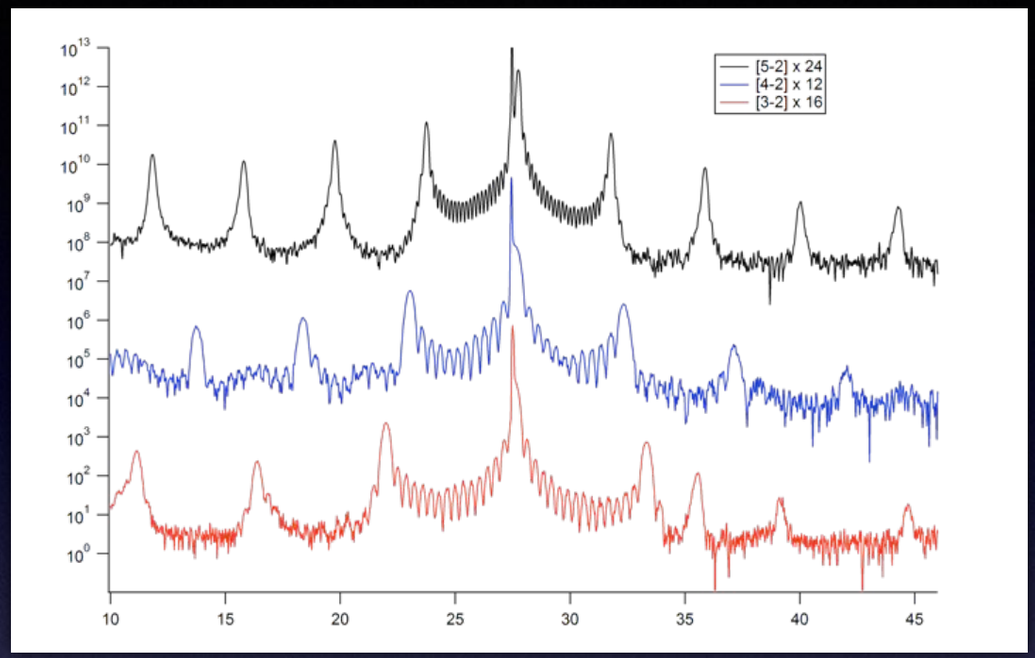
K. Fujiwara, H. Takagi, et al. *Nature Comm.* **4**:*2893* (2013)

future directions : iridate-based heterostructures

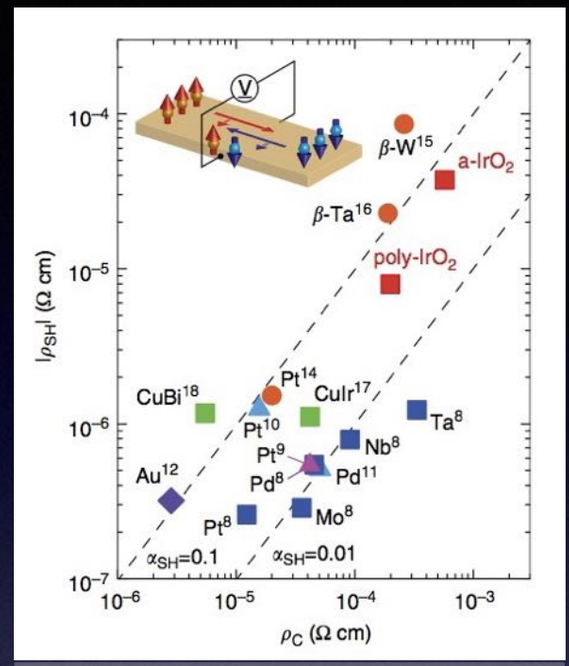
IrO_2 / TiO_2



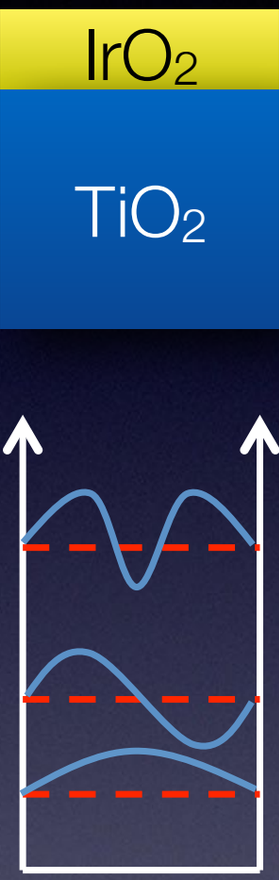
x-ray diffraction



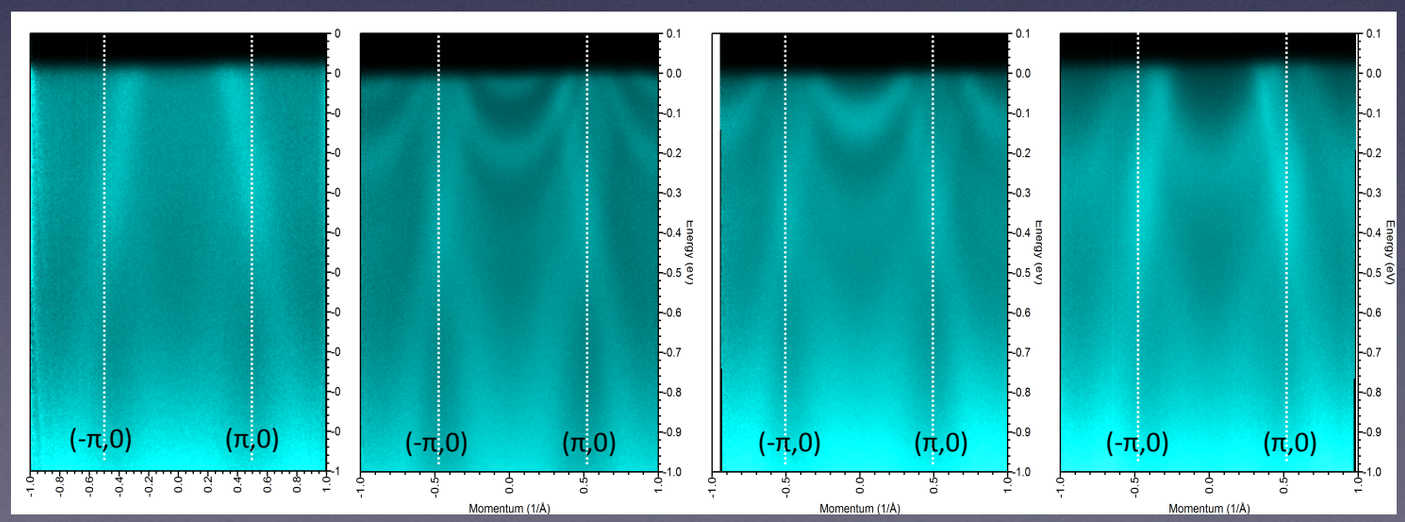
large spin Hall



K. Fujiwara, H. Takagi, et al.
Nature Comm. **4**:*2893* (2013)



20 ML 10 ML 8 ML 4 ML



- IrO_2 grown on TiO_2 (110)
- T = 300 K @ 1.5 x 10^{-6} torr O_3 (adsorption controlled)

- IrO_2 : a = 4.498 A; c = 3.154 A
- TiO_2 : a = 4.594 A; c = 2.959 A

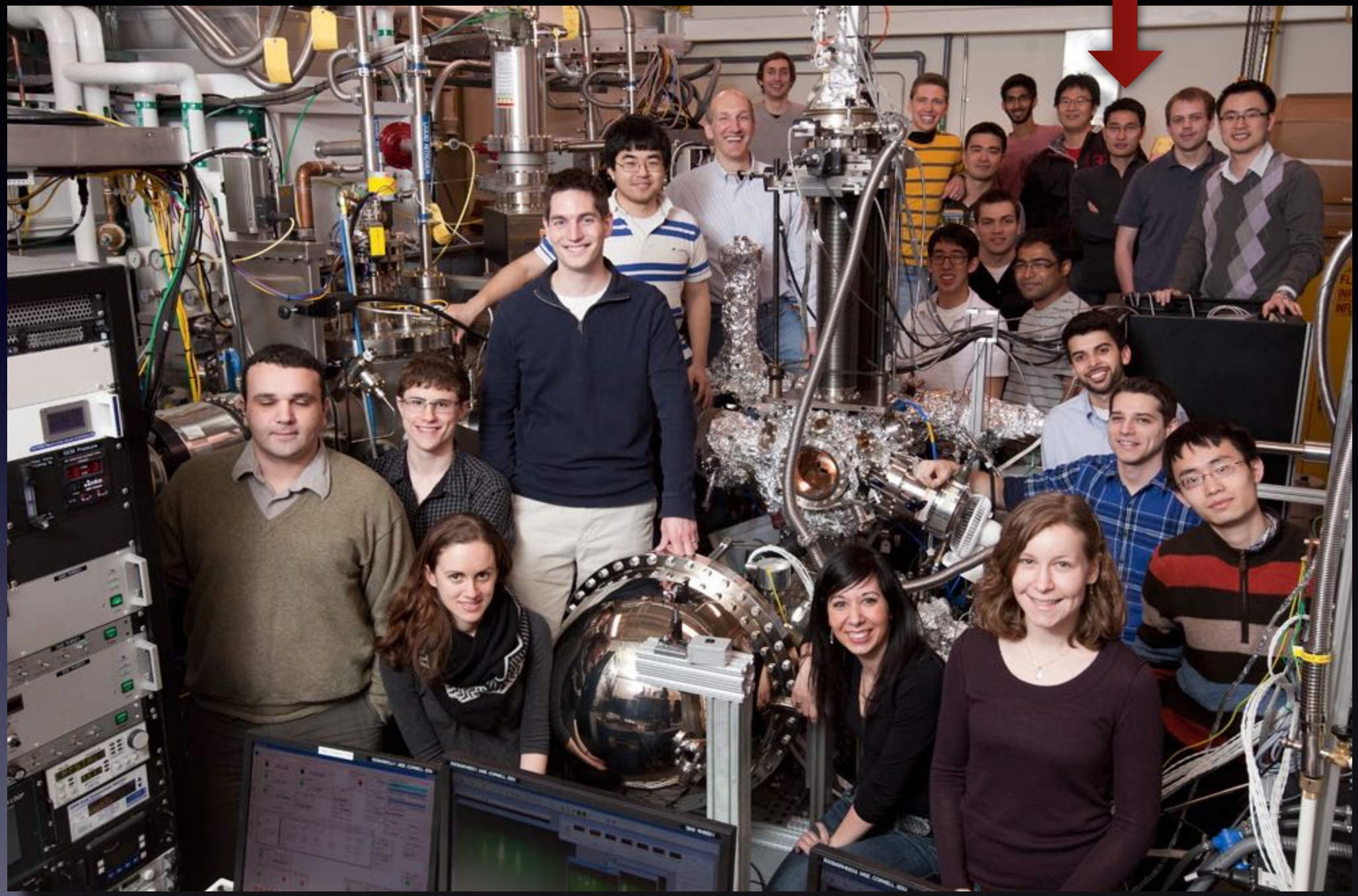
Jason Kawasaki (Kavli Fellow)

final thoughts

- epitaxial stabilization allows us to explore a wider variety of iridate structures
- single-particle excitations in insulating perovskite iridates (Sr_2IrO_4, Ba_2IrO_4, $Sr_3Ir_2O_7$) are best described by small polarons, very similar to the parent cuprates
- [001] & [110] octahedral rotations play a critical role in narrow band semimetal $SrIrO_3$
- metallic bands in $SrIrO_3$ have strongly mixed J_{eff} = 1/2 and 3/2 character

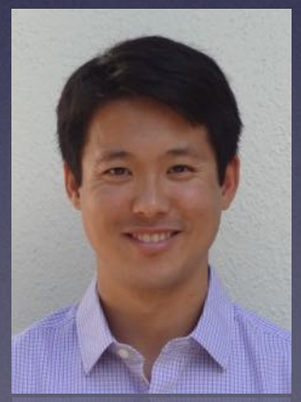
acknowledgements

Yuefeng Nie



Phil King
(@ St. Andrews)

Masaki Uchida
(@ Tokyo)



Jason Kawasaki

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KIC Kavli Institute at Cornell