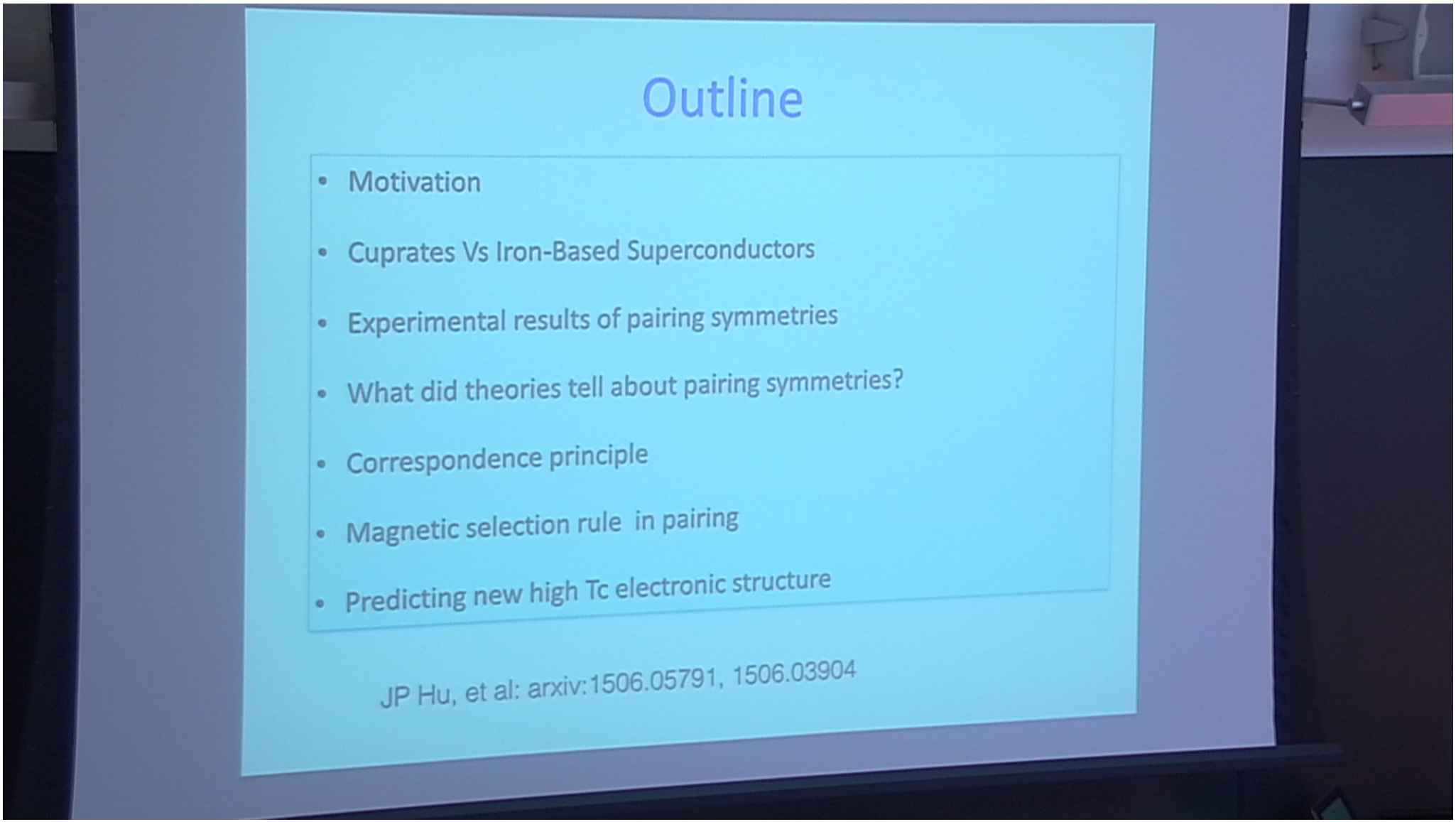
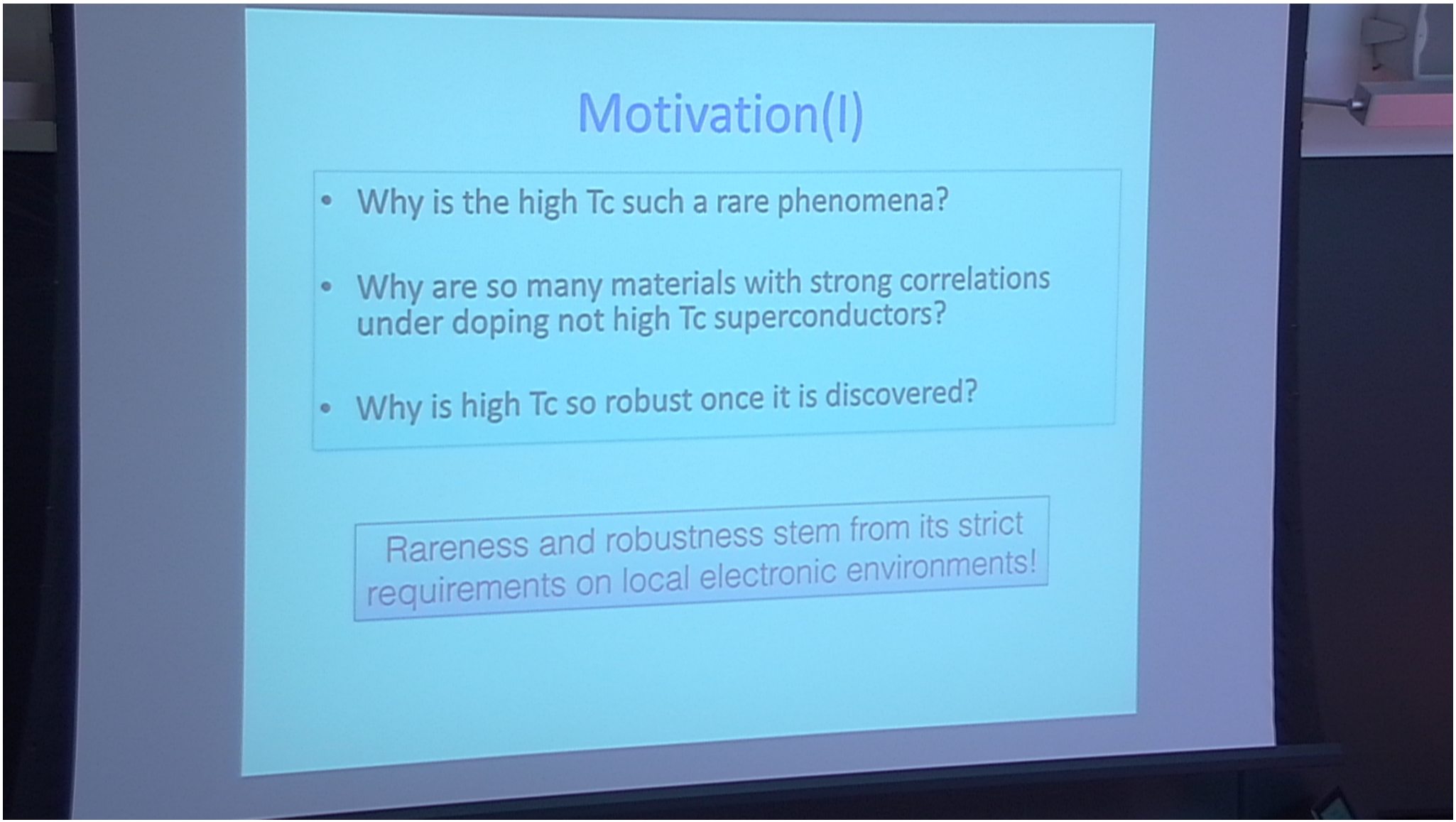
Title: Search the Genes of Unconventional High Temperature Superconductors

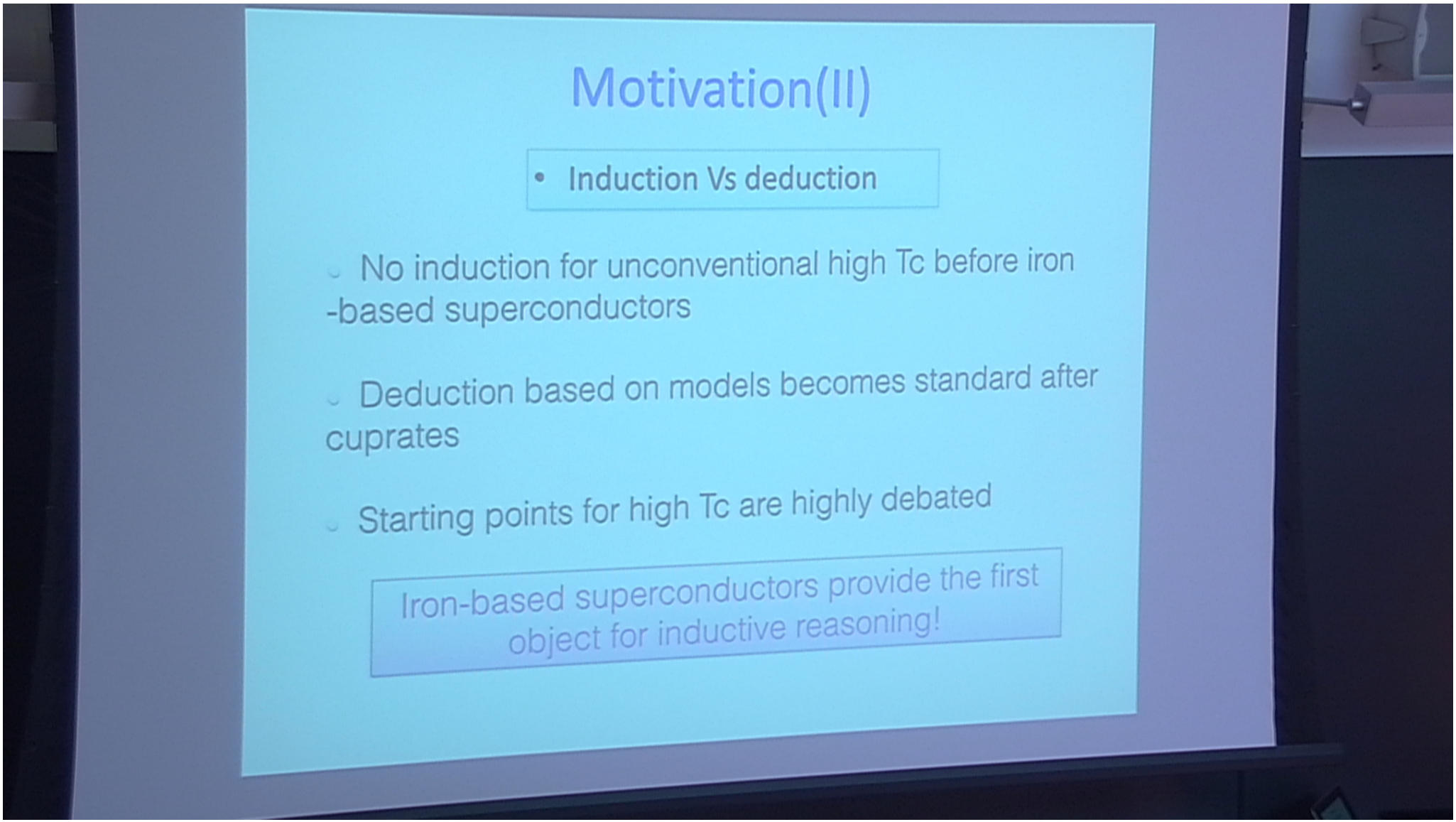
Date: Jul 08, 2015 11:00 AM

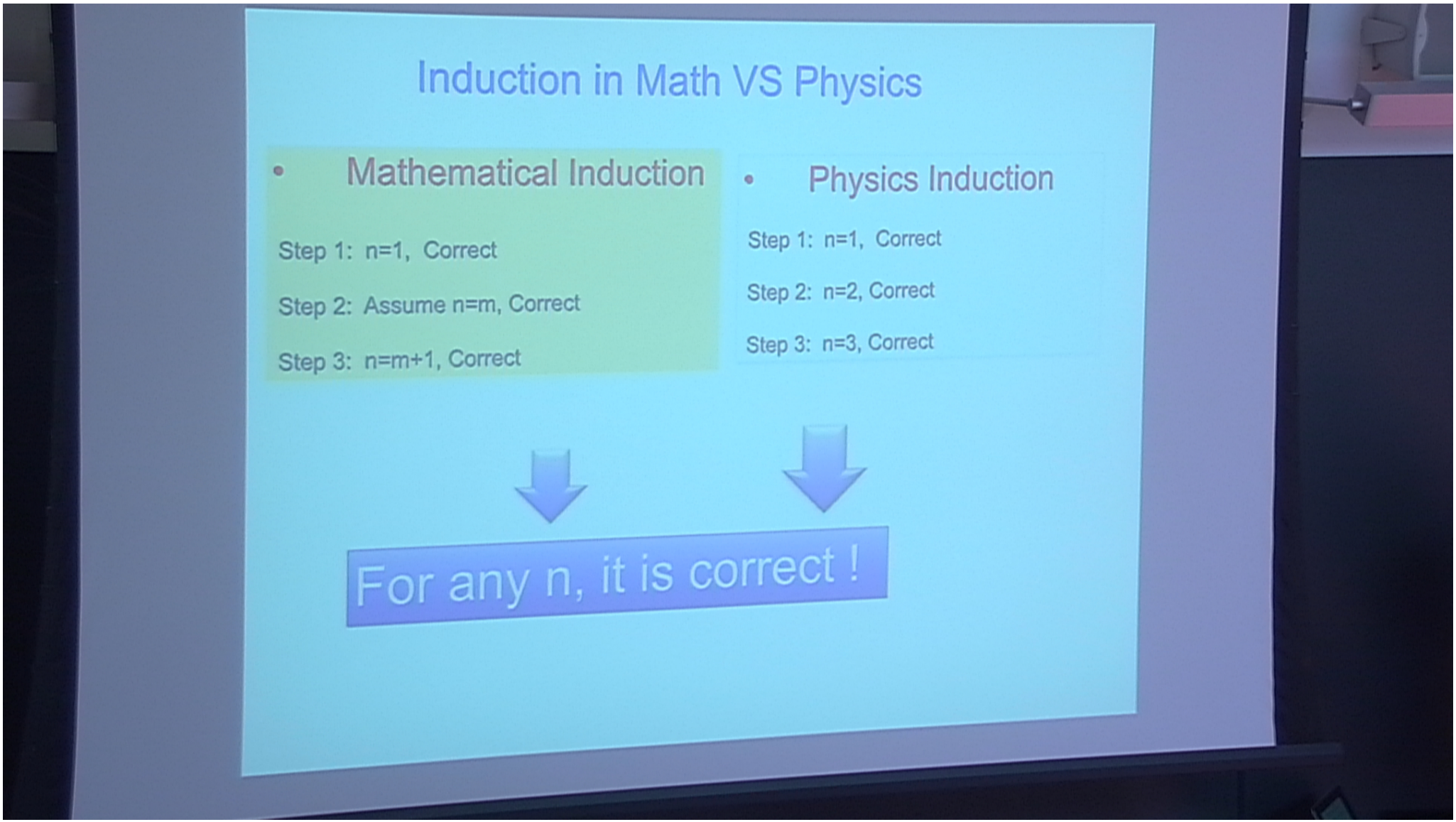
URL: http://pirsa.org/15070068

Abstract: We discuss two basic principles to unify the understanding of both cuprates and iron-based superconductors: (1) the correspondence principleâ€” the short range magnetic exchange interactions and the Fermi surfaces act collaboratively to achieve high Tc superconductivity and determine pairing symmetries; (2) the selective magnetic pairing rule: the superconductivity is only induced by the magnetic exchange couplings from the superexchange mechanism through cation-anion-cation chemical bondings but not those from direct exchange couplings resulted from the direct cation's d-d chemical bondings. These two principles provide a unified explanation why the d-wave pairing symmetry and the s-wave pairing symmetry are robust respectively in cuprates and iron-based superconductors. In the meanwhile, the above two principles can serve as direct guiding rules to search new unconventional high Tc superconductors. We propose that the third classes of unconventional high Tc superconducting candidates in compounds formed by cation-anion trigonal bipyramidal complexes with a d7 filling configuration on the cation ions. Their superconducting states are expected to be dominated by the d+id pairing symmetry. Synthesizing these compounds and verifying the prediction can convincingly establish the high Tc superconducting mechanism and pave a way to design new high Tc superconductors


Outline
Motivation
Cuprates Vs Iron-Based Superconductors
Experimental results of pairing symmetries
What did theories tell about pairing symmetries?
Correspondence principle
Magnetic selection rule in pairing
Predicting new high Tc electronic structure
JP Hu, et al: arxiv:1506.05791, 1506.03904

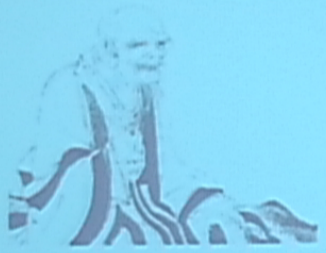

Motivation(I)
• Why is the high Tc such a rare phenomena?
• Why are so many materials with strong correlations under doping not high Tc superconductors?
• Why is high Tc so robust once it is discovered?
Rareness and robustness stem from its strict requirements on local electronic environments!

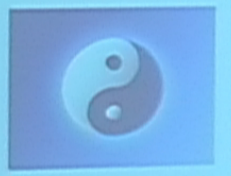

Motivation(II)
• Induction Vs deduction
No induction for unconventional high Tc before iron -based superconductors
Deduction based on models becomes standard after cuprates
Starting points for high Tc are highly debated
Iron-based superconductors provide the first object for inductive reasoning!


Induction in Math VS Physics
Mathematical Induction
Step 1: n=1, Correct
Step 2: Assume n=m, Correct
Step 3: n=m+1, Correct
Physics Induction
Step 1: n=1, Correct
Step 2: n=2, Correct
Step 3: n=3, Correct
For any n, it is correct !

道生一，一生二，二生三，三生万物

The Tao produced One; One produced Two; Two produced Three; Three produced All things.

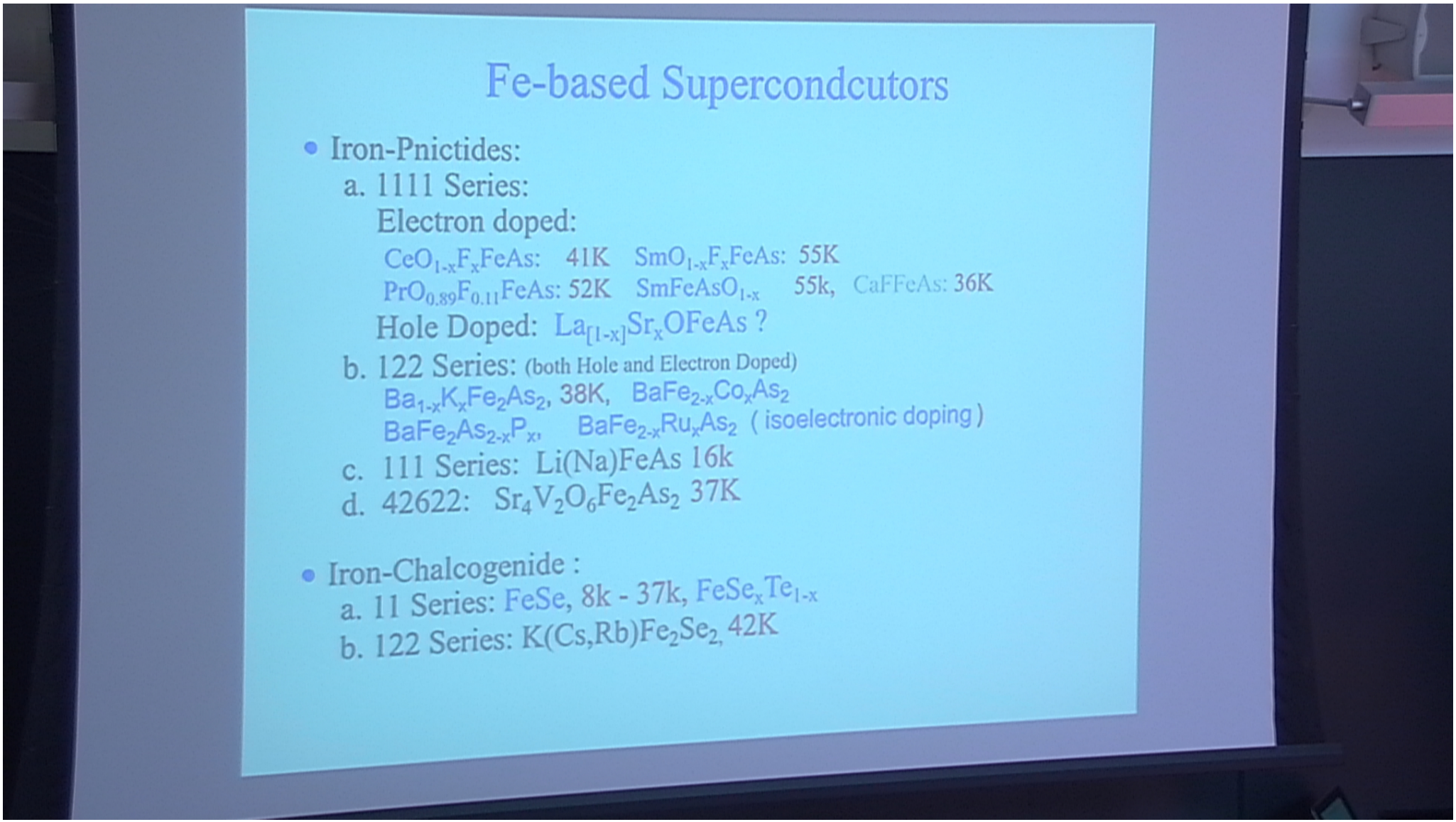




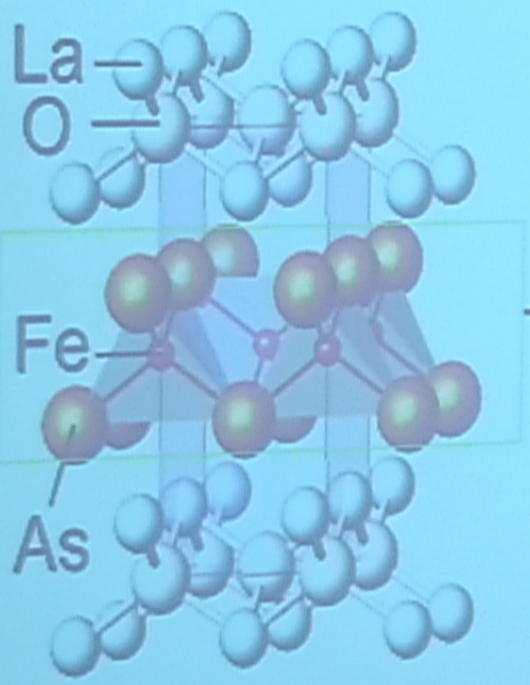
- Curpates
- Iron-based superconductors
- ?

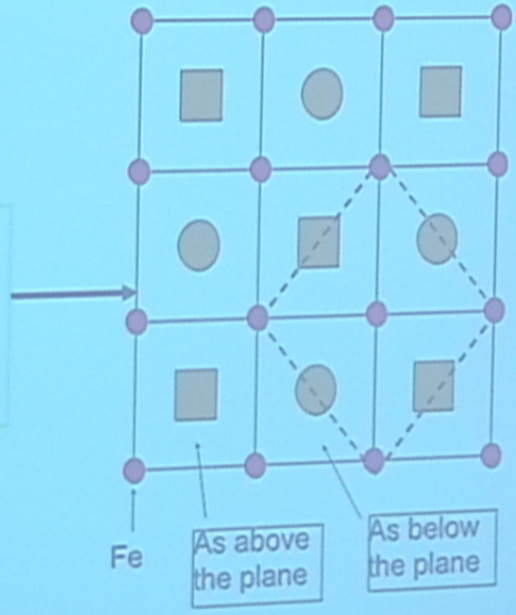
Repeat good things three times:

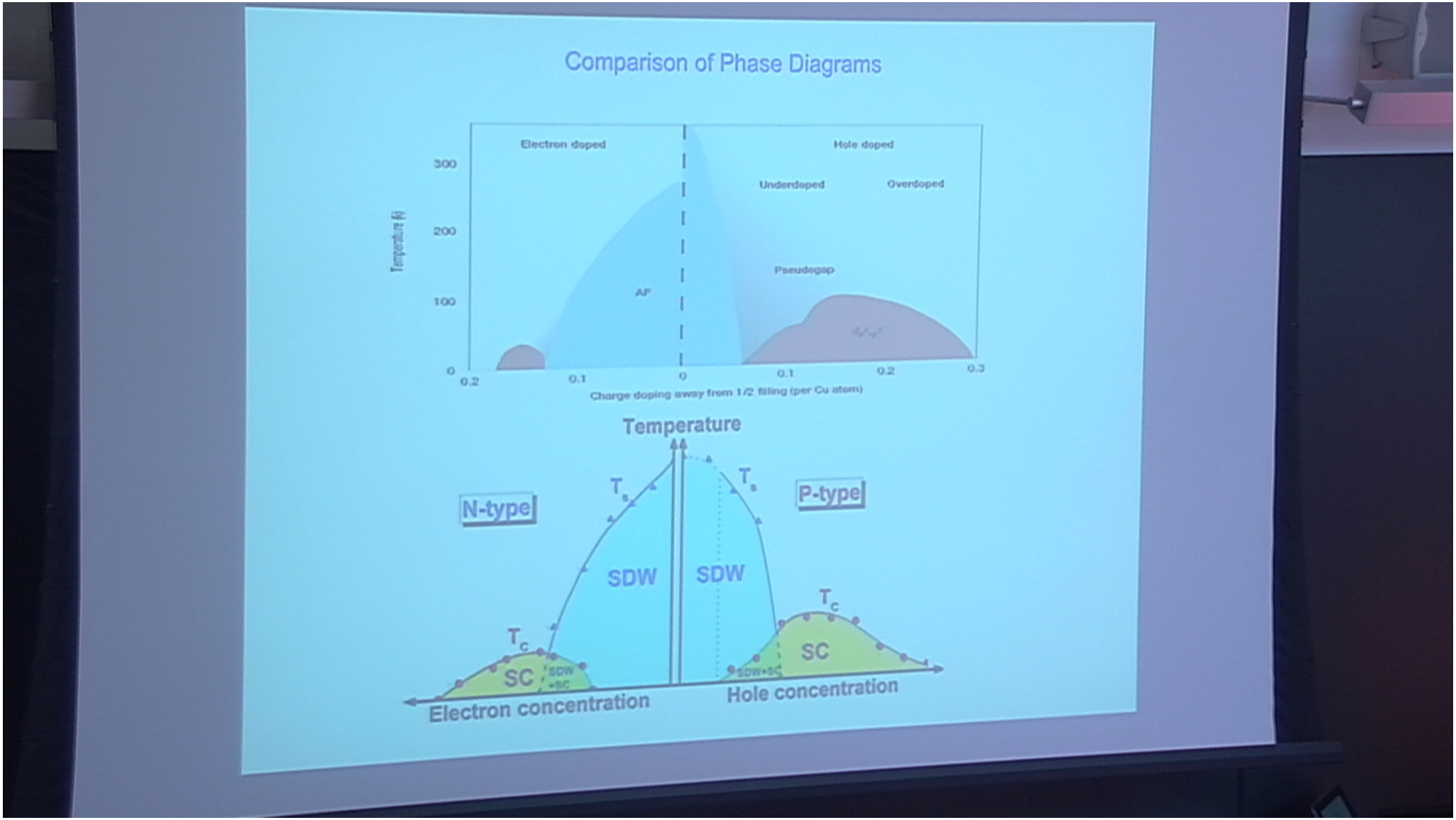
1 = Maybe
2 = Possible
3 = Infinite = Truth

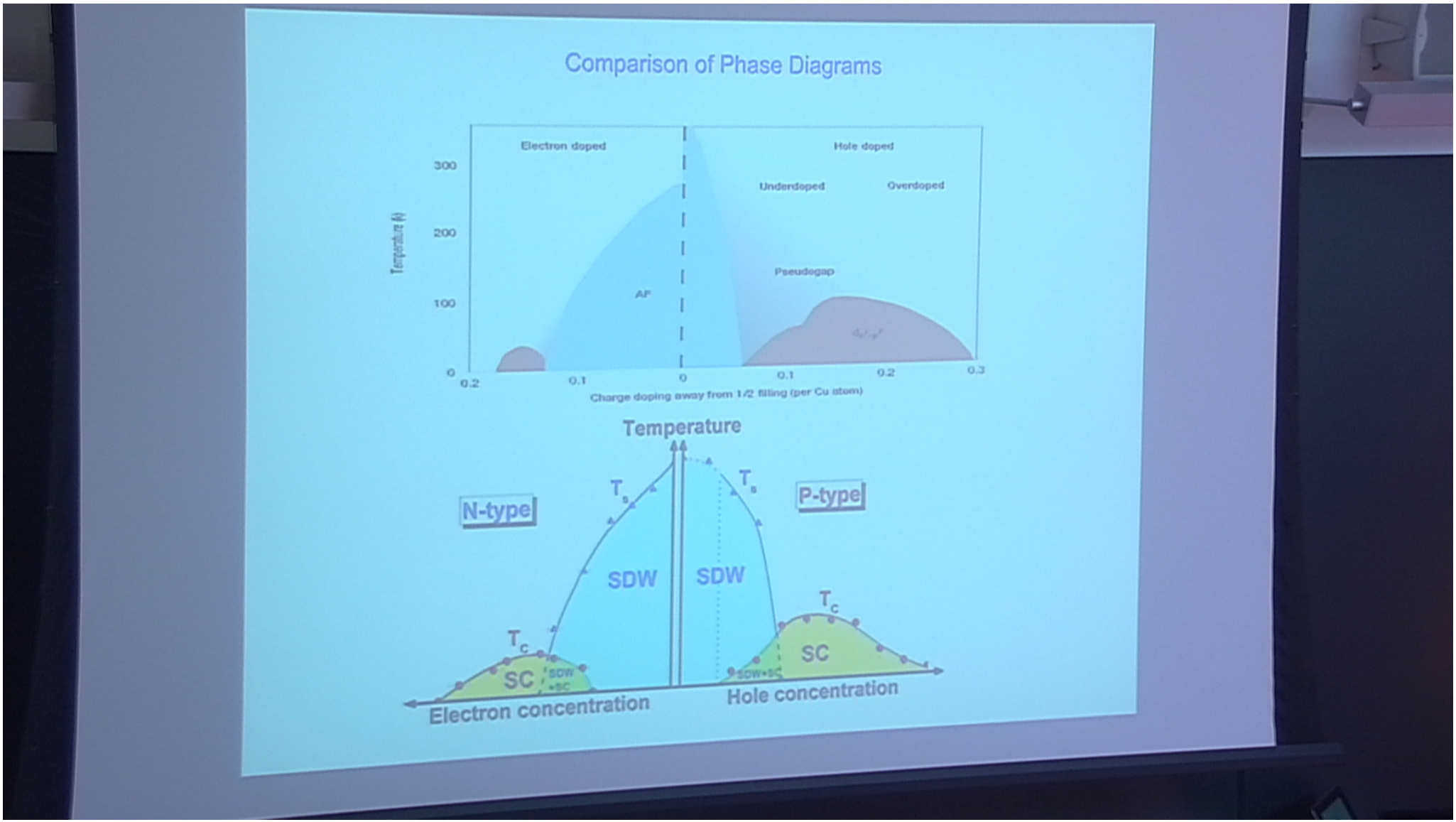

Fe-based Supercondcutors
• Iron-Pnictides:
a. 1111 Series:
Electron doped:
$CeO_{1-x}F_xFeAs$: 41K $SmO_{1-x}F_xFeAs$: 55K
$PrO_{0.89}F_{0.11}FeAs$: 52K $SmFeAsO_{1-x}$ 55k, CaFFeAs: 36K
Hole Doped: $La_{[1-x]}Sr_xOFeAs$?
b. 122 Series: (both Hole and Electron Doped)
$Ba_{1-x}K_xFe_2As_2$, 38K, $BaFe_{2-x}Co_xAs_2$
$BaFe_2As_{2-x}P_x$, $BaFe_{2-x}Ru_xAs_2$ (isoelectronic doping)
c. 111 Series: Li(Na)FeAs 16k
d. 42622: $Sr_4V_2O_6Fe_2As_2$ 37K
• Iron-Chalcogenide :
a. 11 Series: FeSe, 8k - 37k, $FeSe_xTe_{1-x}$
b. 122 Series: $K(Cs,Rb)Fe_2Se_2$, 42K

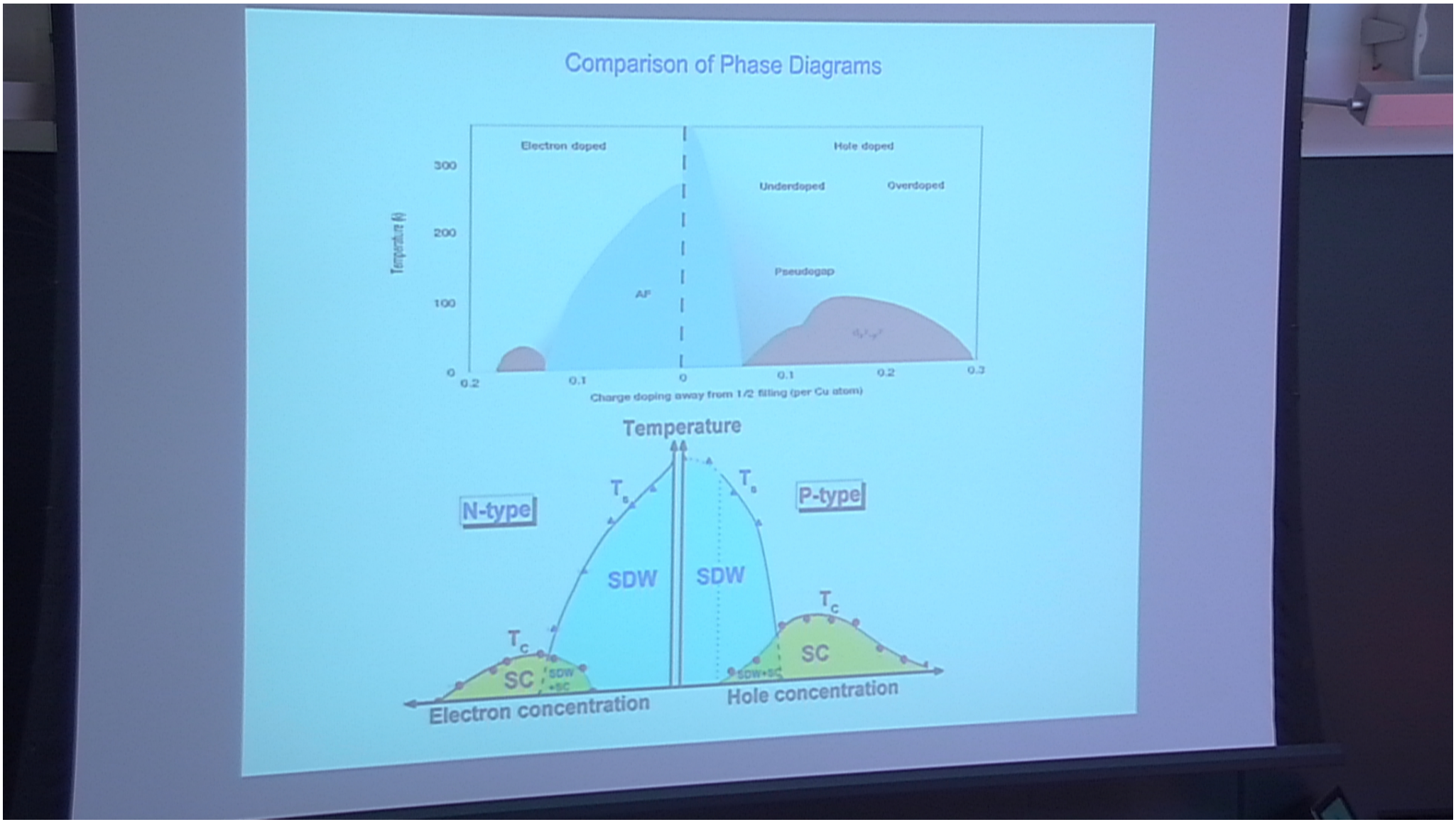
Structure of LaOFeAs

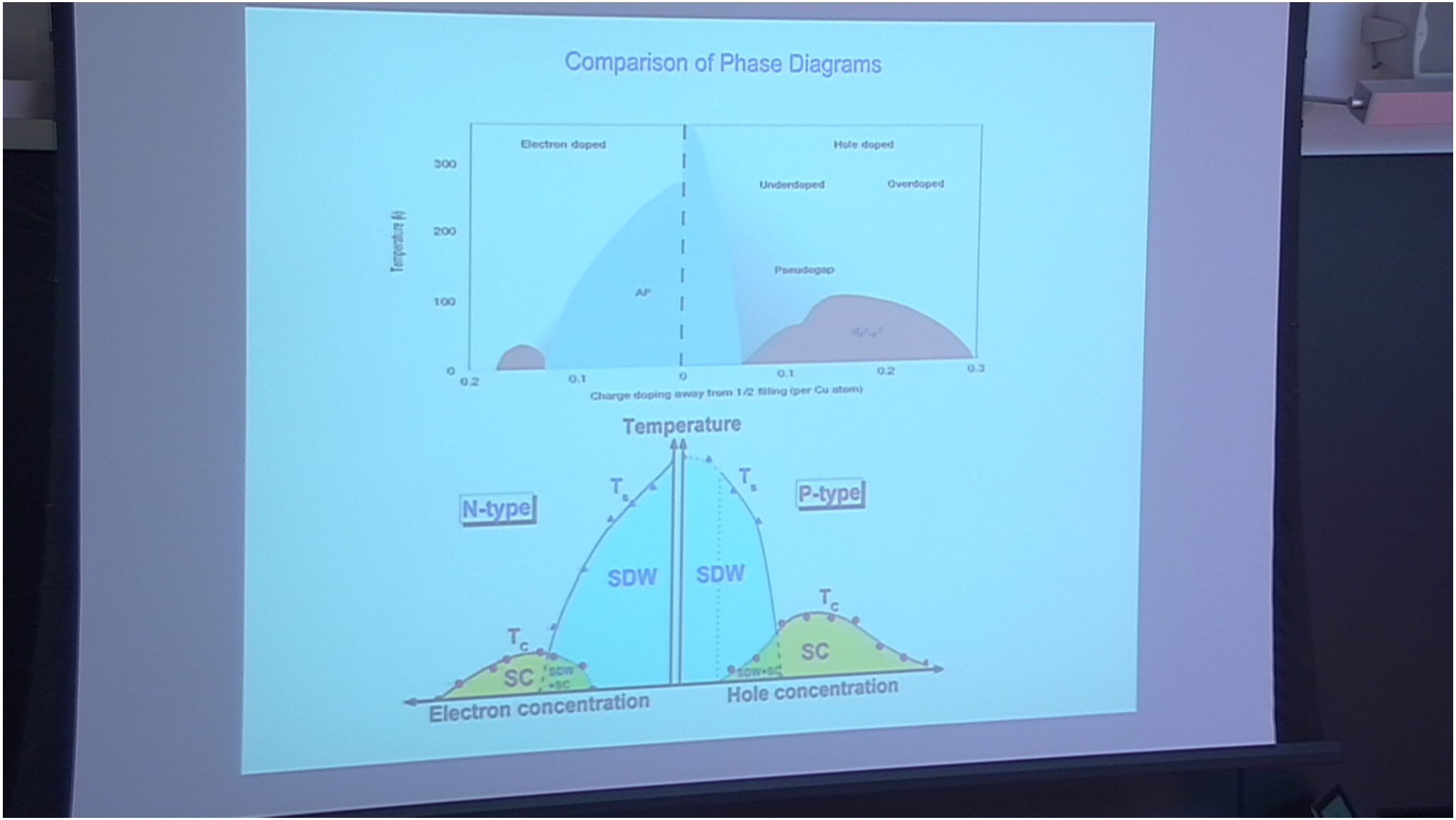


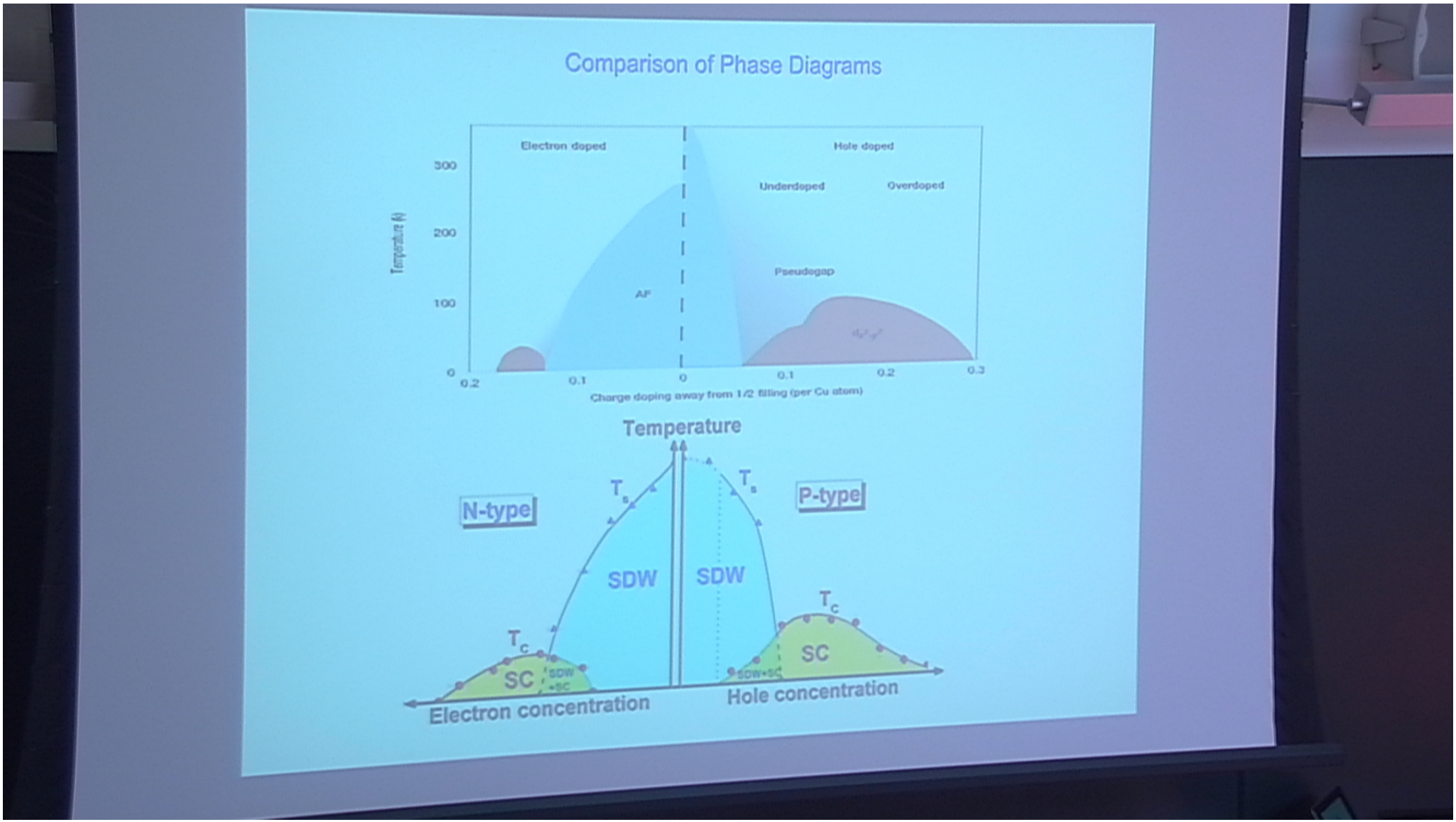



Comparison of Phase Diagrams
Electron doped
Hole doped
Underdoped
Overdoped
Pseudogap
AF
Temperature (K)
300
200
100
0
0.2
0.1
0
0.1
0.2
0.3
Charge doping away from 1/2 filling (per Cu atom)
Temperature
N-type
P-type
T_s
T_s
SDW
SDW
T_c
T_c
SC
SC
SDW+SC
Electron concentration
Hole concentration


Comparison of Phase Diagrams
Electron doped
Hole doped
Underdoped
Overdoped
Pseudogap
AF
300
200
100
0
0.2
0.1
0
0.1
0.2
0.3
Charge doping away from 1/2 filling (per Cu atom)
Temperature
N-type
P-type
SDW
SDW
SC
SC
Electron concentration
Hole concentration


Comparison of Phase Diagrams
Electron doped
Hole doped
Underdoped
Overdoped
Pseudogap
AF
300
200
100
0
0.2
0.1
0
0.1
0.2
0.3
Charge doping away from 1/2 filling (per Cu atom)
Temperature
N-type
P-type
SDW
SDW
SC
SC
Electron concentration
Hole concentration


Comparison of Phase Diagrams
Electron doped
Hole doped
Underdoped
Overdoped
Pseudogap
AF
Temperature (K)
300
200
100
0
0.2
0.1
0
0.1
0.2
0.3
Charge doping away from 1/2 filling (per Cu atom)
Temperature
N-type
P-type
T_s
T_s
SDW
SDW
T_c
T_c
SC
SC
SDW+SC
Electron concentration
Hole concentration


Comparison of Phase Diagrams
Electron doped
Hole doped
Underdoped
Overdoped
Pseudogap
AF
300
200
100
0
0.2
0.1
0
0.1
0.2
0.3
Charge doping away from 1/2 filling (per Cu atom)
Temperature
N-type
P-type
SDW
SDW
SC
SC
Electron concentration
Hole concentration

History Comparison

VOLUME 70, NUMBER 10 PHYSICAL REVIEW LETTERS 8 MARCH 1993

Anomalously Large Gap Anisotropy in the a-b Plane of $Bi_2Sr_2CaCu_2O_{8+\delta}$

Z.-X. Shen,[1,2,3] D. S. Dessau,[1,2,3] B. O. Wells,[1,2,3,4] D. M. King,[2,3] W. E. Spicer,[2,3] A. J. Arko,[1,3] D. Marshall,[2,3] L. W. Lombardo,[1,3] A. Kapitulnik,[1,3] P. Dickinson,[1,3] S. Doniach,[1,3] J. DiCarlo,[1,2,3] A. G. Loeser,[1,2,3] and C. H. Park[1,2,3]

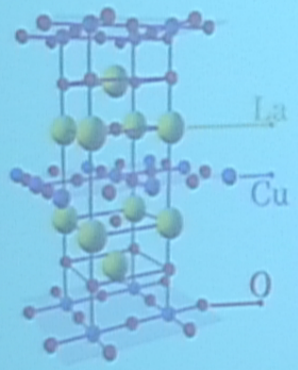
[1]*Department of Applied Physics, Stanford University, Stanford, California 94305*

[2]*Solid State Electronics Laboratory and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, California 94305-4055*

[3]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545*

(Received 11 November 1992)

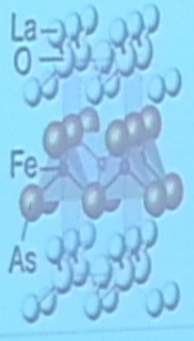
Superconducting gap anisotropy at least an order of magnitude larger than that of the conventional superconductors has been observed in the a-b plane of $Bi_2Sr_2CaCu_2O_{8+\delta}$ in angle-resolved photoemission spectroscopy. For samples with T_c of 88 K, the gap size reaches a maximum of approximately 20 meV along the Cu-O bond direction, and a minimum of much smaller or vanishing magnitude 45° away. The experimental data are discussed within the context of various theoretical models. In particular, a detailed comparison with what is expected from a superconductor with a $d_{x^2-y^2}$ order parameter is carried out, yielding a consistent picture.



Discover: 1986

d-wave: 1993

Establish: 2000



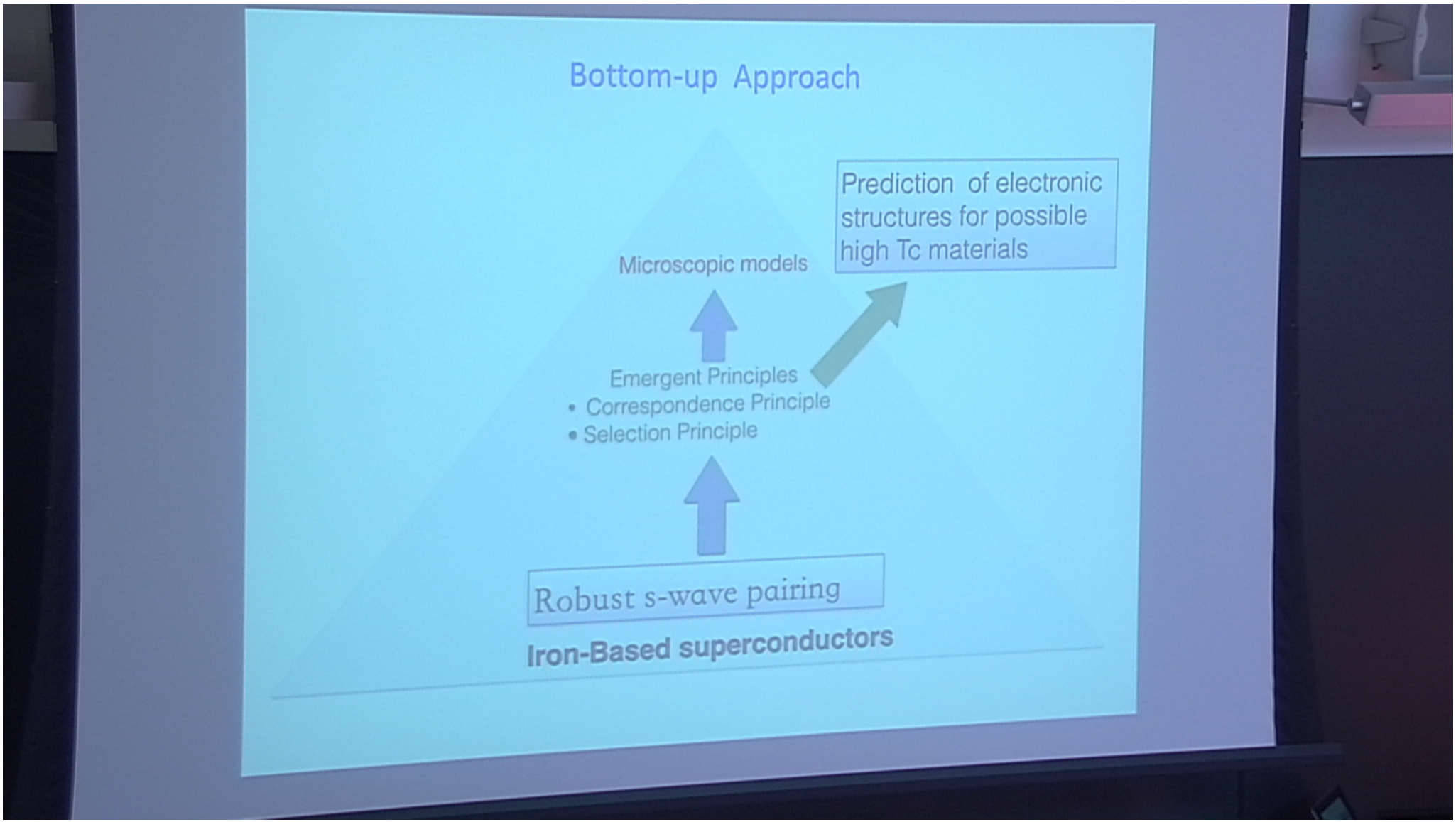
Discover: 2008

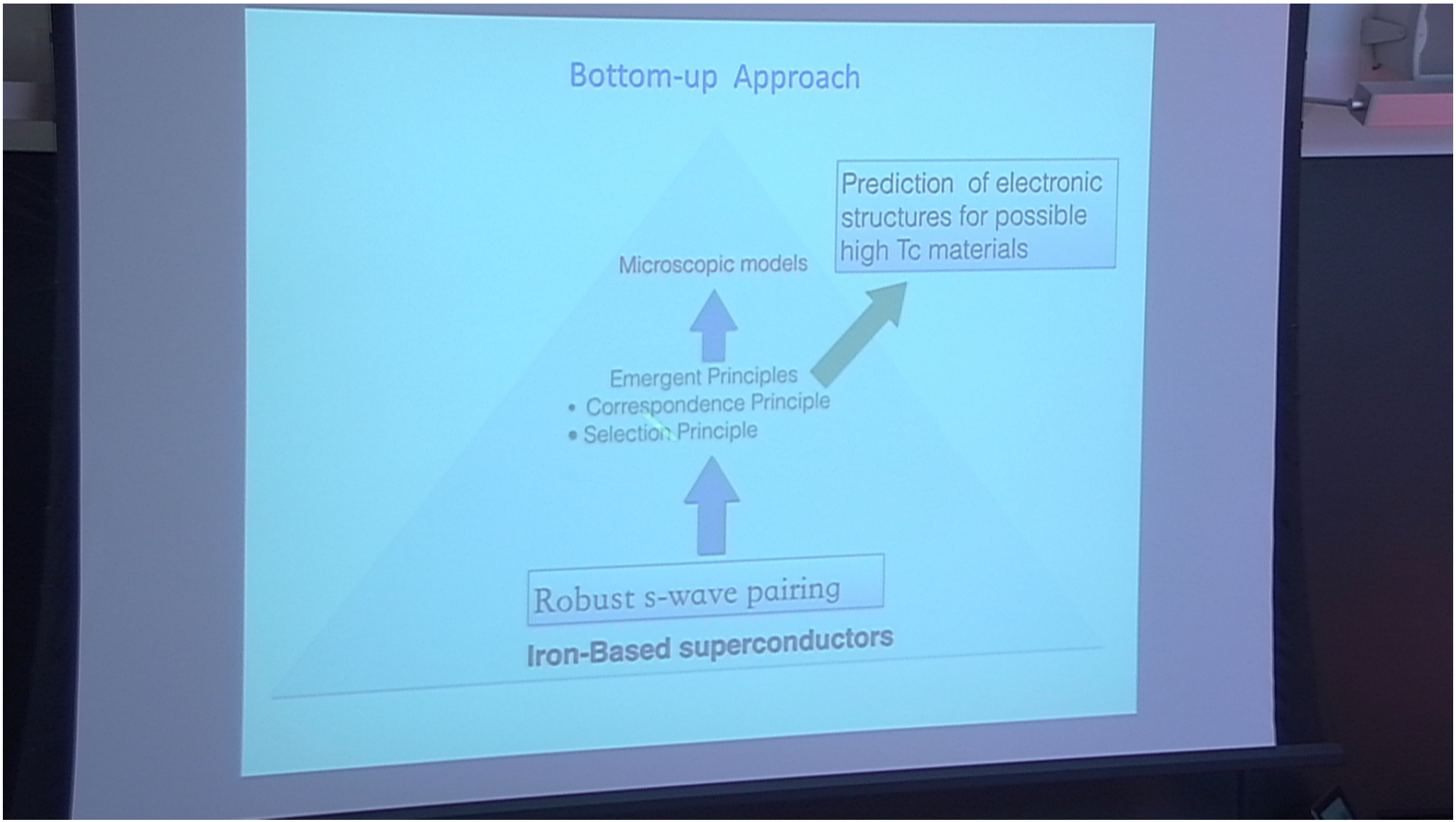
? –wave: 2015?

Establish: ?

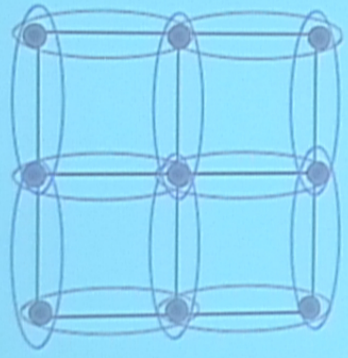
Pairing Symmetry

- black or white
- important to mechanism

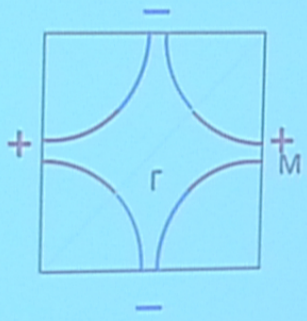

Bottom-up Approach
Prediction of electronic structures for possible high Tc materials
Microscopic models
Emergent Principles
• Correspondence Principle
• Selection Principle
Robust s-wave pairing
Iron-Based superconductors


Bottom-up Approach
Prediction of electronic structures for possible high Tc materials
Microscopic models
Emergent Principles
• Correspondence Principle
• Selection Principle
Robust s-wave pairing
Iron-Based superconductors

How d-wave Pairing Symmetry is determined in Curpates



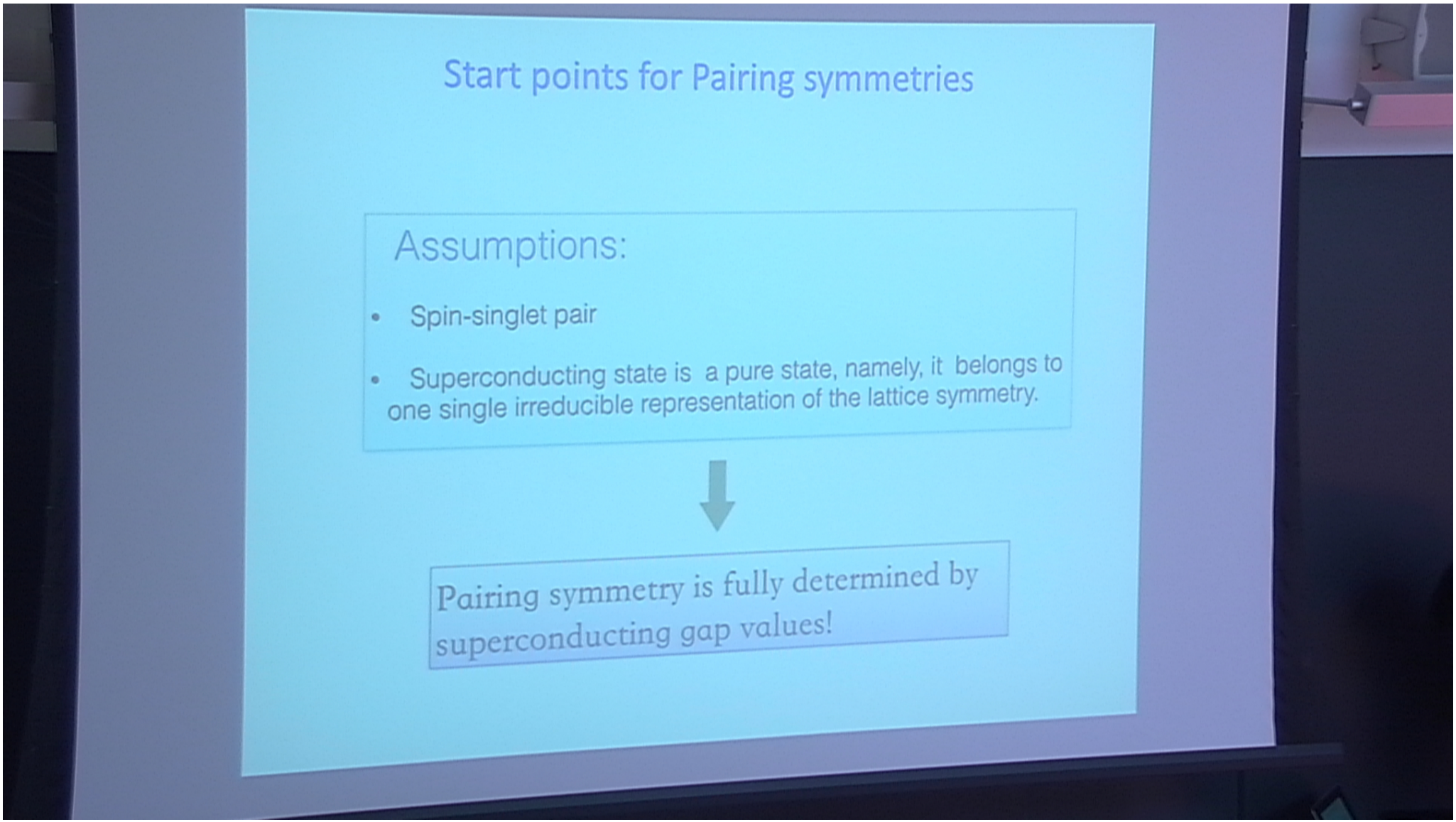
$$\Delta(r) = |\Delta(r)| e^{i\phi(r)}$$

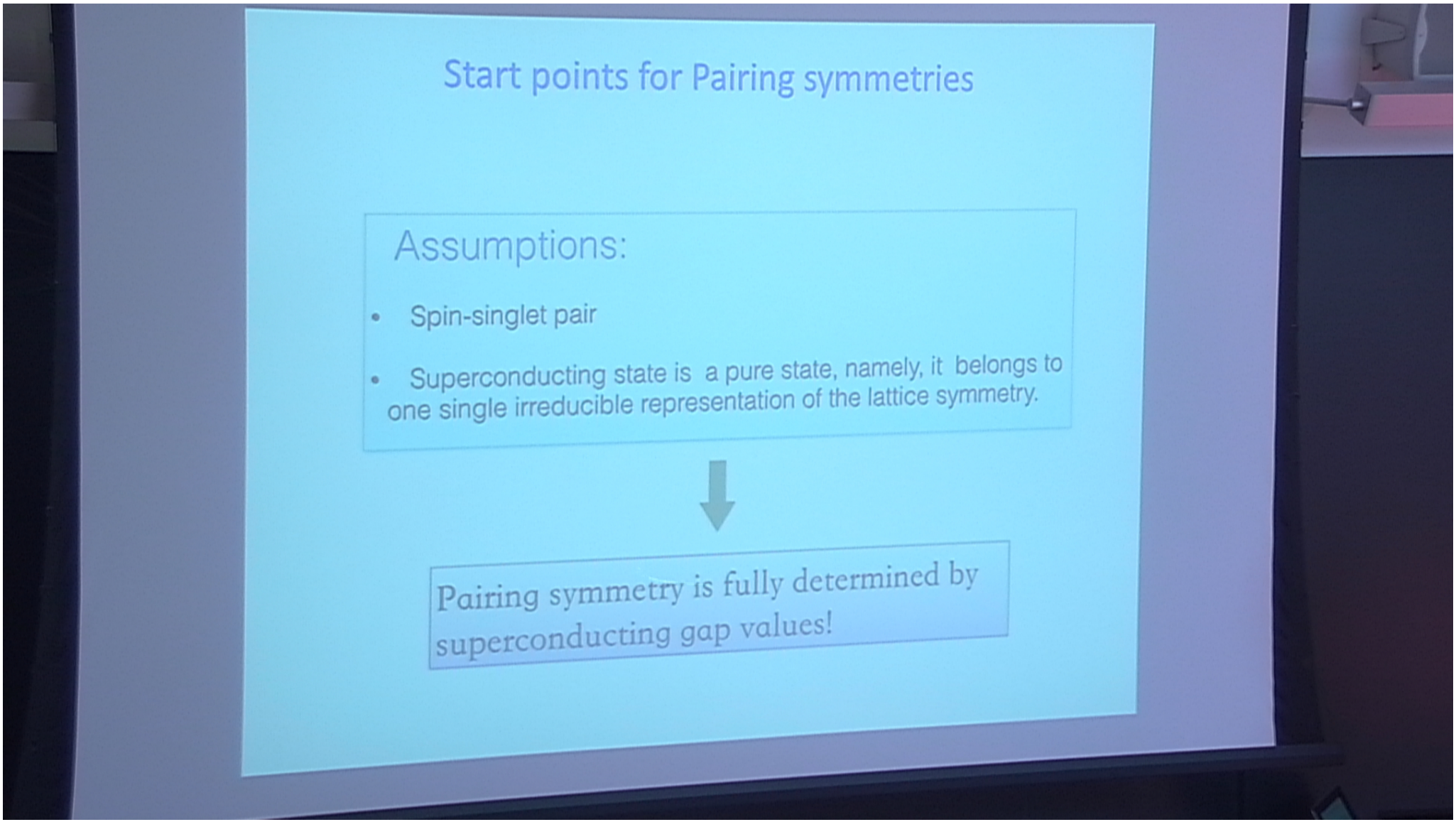


$$\Delta(k) = |\Delta(k)| e^{i\phi(k)}$$

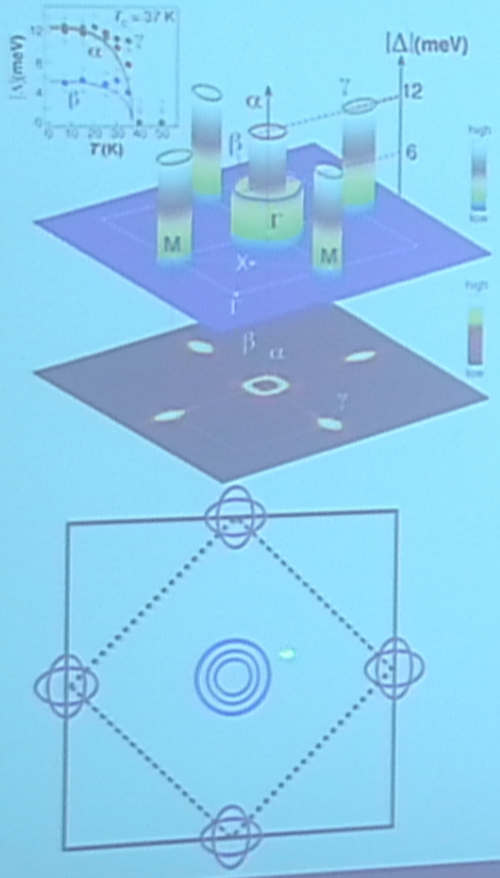
d-wave:

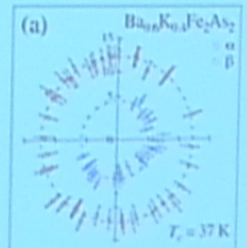
- Gapless nodes: affect many physical properties
- Sign change in in both real space and momentum space: phase sensitive measurements

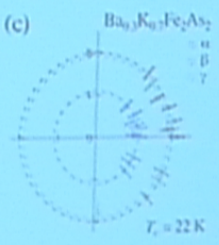

Start points for Pairing symmetries
Assumptions:
• Spin-singlet pair
• Superconducting state is a pure state, namely, it belongs to one single irreducible representation of the lattice symmetry.
Pairing symmetry is fully determined by superconducting gap values!

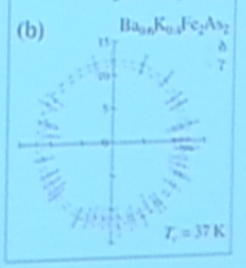

Start points for Pairing symmetries
Assumptions:
• Spin-singlet pair
• Superconducting state is a pure state, namely, it belongs to one single irreducible representation of the lattice symmetry.
Pairing symmetry is fully determined by superconducting gap values!

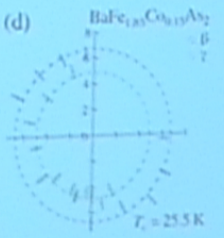
Iron-Based Superconductors: Gap structure







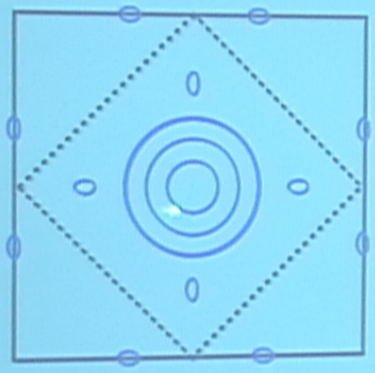


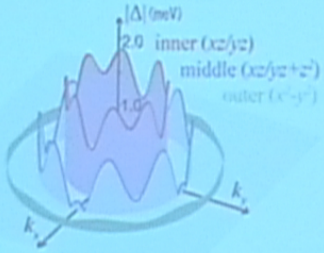


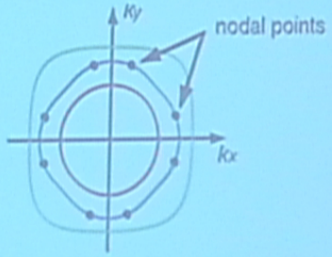
- Full Gap structure on both electron and hole doped 122

H. Ding et al: EPL 8 47001 (2008)
K. Terashima et al: PNAS 106 7330 (2009).
PRB 83:020502(R)

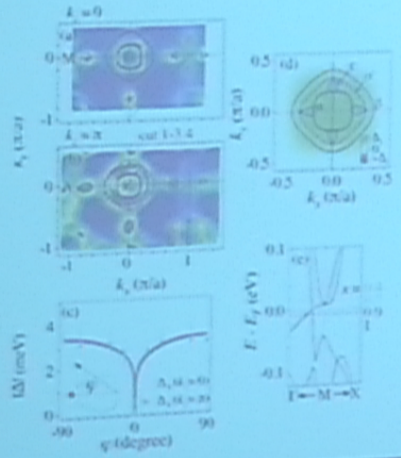
Iron-Based Superconductors: Heavy Hole doping(FeAs)







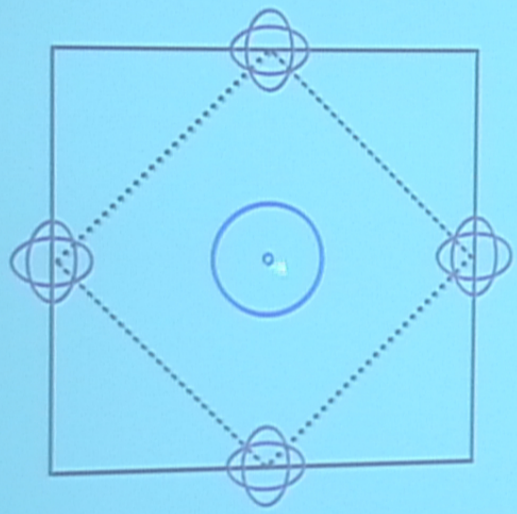
KFe2As2
K. Okazaki et al, Science 337 1314 (2012)

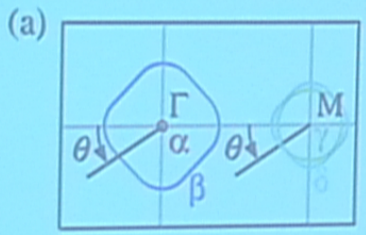


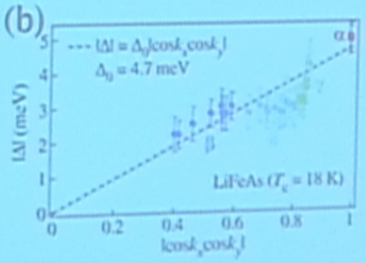
- Full Gap for inner Hole pockets
- Nodes develops on the outer hole pockets
- The gap size is larger in the the inner hole pocket

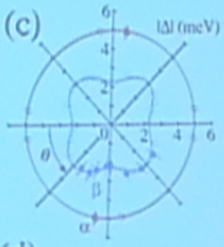
K0.9Fe2As2
N. Xu et al, PRB ,88 220508 (2013)

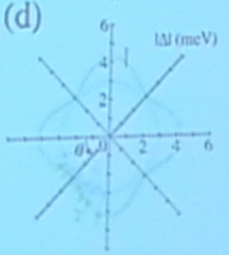
Iron-Based Superconductors: Gap structure (LiFeAs)







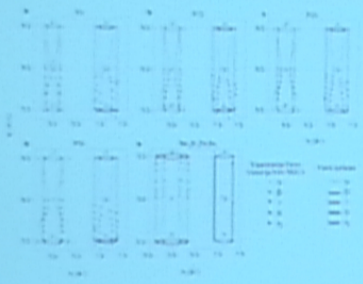


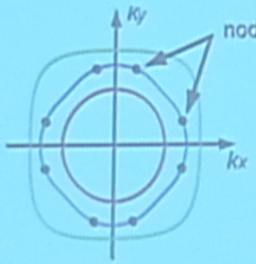


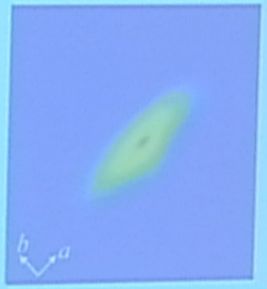
K. Umezawa et al, PRL 108 037002 (2012)

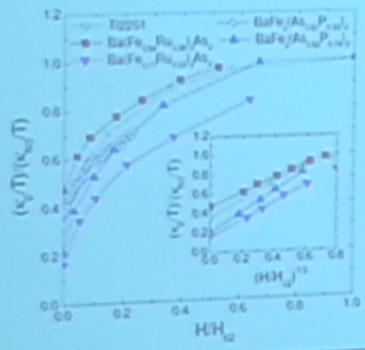
- Full Gap
- Large superconductivity order exists even if the pockets sinks below Fermi surfaces
- The gap size is larger in the the inner hole pocket

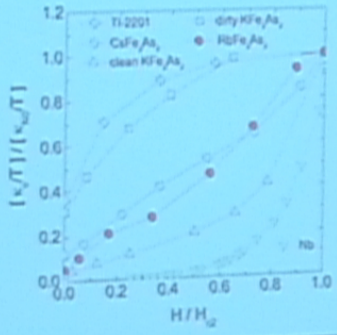
Iron-Based Superconductors: Accidental nodes

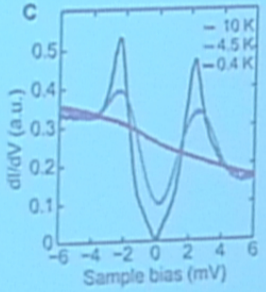










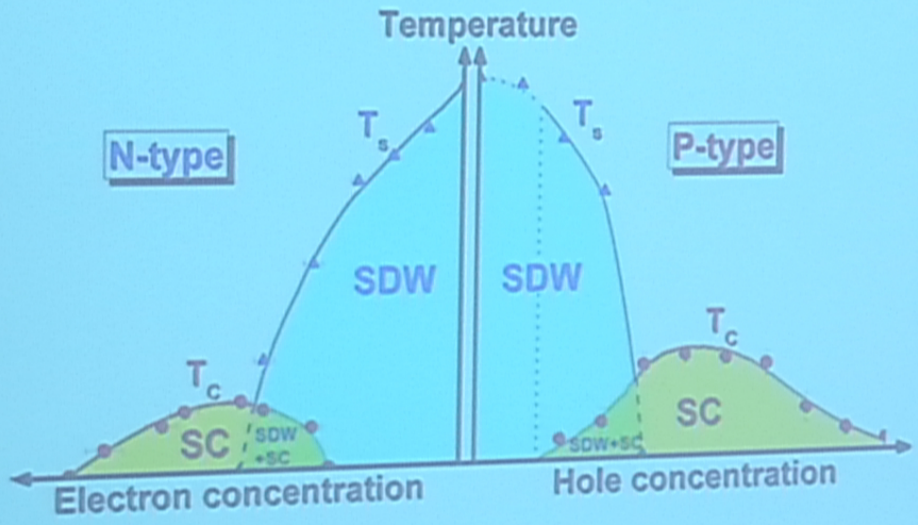


$BaFe_2As_{2-x}P_x$
X. Qiu, et al. PRX, 011010 (2012)
Y. Zhang, et al. Nature Phys. 8,371 (2012)

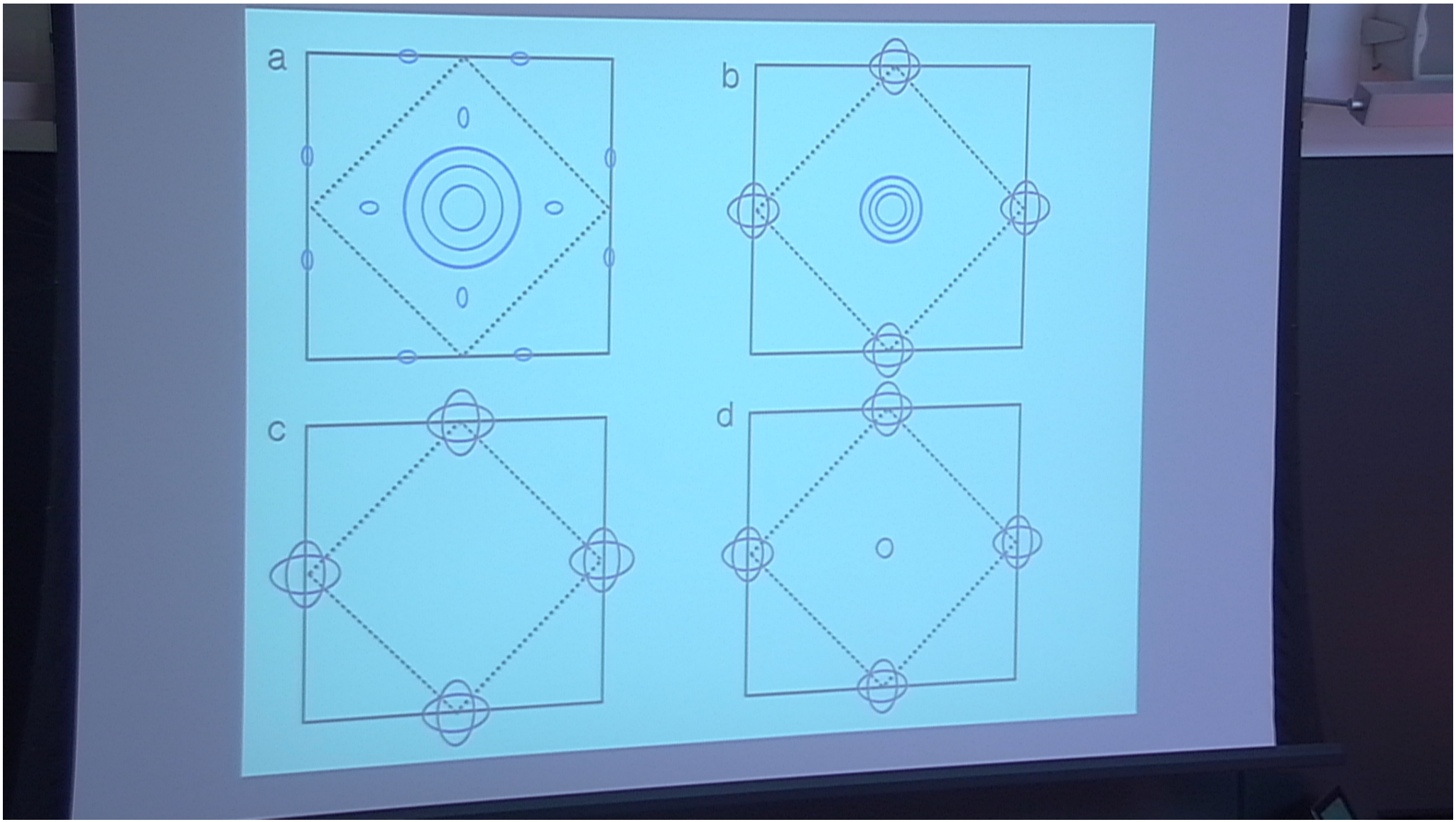
AFe2As2
Z. Zhang, et al. PRB, 91 024502 (2015)
K. Okazaki et al. Science 337 1314 (2012)

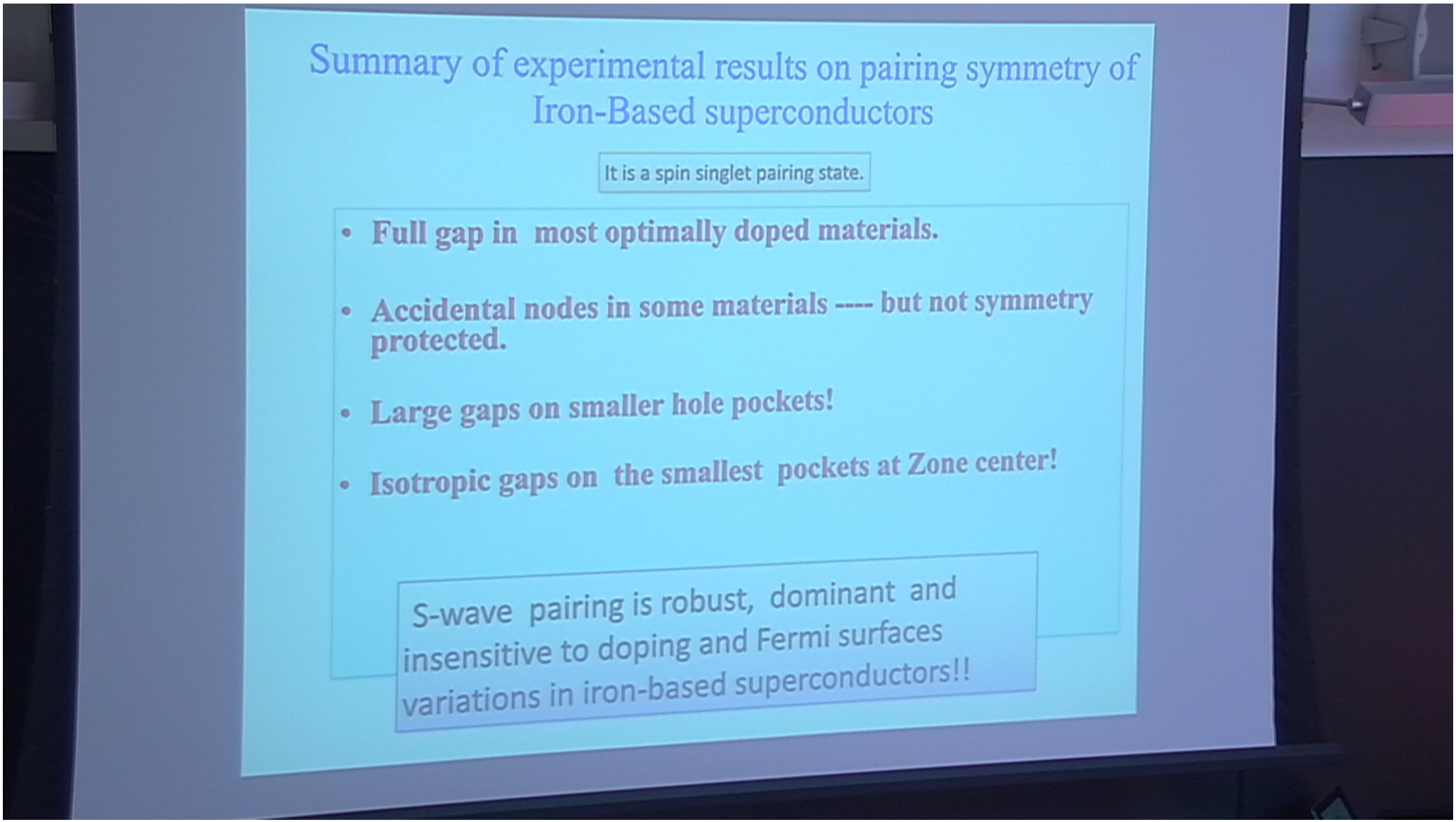
FeSe (strong orthorhombic)
CL Song et al, Science, 332 1410 (2011)

Phase Diagrams



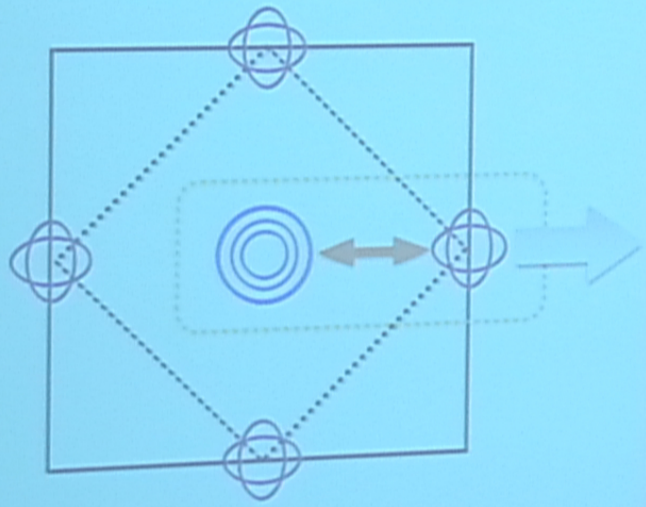
Smooth phase diagram is also against pairing symmetry change.


a
b
c
d


Summary of experimental results on pairing symmetry of Iron-Based superconductors
It is a spin singlet pairing state.
• Full gap in most optimally doped materials.
• Accidental nodes in some materials ---- but not symmetry protected.
• Large gaps on smaller hole pockets!
• Isotropic gaps on the smallest pockets at Zone center!
S-wave pairing is robust, dominant and insensitive to doping and Fermi surfaces variations in iron-based superconductors!!

Standard Model (I): Hubbard-Type model

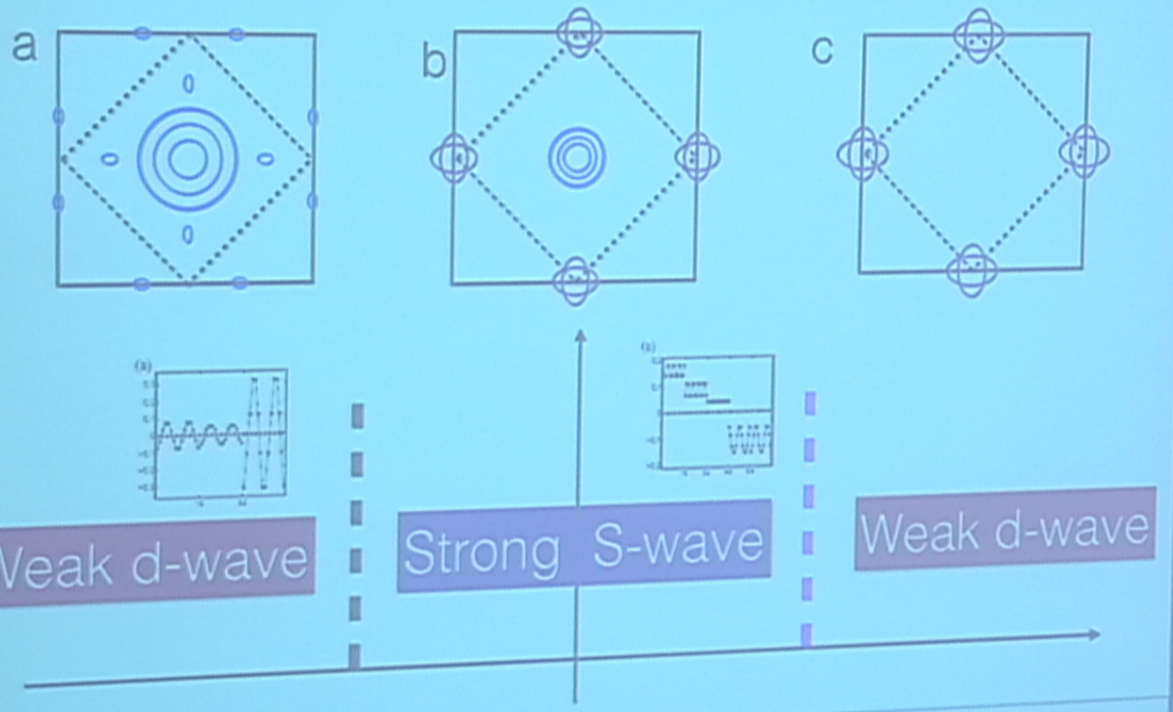
$$\hat{H}_U = \hat{H}_0 + \hat{H}_I,$$
$$\hat{H}_I = \sum_i [\sum_{a \neq b} (J_H \hat{S}_{ai} \cdot \hat{S}_{bi} + U' \hat{n}_{ai\uparrow} \hat{n}_{bi\downarrow}) + U \hat{n}_{ai\uparrow} n_{ai\downarrow}]$$



- Robust S-wave at near nesting condition
- Driven by repulsive interaction between electron and hole pockets: S±
- Strong superconductivity is achieved near nesting condition.

Mazin, Kuroki, Dunghai Lee, Chubukov, Hirschfeld, Scalapino…

Standard Hubbard-Type model results



- S-wave is not robust against doping.
- d-wave symmetry is expected when only electron pockets exist.
- d-wave is expected to be much weaker.

Standard Model (II): t-J-Type effective model

$$\hat{H}_{tJ} = \hat{\tilde{H}}_0 + \sum_{<ij>} J_{ij} \hat{S}_i \cdot \hat{S}_j$$

To Achieve High Tc:

- Strong renormalized band structure. J/t has to be larger than a critical value (around 0.1)
- Correspondence Principle: Collaboration between the form factors of effective magnetic exchange coupling and Fermi surfaces to determine pairing symmetry

Robust S-wave:

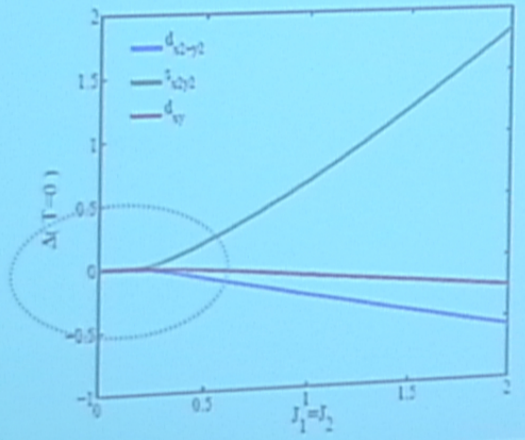
- Magnetic selection rule in pairing: only superexchange magnetism is important in driving pairing

Standard Model (II): t-J-Type effective model

$$\hat{H}_{tJ} = \hat{\tilde{H}}_0 + \sum_{<ij>} J_{ij} \hat{S}_i \cdot \hat{S}_j$$

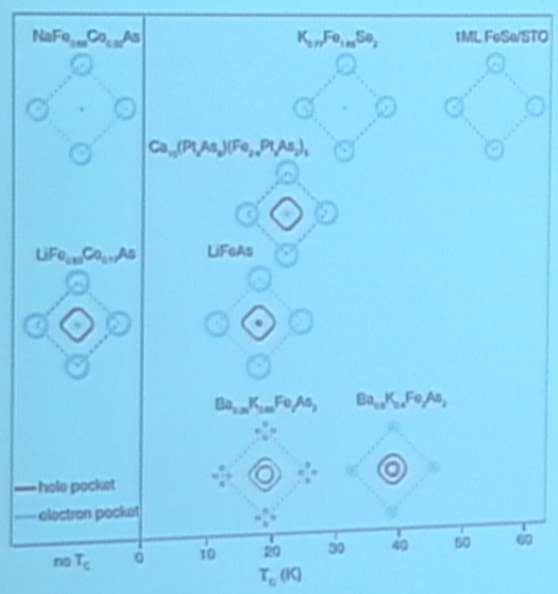
To Achieve High Tc:

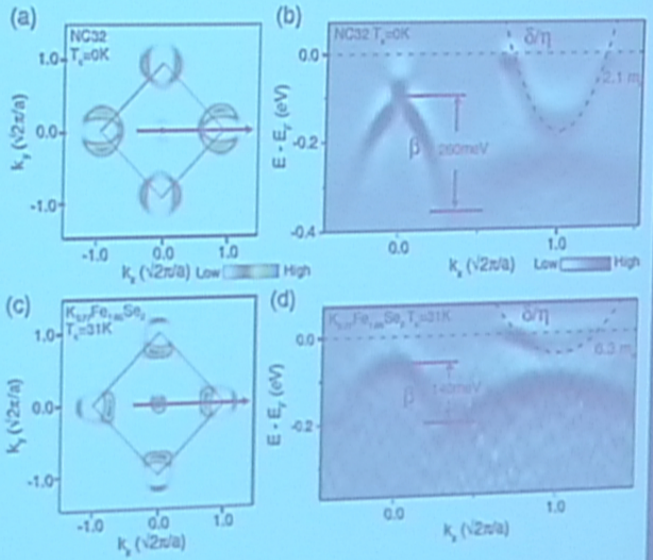
- Strong renormalized band structure. J/t has to be larger than a critical value (around 0.1)



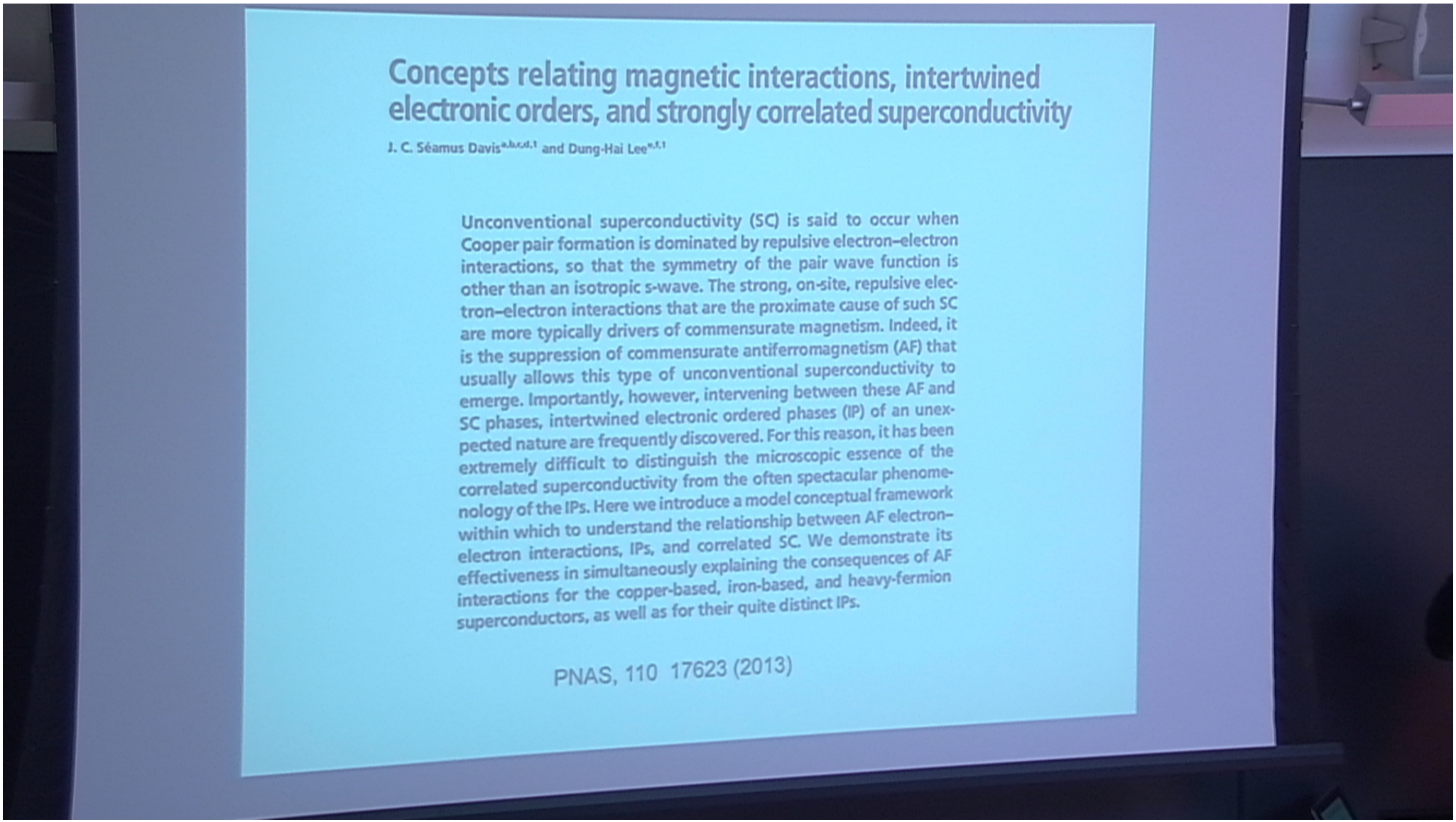
K.Seo, A. B. Bernevig, JP Hu, PRL101,206404 (2008)

Effect of renormalization on High Tc

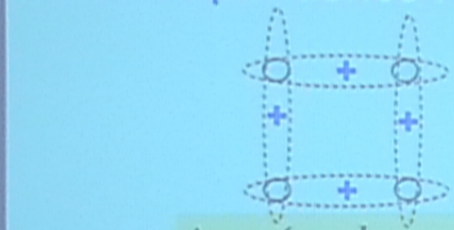




Z.R. YE, et al PRX 4, 031041 (2014)


Concepts relating magnetic interactions, intertwined electronic orders, and strongly correlated superconductivity
J. C. Séamus Davis[a,b,c,d,1] and Dung-Hai Lee[e,f,1]
Unconventional superconductivity (SC) is said to occur when Cooper pair formation is dominated by repulsive electron–electron interactions, so that the symmetry of the pair wave function is other than an isotropic s-wave. The strong, on-site, repulsive electron–electron interactions that are the proximate cause of such SC are more typically drivers of commensurate magnetism. Indeed, it is the suppression of commensurate antiferromagnetism (AF) that usually allows this type of unconventional superconductivity to emerge. Importantly, however, intervening between these AF and SC phases, intertwined electronic ordered phases (IP) of an unexpected nature are frequently discovered. For this reason, it has been extremely difficult to distinguish the microscopic essence of the correlated superconductivity from the often spectacular phenomenology of the IPs. Here we introduce a model conceptual framework within which to understand the relationship between AF electron–electron interactions, IPs, and correlated SC. We demonstrate its effectiveness in simultaneously explaining the consequences of AF interactions for the copper-based, iron-based, and heavy-fermion superconductors, as well as for their quite distinct IPs.
PNAS, 110 17623 (2013)

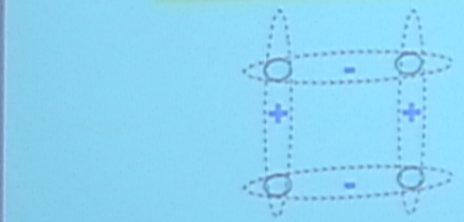
Correspondence Principle of Pairing Symmetry: Cuprates



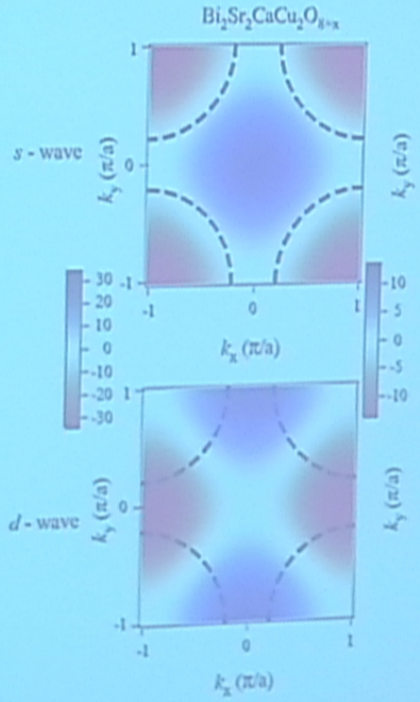
$$\Delta_s \propto (\cos k_x + \cos k_y)$$

$$J\sum_{<ij>} S_i S_j$$

$$\Delta_d \propto (\cos k_x - \cos k_y)$$

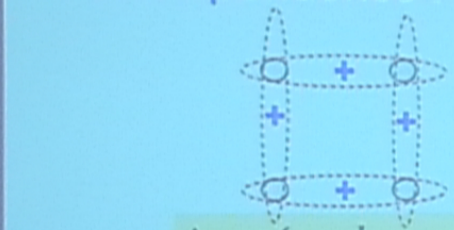


Win



- AFM exchange provides pairing force and possible choices of pairing symmetries.
- Fermi surface topology selects the pairing symmetry.

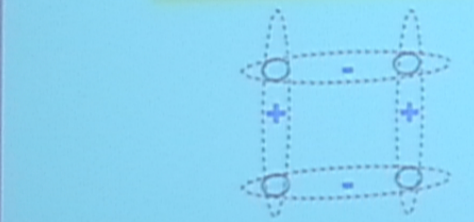
Correspondence Principle of Pairing Symmetry: Cuprates



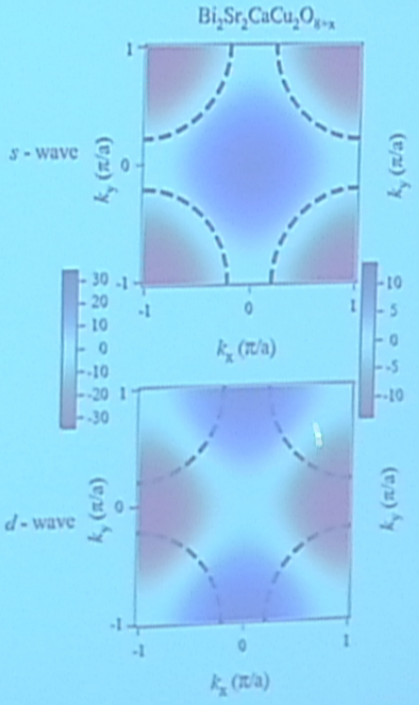
$$\Delta_s \propto (\cos k_x + \cos k_y)$$

$$J \sum_{<ij>} S_i S_j$$

$$\Delta_d \propto (\cos k_x - \cos k_y)$$



Win

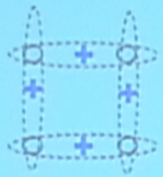


- AFM exchange provides pairing force and possible choices of pairing symmetries.
- Fermi surface topology selects the pairing symmetry.

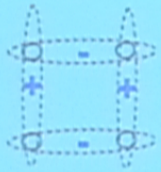
Pairing symmetry in two band-{t}-J_1-J_2 model

J_1

S wave pairing
$\cos k_x + \cos k_y$



d wave pairing
$\cos k_x - \cos k_y$



J_2

S wave pairing
$\cos k_x \cos k_y$

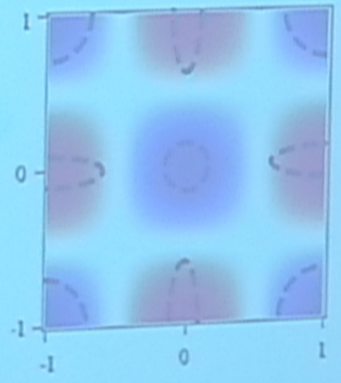
d wave pairing
$\sin k_x \sin k_y$

$$2T_c = J_2 \sum_k (f(k))^2 g(x(k, T_c))$$

Symmetry factors

Function peaks at Fermi surfaces

$Ba_{0.6}K_{0.4}Fe_2As_2$



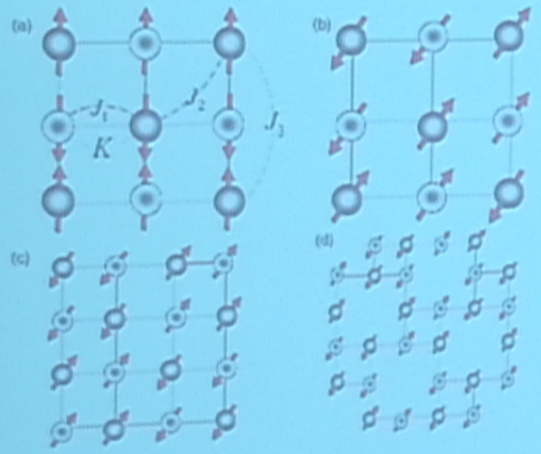
K.Seo, A. B. Bernevig, JP Hu, PRL101,206404 (2008)

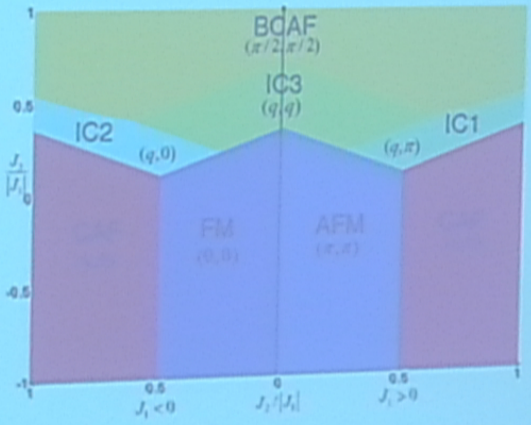
Minimum Magnetic Model

Unified minimum effective model of magnetic properties of iron-based superconductors

Jiangping Hu,[1,2,*] Bao Xu,[1] Wuming Liu,[1] Ning-Ning Hao,[1] and Yupeng Wang[1]

PHYSICAL REVIEW B 85, 144403 (2012)





$$H = \sum_{ij,n} \left[J_{ij} \vec{S}_i^n \cdot \vec{S}_j^n - K_{ij} \left(\vec{S}_i^n \cdot \vec{S}_j^n \right)^2 \right] + J_c \sum_{i,n} \vec{S}_i^n \cdot \vec{S}_i^{n+1}$$

A. L. Wysocki, Nature Physics 7 485 (2011)

Minimum Magnetic Model

Unified minimum effective model of magnetic properties of iron-based superconductors

Jiangping Hu,[1,2,*] Bao Xu,[1] Wuming Liu,[1] Ning-Ning Hao,[1] and Yupeng Wang[1]

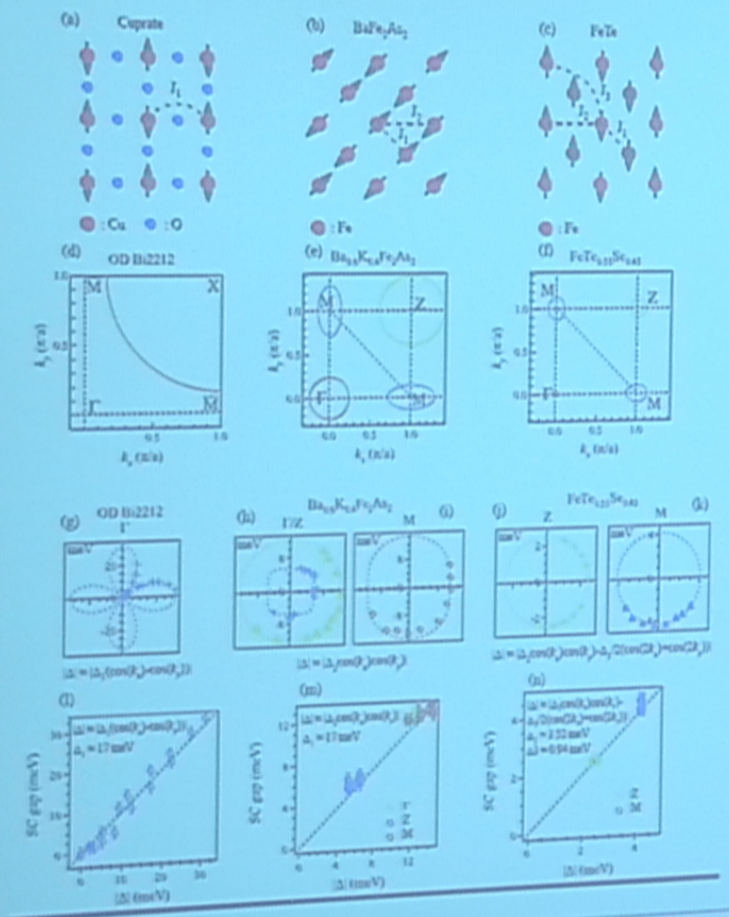
PHYSICAL REVIEW B 85, 144403 (2012)

$$H = \sum_{ij,n} \left[J_{ij} \vec{S}_i^n \cdot \vec{S}_j^n - K_{ij} (\vec{S}_i^n \cdot \vec{S}_j^n)^2 \right] + J_c \sum_{i,n} \vec{S}_i^n \cdot \vec{S}_i^{n+1}$$

TABLE I. The values of the magnetic exchange interactions in $J_1 - J_2 - J_3 - K$ model obtained from the experimental results of different parent compounds of iron-based superconductors.[10–12,16]

Material	Phases	(Q_x, Q_y)	J_1S	J_2S	J_3S	KS^2	J_cS
$CaFe_2As_2$	CAF	$(0,1)\pi$	22	19	...	14	5
$BaFe_2As_2$	CAF	$(0,1)\pi$	25	14	...	17	2
FeTe	BCAF	$(\frac{1}{2},\frac{1}{2})\pi$	−34	18.5	9.5	9	...
$K_{0.8}Fe_{1.6}Se_2$	BAF_v	$(\frac{1}{5},\frac{1}{5})\pi$	−10	16	9	12	1.4

- From iron-pnictides: AFM J1>0;For Iron-chalcogendies: FM J1<0
- J_1 is not universal, but J2 is universal
- J_3 is significant and AFM in Iron chalcogendies
- K term is significant in NN bonds



- Curpates:

  J_1

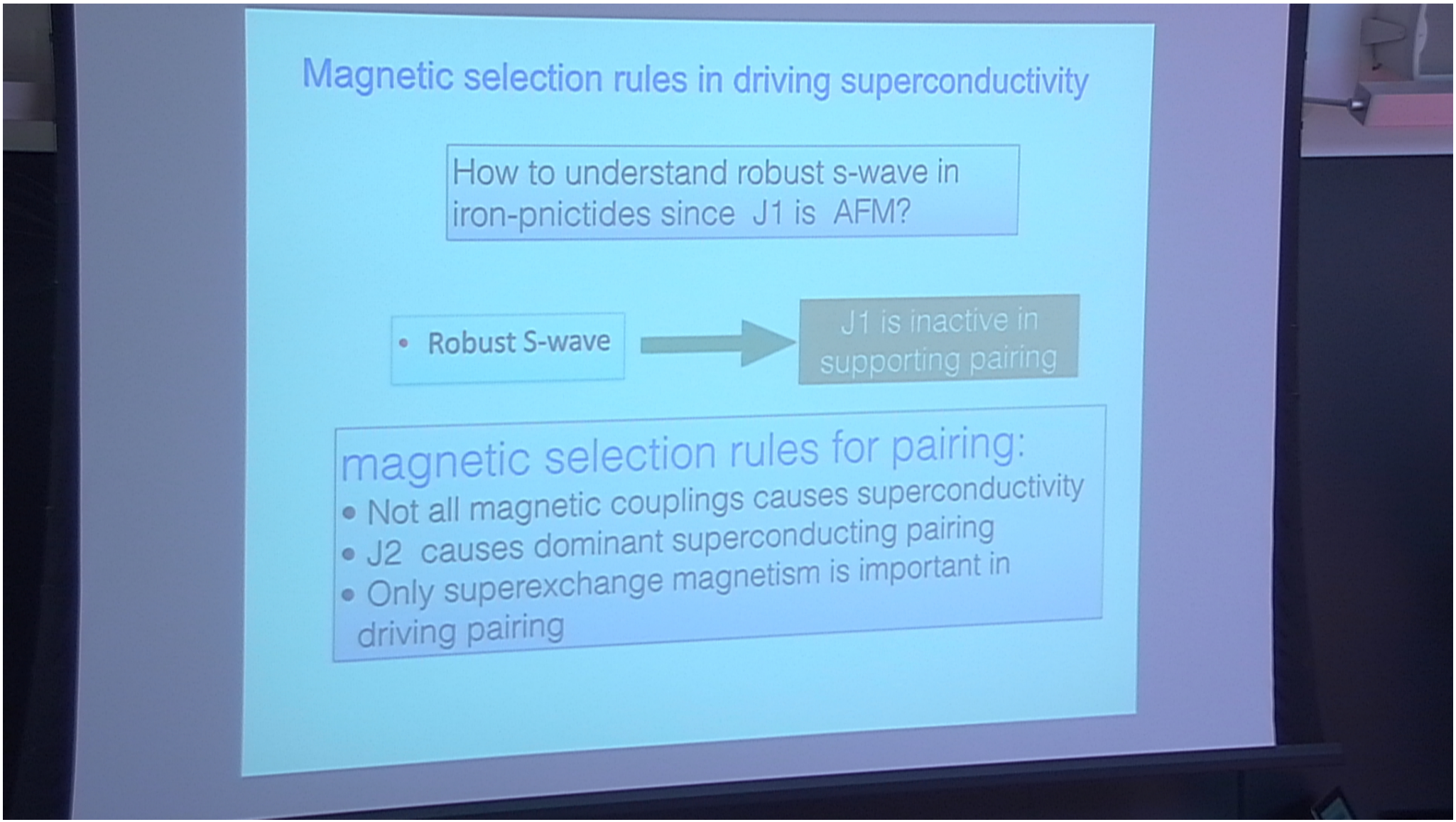
- Ferropnictides

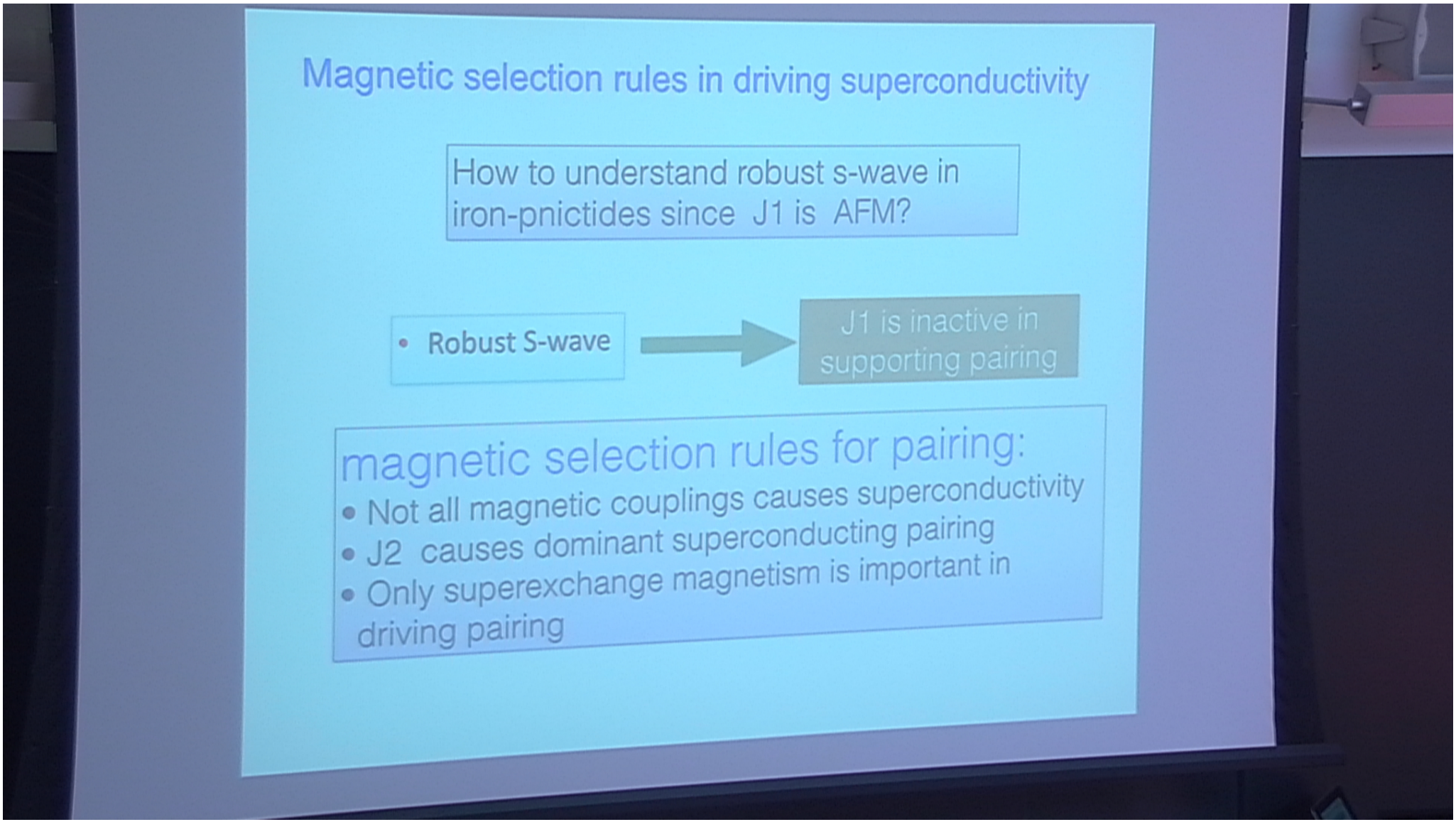
  J_1 , J_2

- Ferrochalcogenites

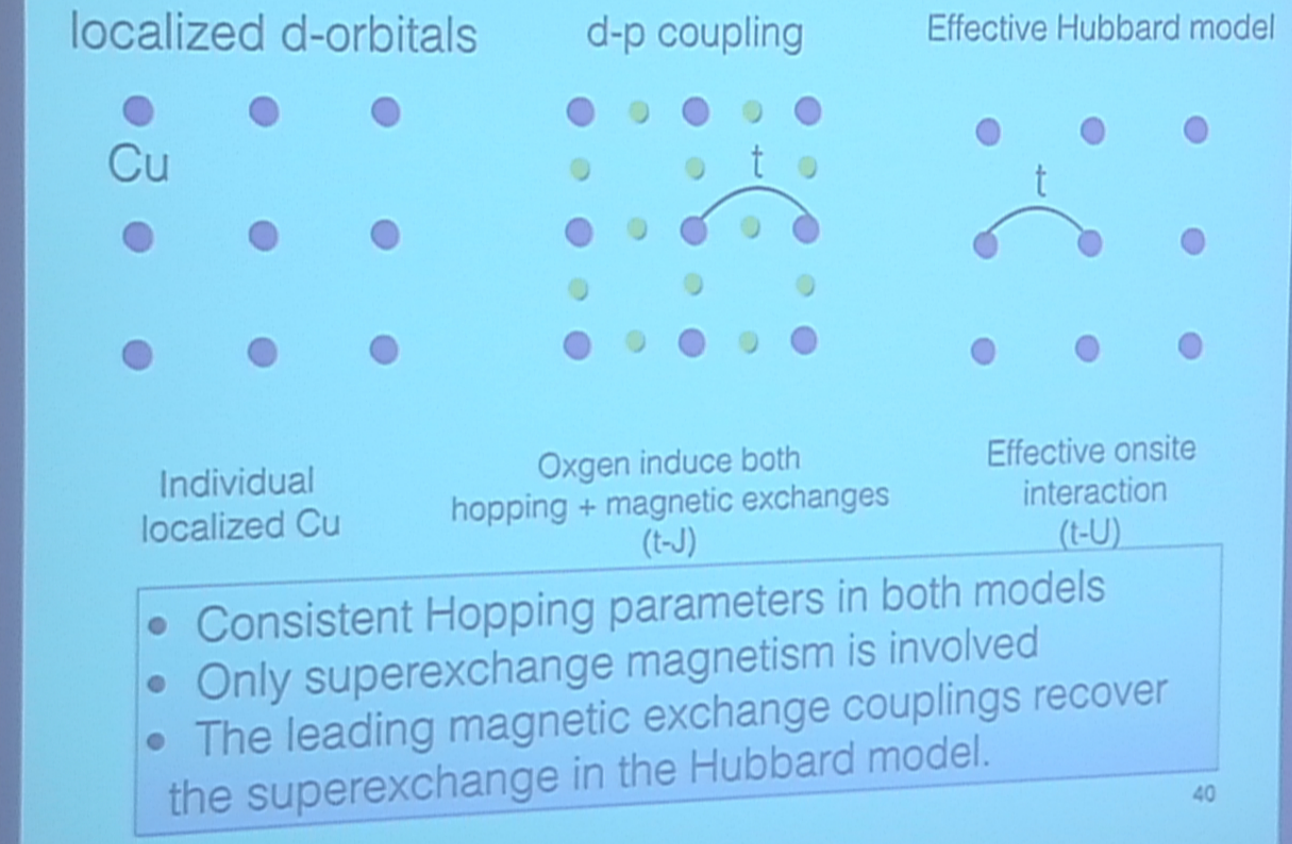
  J_2 , J_3

J.P. Hu and H. Ding, Scientific Reports 2, 38, 2012


Magnetic selection rules in driving superconductivity
How to understand robust s-wave in iron-pnictides since J1 is AFM?
• Robust S-wave
J1 is inactive in supporting pairing
magnetic selection rules for pairing:
• Not all magnetic couplings causes superconductivity
• J2 causes dominant superconducting pairing
• Only superexchange magnetism is important in driving pairing


Magnetic selection rules in driving superconductivity
How to understand robust s-wave in iron-pnictides since J1 is AFM?
• Robust S-wave
J1 is inactive in supporting pairing
magnetic selection rules for pairing:
• Not all magnetic couplings causes superconductivity
• J2 causes dominant superconducting pairing
• Only superexchange magnetism is important in driving pairing

Consistency in predicting d-wave pairing symmetry in cuprates

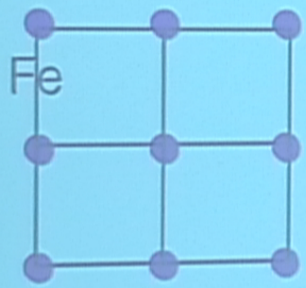


- Consistent Hopping parameters in both models
- Only superexchange magnetism is involved
- The leading magnetic exchange couplings recover the superexchange in the Hubbard model.

40

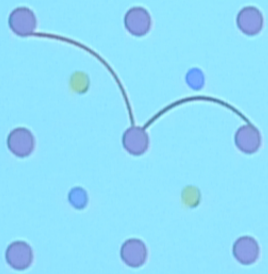
Difference in iron-based superconductors

nonlocalized d-orbitals



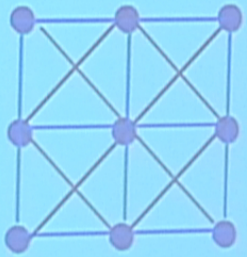
Metallic Fe states

d-p coupling



As(Se) induce additional hopping + magnetic exchanges

Effective Hubbard-type model



Effective onsite interaction

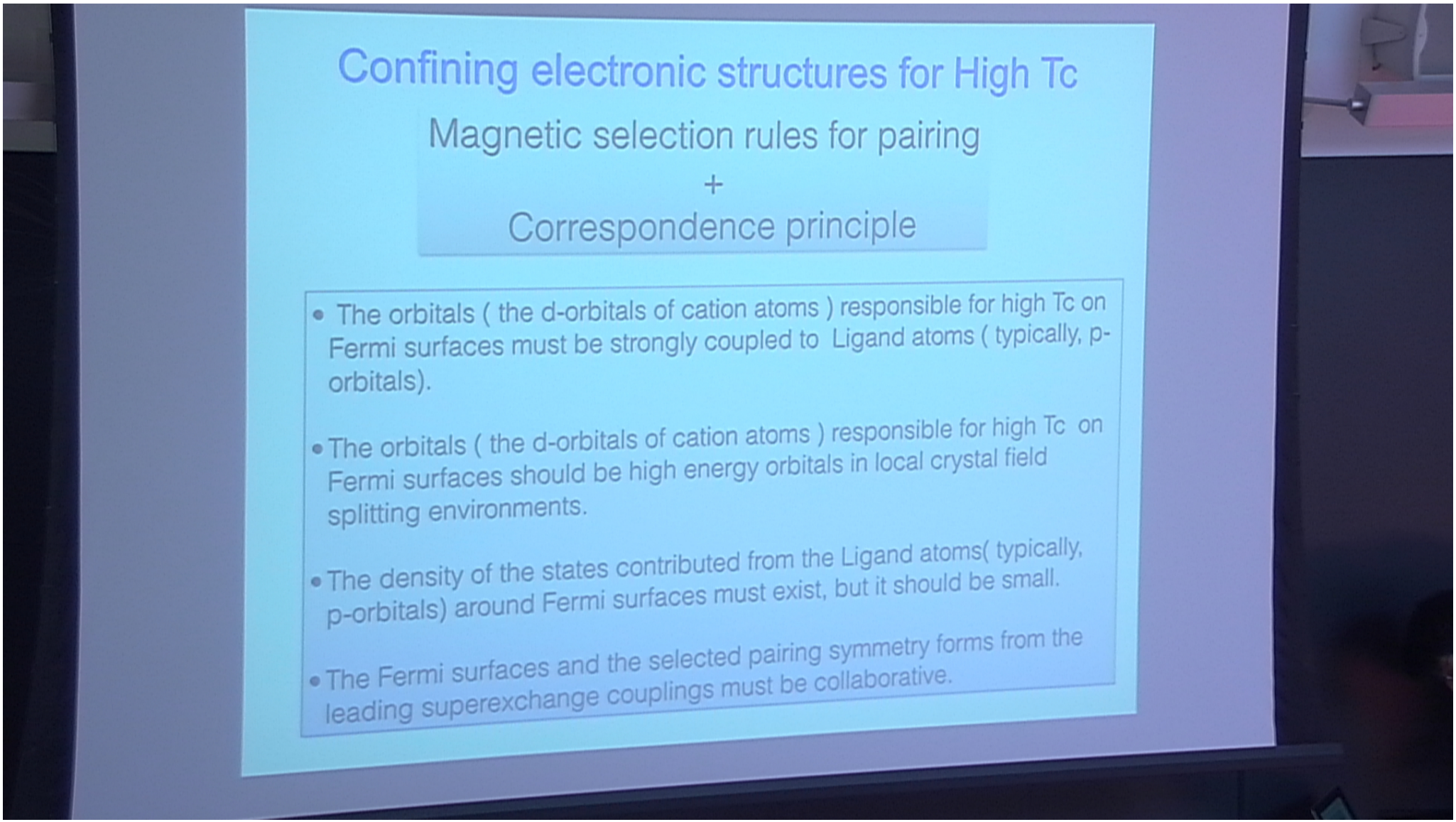
- Large hopping already exists between two NN Fe sites
- Direct exchange mechanism is strongly involved in NN magnetic exchange coupling.
- Effective model (t-U) treats all magnetism equally and does not distinguish the true superexchange couplings from other processes.
- Only J2 from NNN sites are truly superexchange-dominated

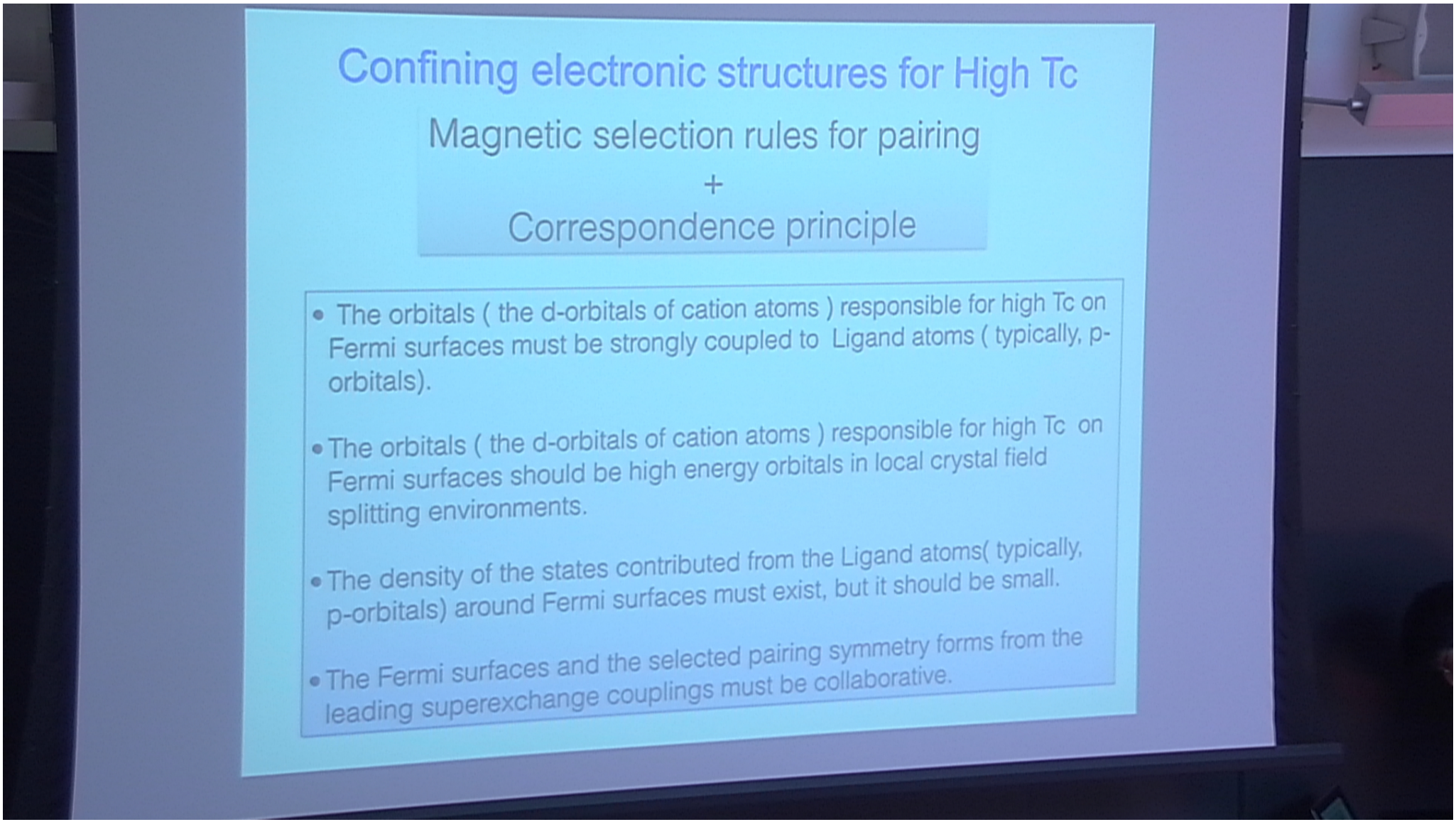
Thoughts for Fixing the effective model

S-wave stablizer?

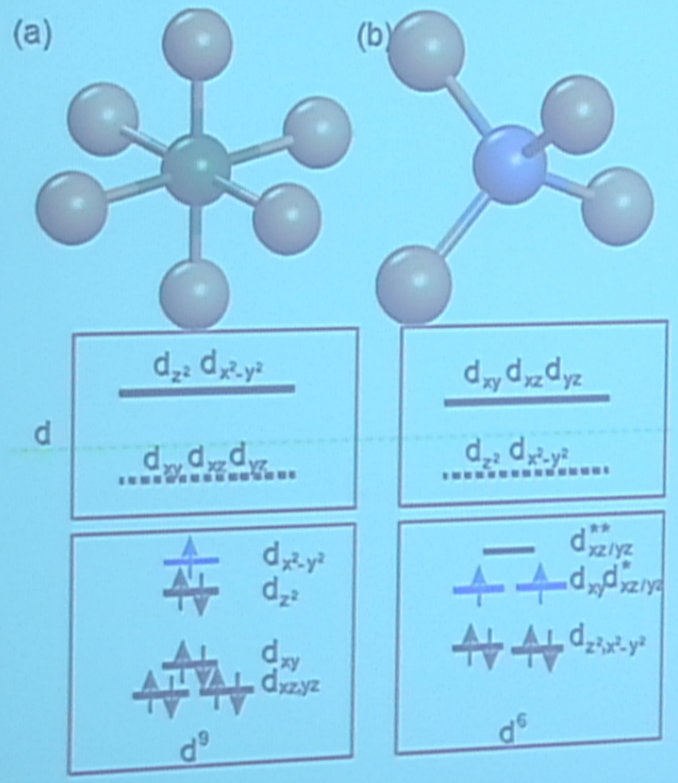
$$\hat{H}_U = \hat{H}_0 + \hat{H}_I,$$
$$\hat{H}_I = \sum_i [\sum_{a \neq b} (J_H \hat{S}_{ai} \cdot \hat{S}_{bi} + U' \hat{n}_{ai\uparrow} n_{bi\downarrow}) + U \hat{n}_{ai\uparrow} n_{ai\downarrow}]$$

- Additional terms to suppress the NN Pairing. V term?
- Derive magnetism from d-p?
- Effective model defined in iron-sublattice (one step of real space RG)
- Separate superexchange mechanisms from direct exchange


Confining electronic structures for High Tc
Magnetic selection rules for pairing
+
Correspondence principle
• The orbitals (the d-orbitals of cation atoms) responsible for high Tc on Fermi surfaces must be strongly coupled to Ligand atoms (typically, p-orbitals).
• The orbitals (the d-orbitals of cation atoms) responsible for high Tc on Fermi surfaces should be high energy orbitals in local crystal field splitting environments.
• The density of the states contributed from the Ligand atoms(typically, p-orbitals) around Fermi surfaces must exist, but it should be small.
• The Fermi surfaces and the selected pairing symmetry forms from the leading superexchange couplings must be collaborative.


Confining electronic structures for High Tc
Magnetic selection rules for pairing
+
Correspondence principle
• The orbitals (the d-orbitals of cation atoms) responsible for high Tc on Fermi surfaces must be strongly coupled to Ligand atoms (typically, p-orbitals).
• The orbitals (the d-orbitals of cation atoms) responsible for high Tc on Fermi surfaces should be high energy orbitals in local crystal field splitting environments.
• The density of the states contributed from the Ligand atoms(typically, p-orbitals) around Fermi surfaces must exist, but it should be small.
• The Fermi surfaces and the selected pairing symmetry forms from the leading superexchange couplings must be collaborative.

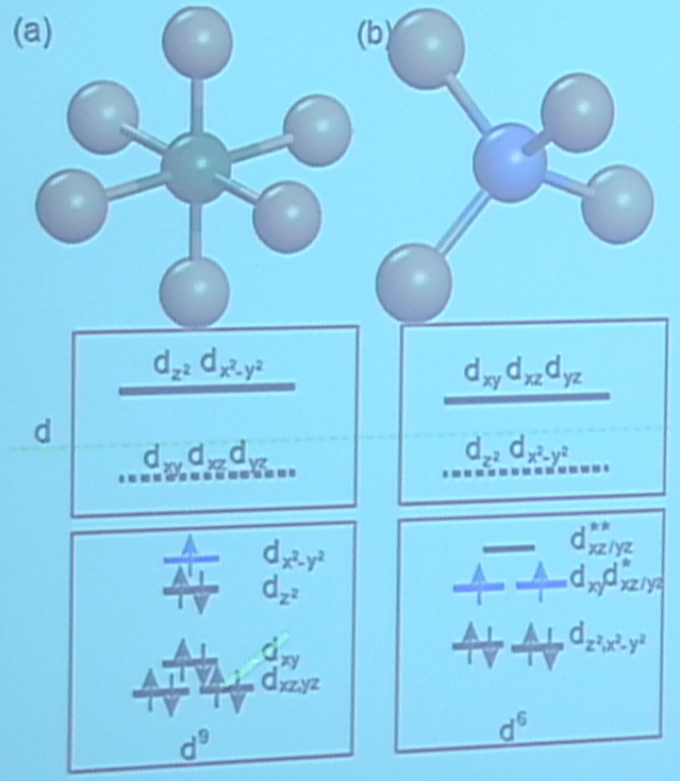
Cuprates vs iron-based superconductors



- Octahedral: d9 is unique to achieve high Tc
- Tetrahedral: d6 is unique to achieve high tc
- ?

46

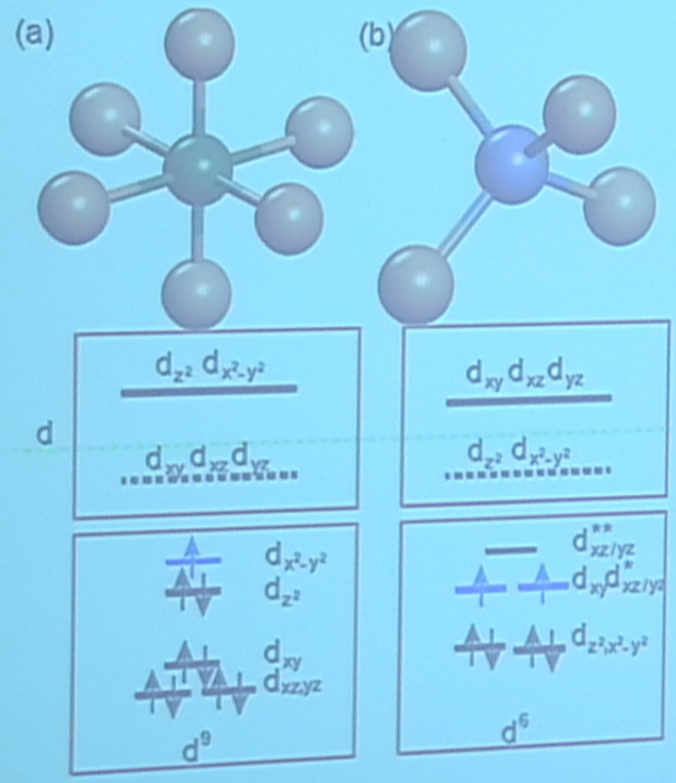
Cuprates vs iron-based superconductors



- Octahedral: d9 is unique to achieve high Tc
- Tetrahedral: d6 is unique to achieve high tc
- ?

46

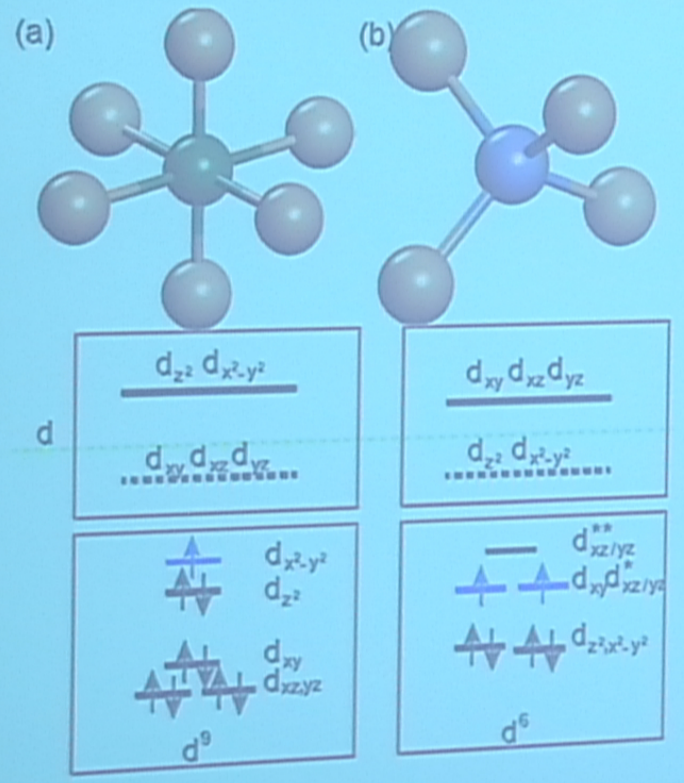
Cuprates vs iron-based superconductors



- Octahedral: d9 is unique to achieve high Tc
- Tetrahedral: d6 is unique to achieve high tc
- ?

46

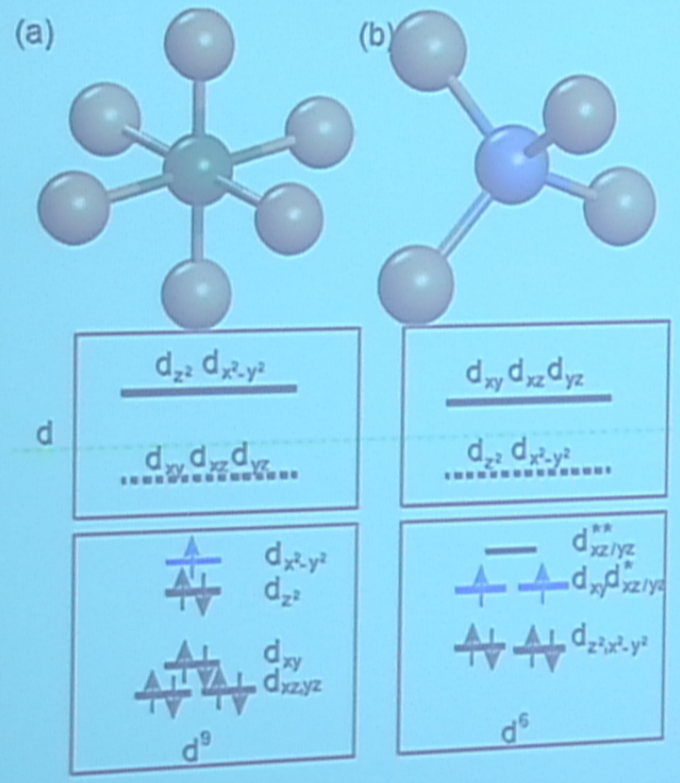
Cuprates vs iron-based superconductors



- Octahedral: d9 is unique to achieve high Tc
- Tetrahedral: d6 is unique to achieve high tc
- ?

46

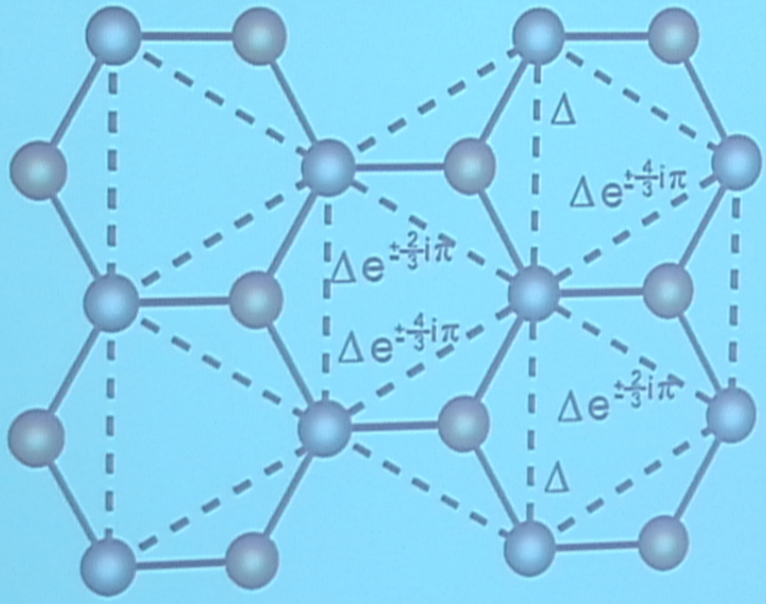
Cuprates vs iron-based superconductors



- Octahedral: d9 is unique to achieve high Tc
- Tetrahedral: d6 is unique to achieve high tc
- ?

46

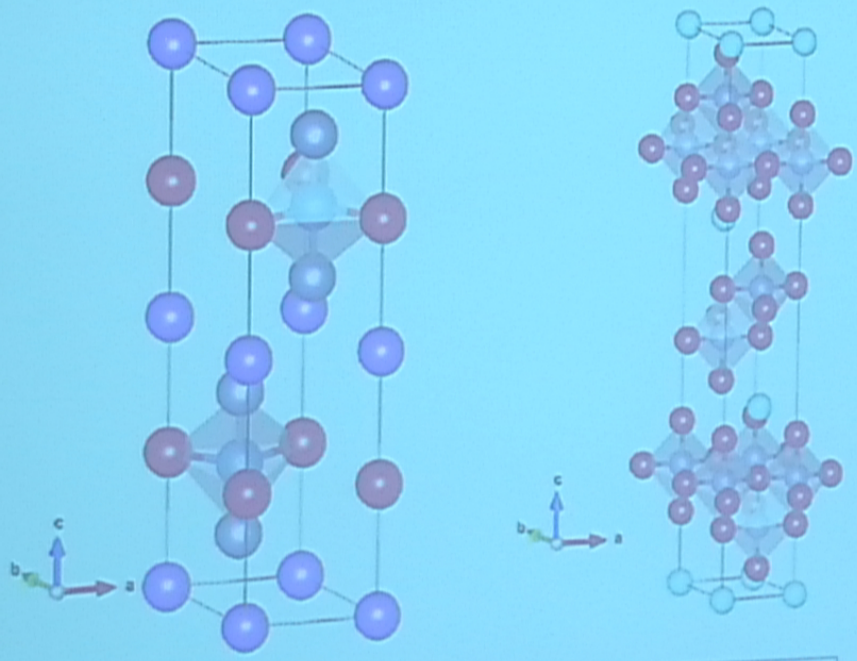
Triangle lattice by corner shared Triangular Bipyramidal



- Two Dimensional Triangle lattice

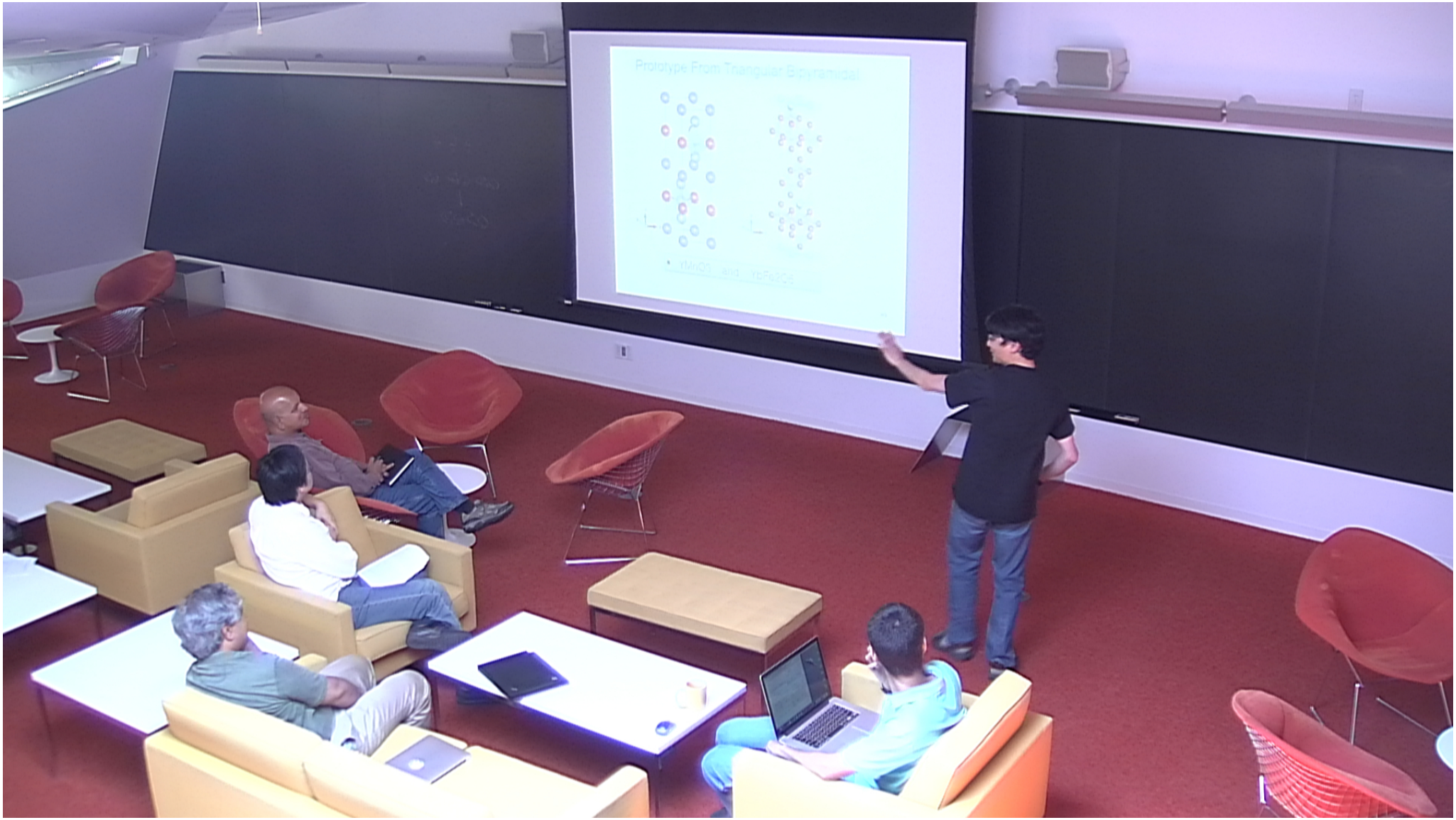
48

Prototype From Triangular Bipyramidal



- $YMnO_3$ and $YbFe_2O_5$

49


Prototype From Triangular Bipyramidal

Band Structure for YNiO3

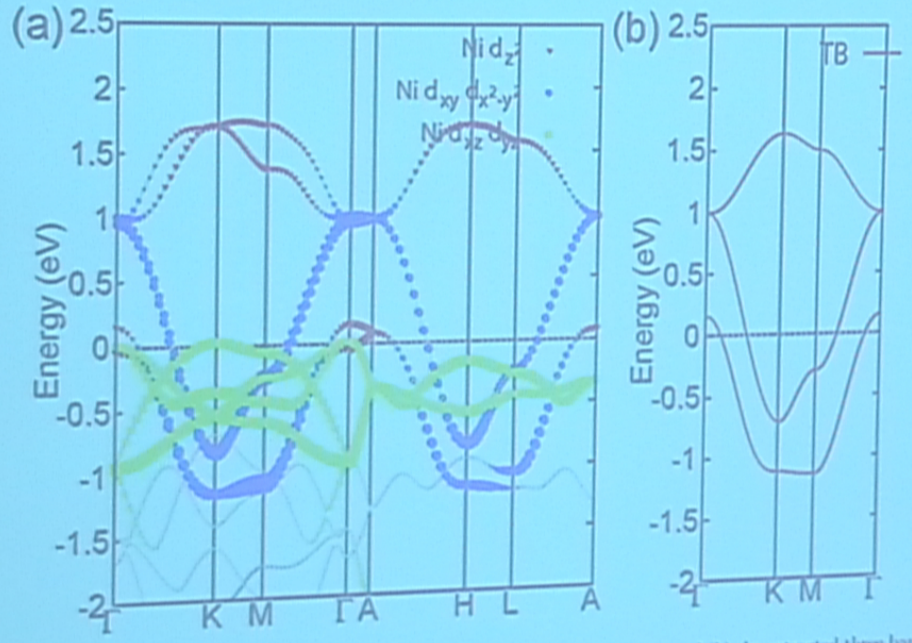
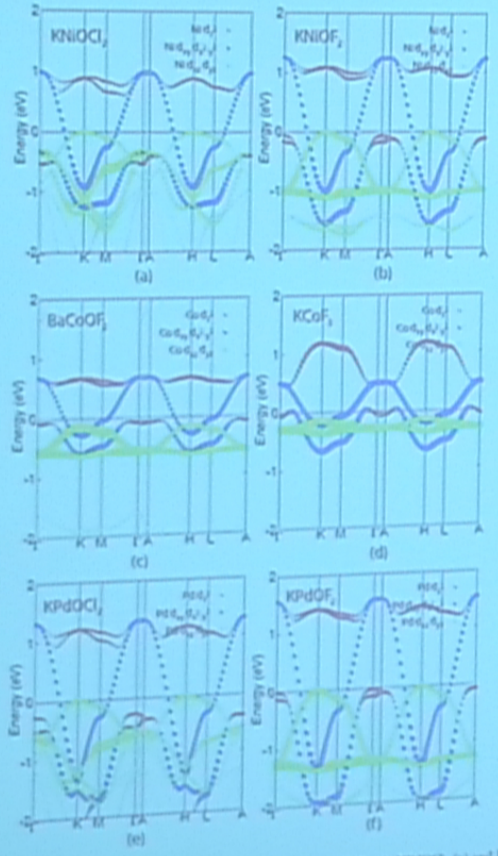


FIG. 3: (a) The band structures of $YNiO_3$ obtained from the first principle calculations and (b) the extracted three bands for the tight binding model. The orbital characters of the bands in (a) are indicated by the different colors specified in the right top corner of the figure.

51

Possible alternatives

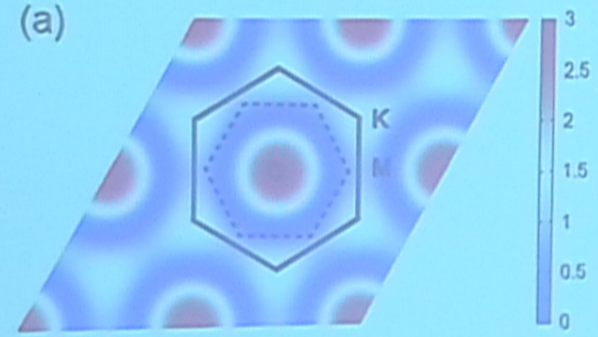


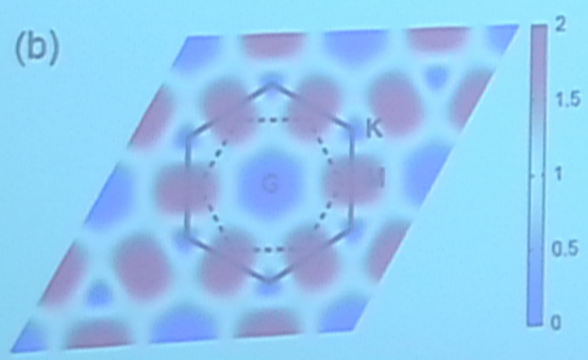
- The targeted band is robust
- There are many series of materials: Co2+, Ni3+, (Palladium)Pd3+ (Rhodium)Rh2+

53

FIG. 8. The band structures of $KNiOCl_3$ (a), $KNiOF_3$ (b), $BaCoOF_3$ (c), $KCoF_3$ (d) $KPdOCl_3$ (e) and $KPdOF_3$ (f).

Pairing Symmetry and Tc





- S-wave has little weight
- d+id has very large weight
- Energy Scale:

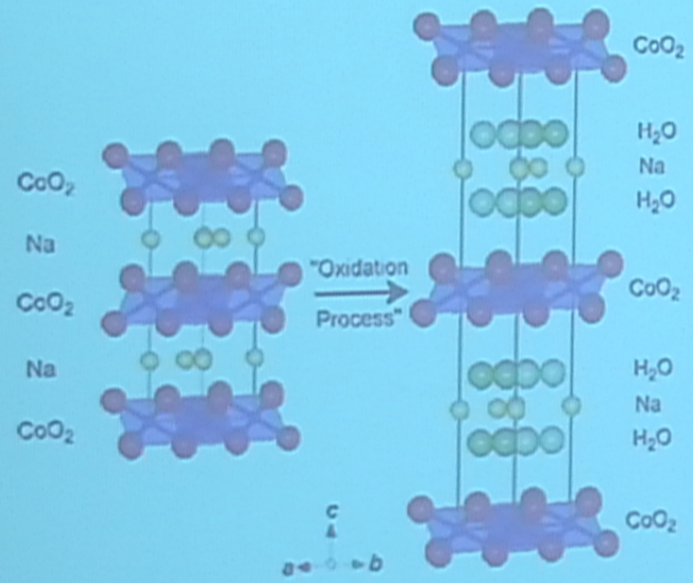
Cuprates

Ni/Co-based

iron-based

54

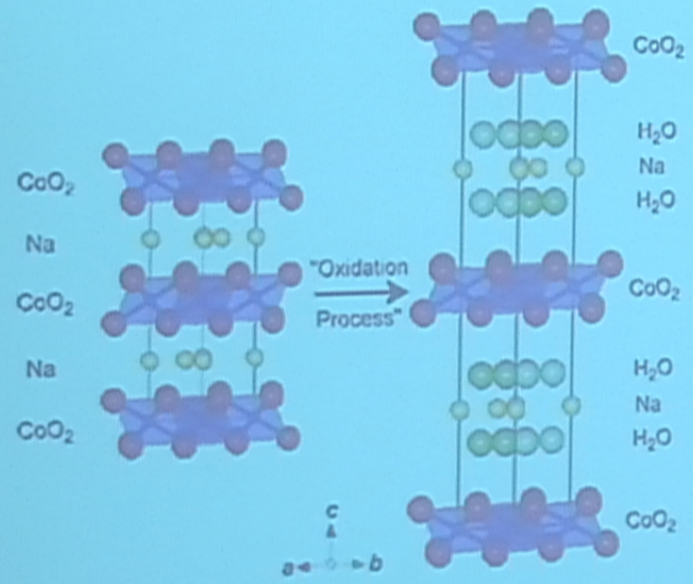
Comparison to NaCoO2



- Co3+ in Octahedral complex
- short lattice constants (co-co direct exchange)

56

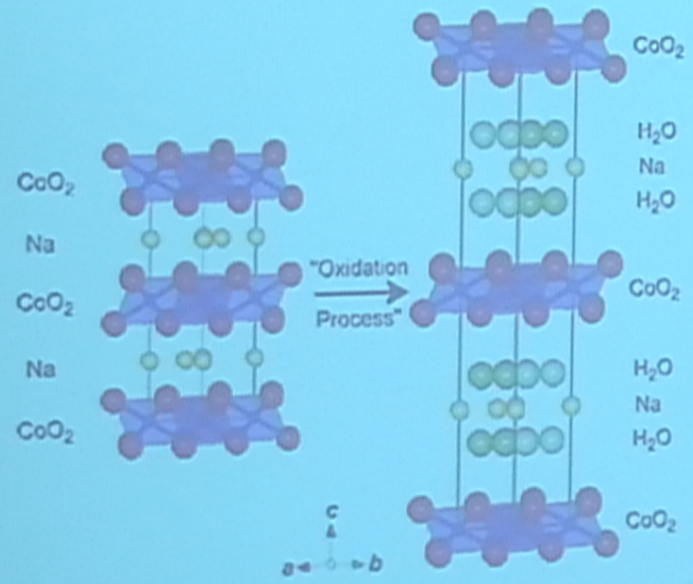
Comparison to NaCoO2



- Co3+ in Octahedral complex
- short lattice constants (co-co direct exchange)

56

Comparison to NaCoO2



- Co3+ in Octahedral complex
- short lattice constants (co-co direct exchange)

56