Searching for next unconventional high temperature superconductors

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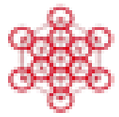
3/28/2017

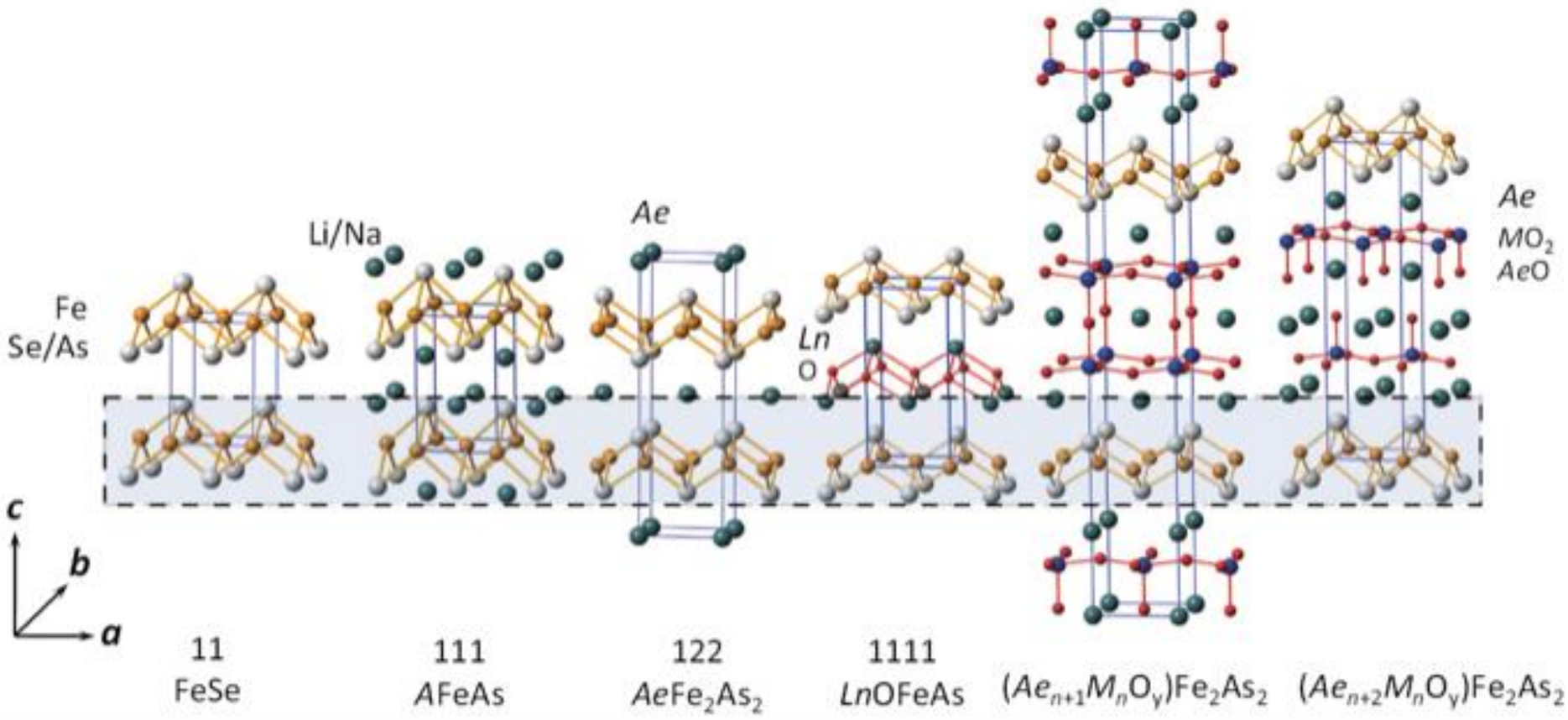


Kavli Institute for Theoretical Sciences
University of Chinese Academy of Sciences (UCAS)

Welcome to KITS!

Major Progress in the Past Ten Years:

The discovery of iron-based superconductors



The second family of unconventional high Tc superconductors

Why did the entire high Tc research community fail to provide any clue about iron-based superconductors?

Motivation:
Why does iron high Tcs bring new hope?

- Induction Vs deduction

- No induction for unconventional high Tc before iron -based superconductors

- Deduction method based on models becomes standard after cuprates

Iron-based superconductors provide the first class of materials for inductive reasoning!

Motivation

21	22	23	24	25	26	27	28	29	30
Sc	**Ti**	**V**	**Cr**	**Mn**	**Fe**	**Co**	**Ni**	**Cu**	**Zn**
44.9559	47.867	50.9415	51.9961	54.938	55.845	58.9332	58.6934	63.546	65.4089
Scandium	Titanium	Vanadium	Chromium	Manganese	Iron	Cobalt	Nickel	Copper	Zinc
39	40	41	42	43	44	45	46	47	48
Y	**Zr**	**Nb**	**Mo**	**Tc**	**Ru**	**Rh**	**Pd**	**Ag**	**Cd**
88.9058	91.224	92.9064	85.94	98	101.07	102.9055	106.42	107.8682	112.411
Yitrium	Zirconium	Niobium	Molybdenum	Technetium	Ruthenium	Rbodium	Palladium	Silver	Cadmium
71	72	73	74	75	76	77	78	79	80
Lu	**Hf**	**Ta**	**W**	**Re**	**Os**	**Ir**	**Pt**	**Au**	**Hg**
174.967	178.49	180.9497	183.84	186.207	190.23	192.217	195.084	196.9666	200.59
Lutetium	Hafnium	Tantalum	Tungsten	Rhenium	Osmium	Iridium	Platinum	Gold	Mercury

Are Fe and Cu special ?
Is there a single trait to separate them from other materials? If yes, what is it?

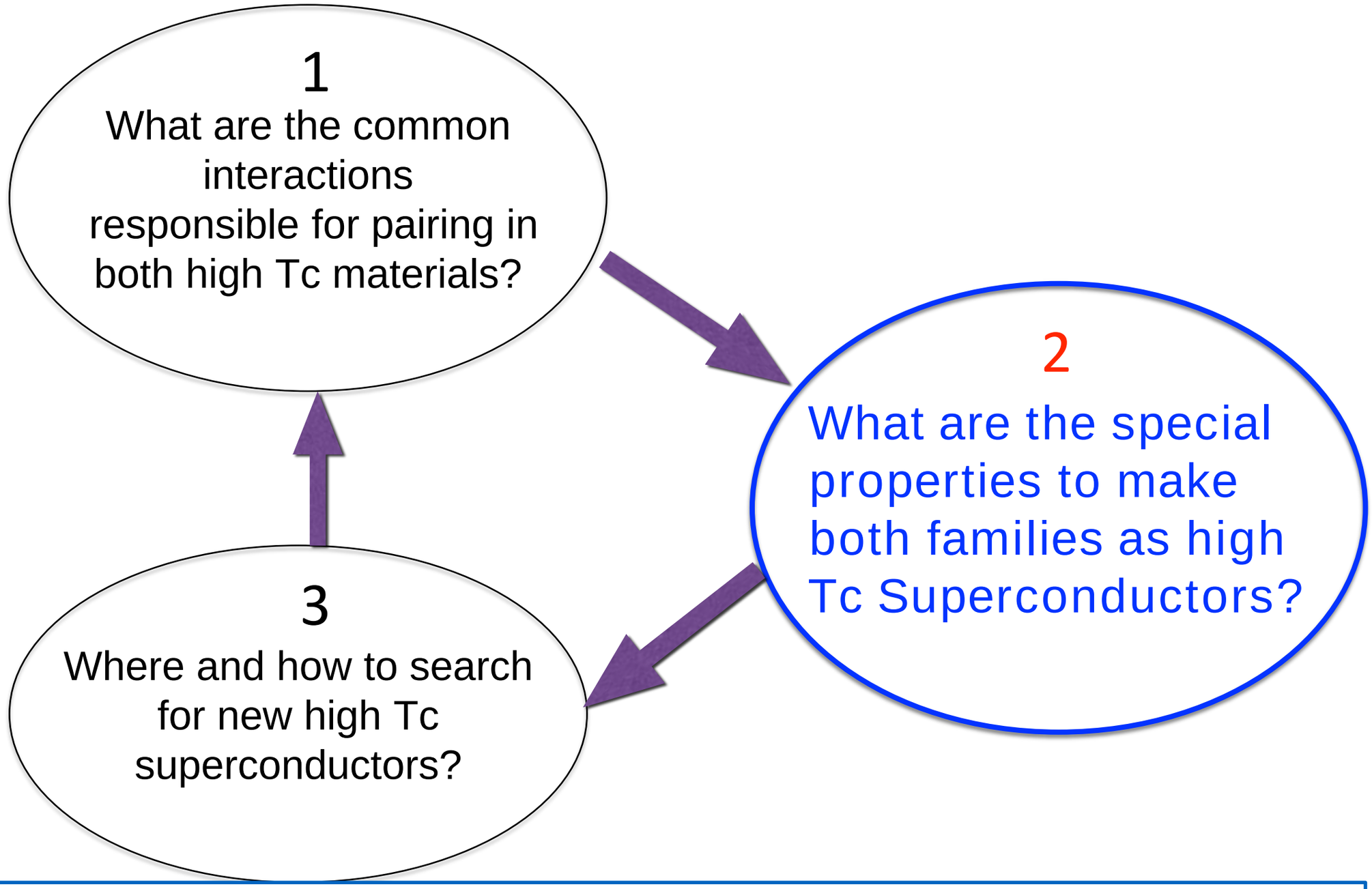
Motivation

- 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!

The genes for high Tc!!

Self-contained Questions



Chance to settle unconventional high Tc mechanism:

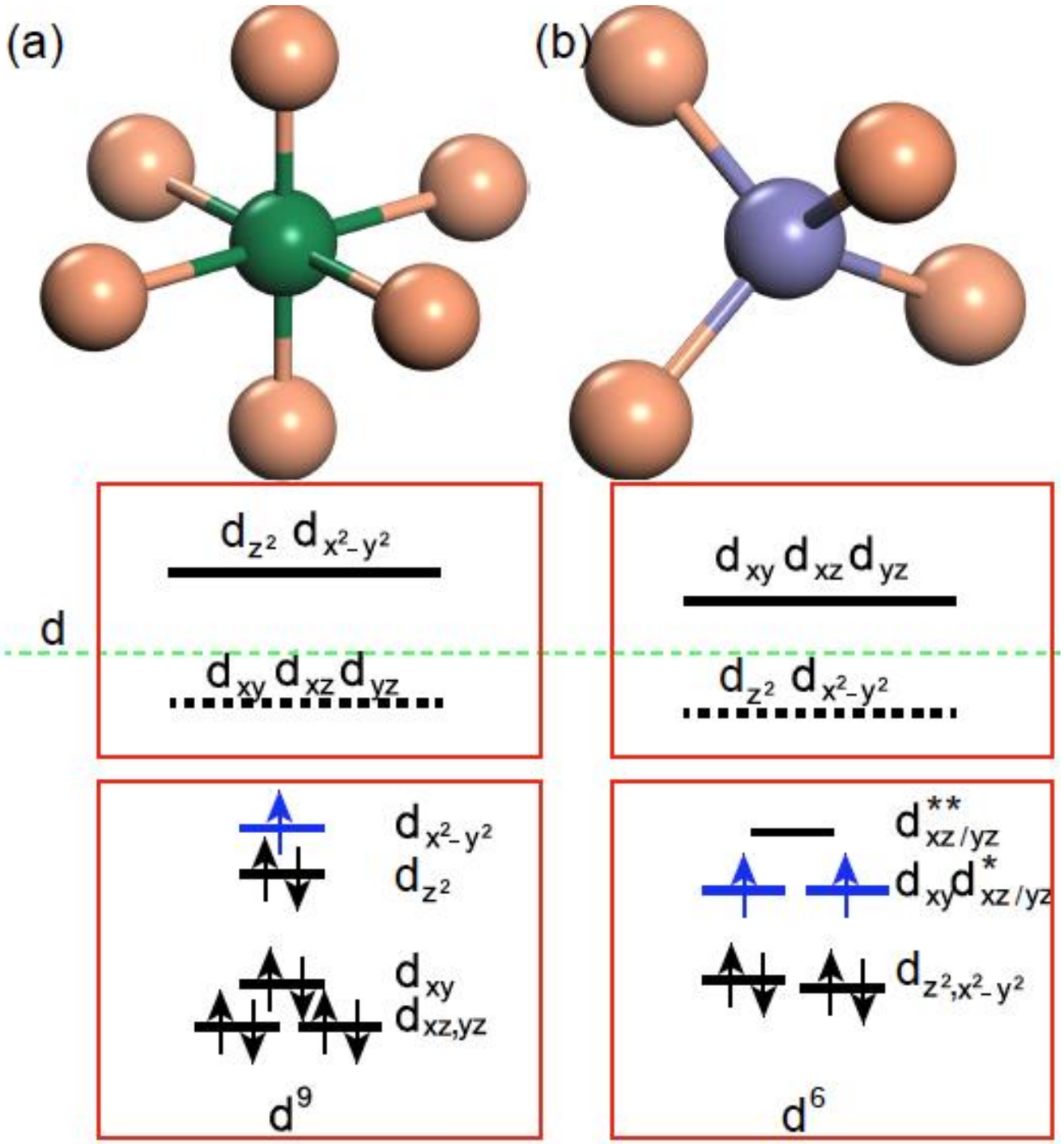
Theoretically predict it before the third family of high Tc superconductors is discovered!!!

Genes for high Tc

Those d-orbitals with the strongest coupling to the in-plane anion p orbitals are isolated near Fermi energy.

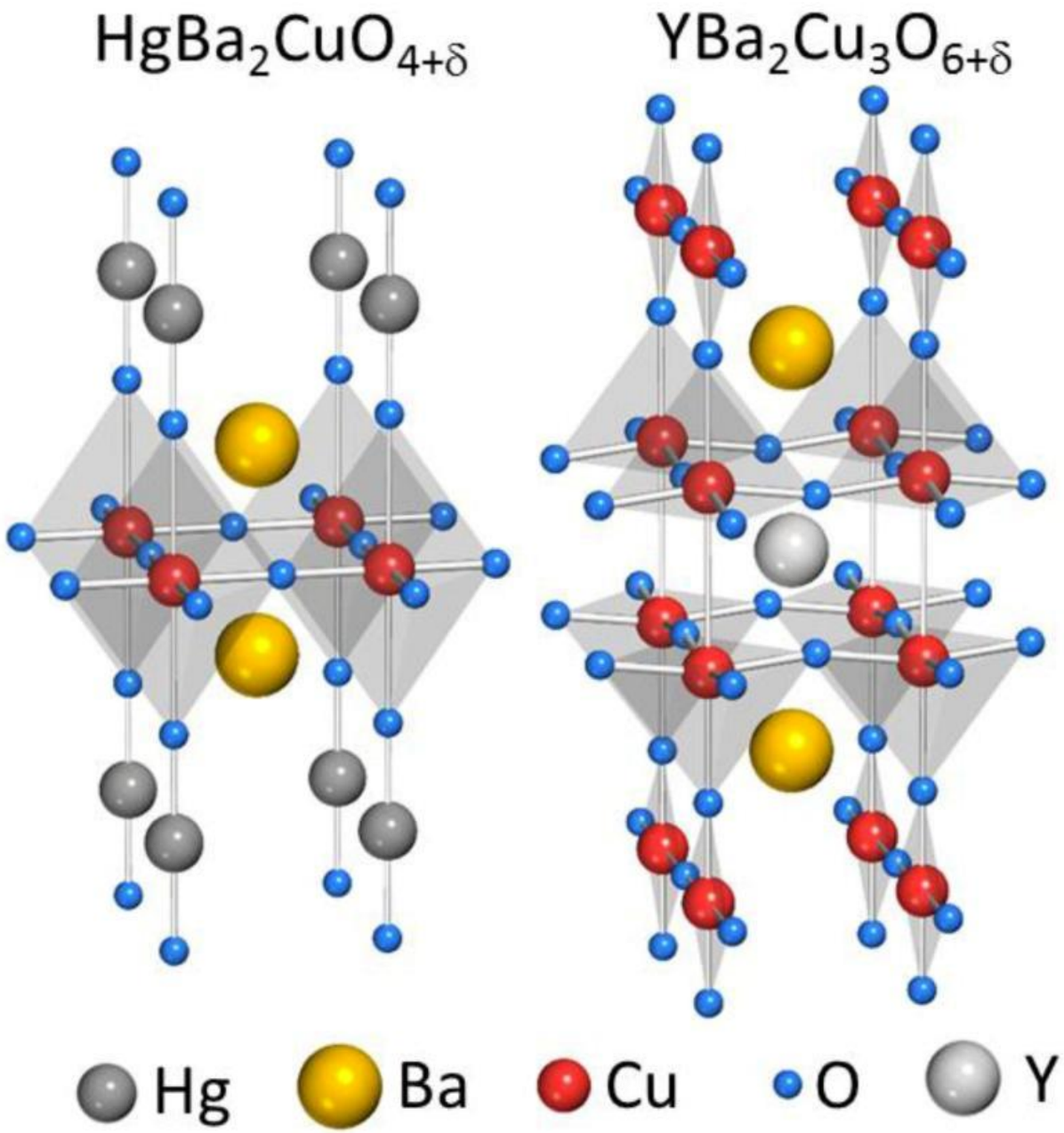
- An electronic environment to allow the AFM superexchange to provide pairing.

Cuprates vs iron-based superconductors



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

Octahedron, Perovskite structure and Cuprates



- Single d-orbital: d_{x2-y2}
- The d_{x2-y2} orbital has the highest energy in the d shell
- Jahn-Teller distortion (c>a=b) lows d_z^2
- d^9 is unique to achieve high Tc

Orbital Distillation

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Physics Procedia 45 (2013) 13 – 16

Physics Procedia

ISS2012

Three-orbital study on the orbital distillation effect in the high T_c cuprates

H. Sakakibara[a*], K. Suzuki[b], H. Usui[a], K. Kuroki[a], R. Arita[b,e], D.J. Scalapino[c], H. Aoki[d]

- Tc is drastically reduced with the rising of d_z^2 orbitals to Fermi energy

K_2CuF_4

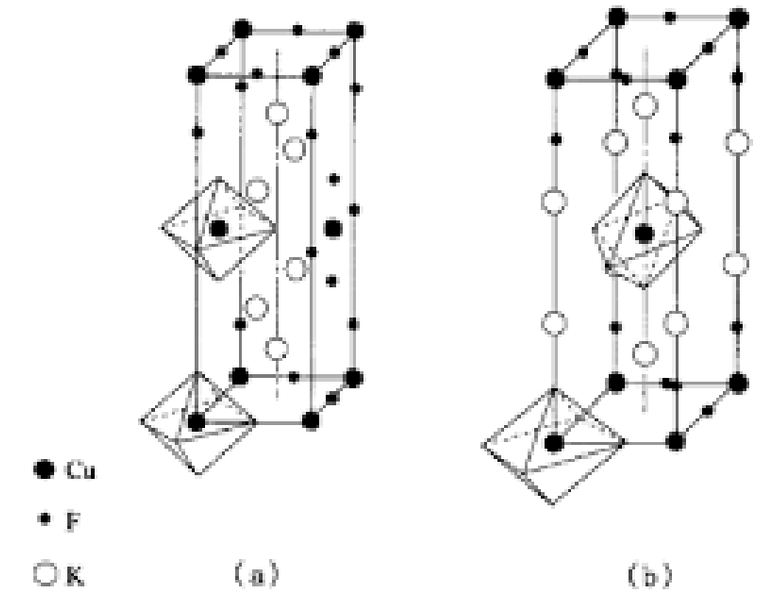
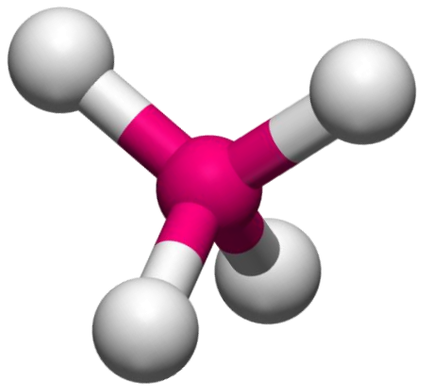
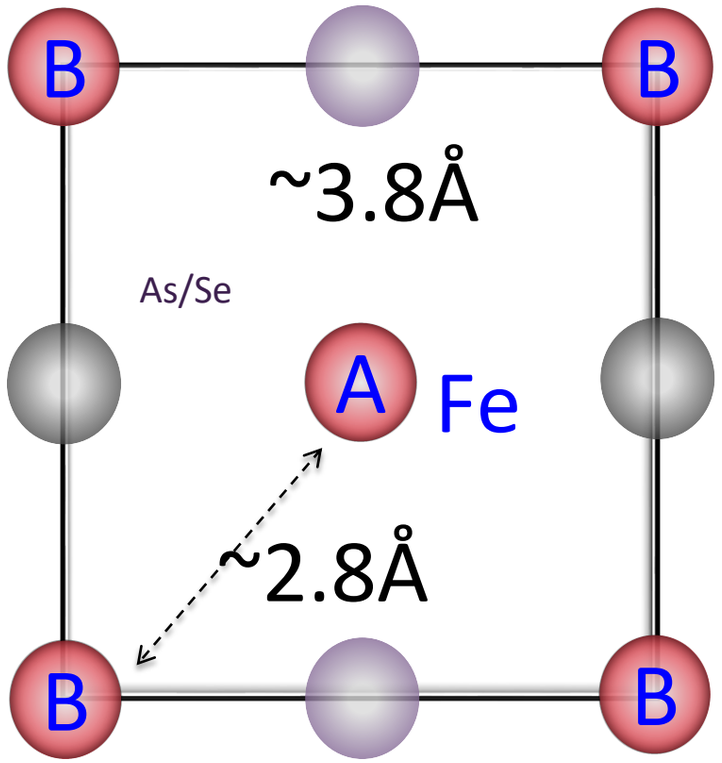


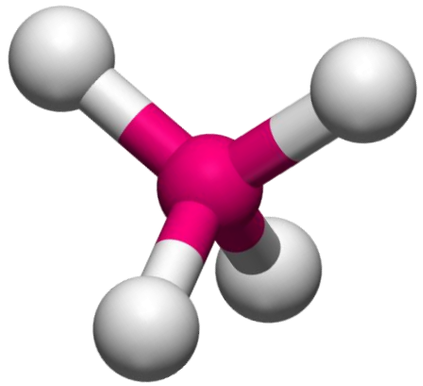
Fig. 2. Schematic structures of two kinds of K_2CuF_4: (a) in the high-pressure phase and (b) at ambient pressure.

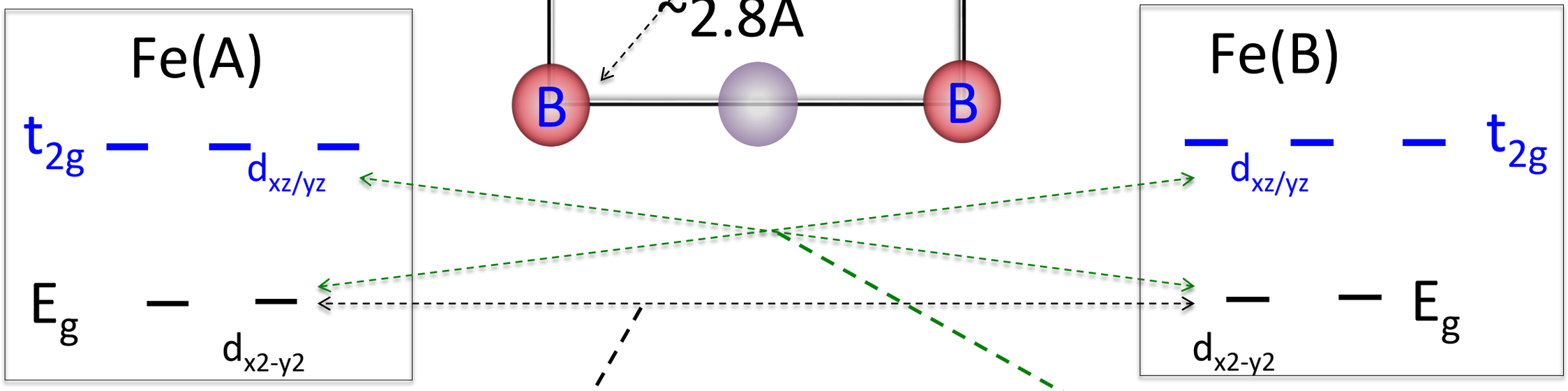
- Jahn-Teller distortion: a>c>b
- Jahn-Teller distortion does not low d_z^2
- The d_{x2-y2} orbital is not isolated.

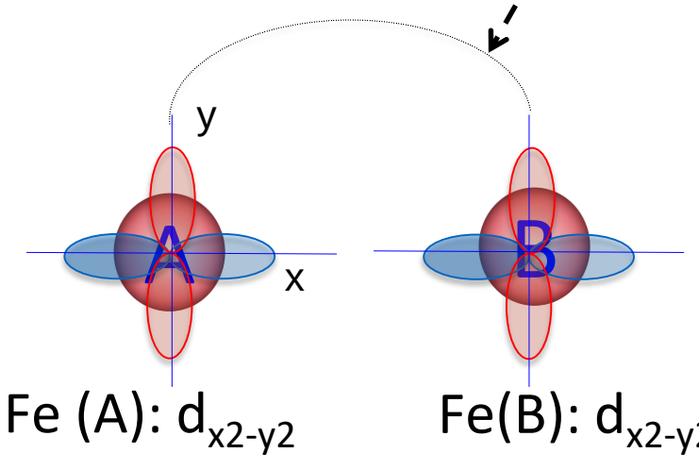
Tetrahedron and iron-based superconductors

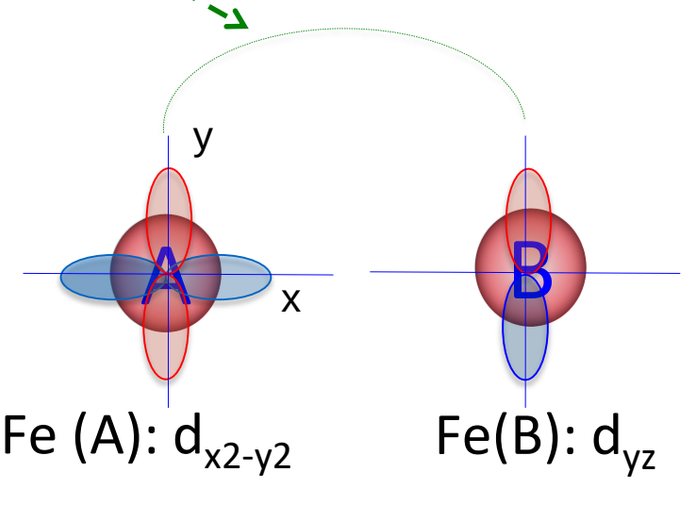












Local electronic structure in iron-based superconductors

- Analyzing local electron environment of Fe needs to include the NN Fe atoms.
- Short distance between two NN Fe
- Direct chemical bonding between two NN Fe
- Large coupling between E_g (d_{x2-y2}) and t_{2g} ($d_{xz/yz}$) orbitals

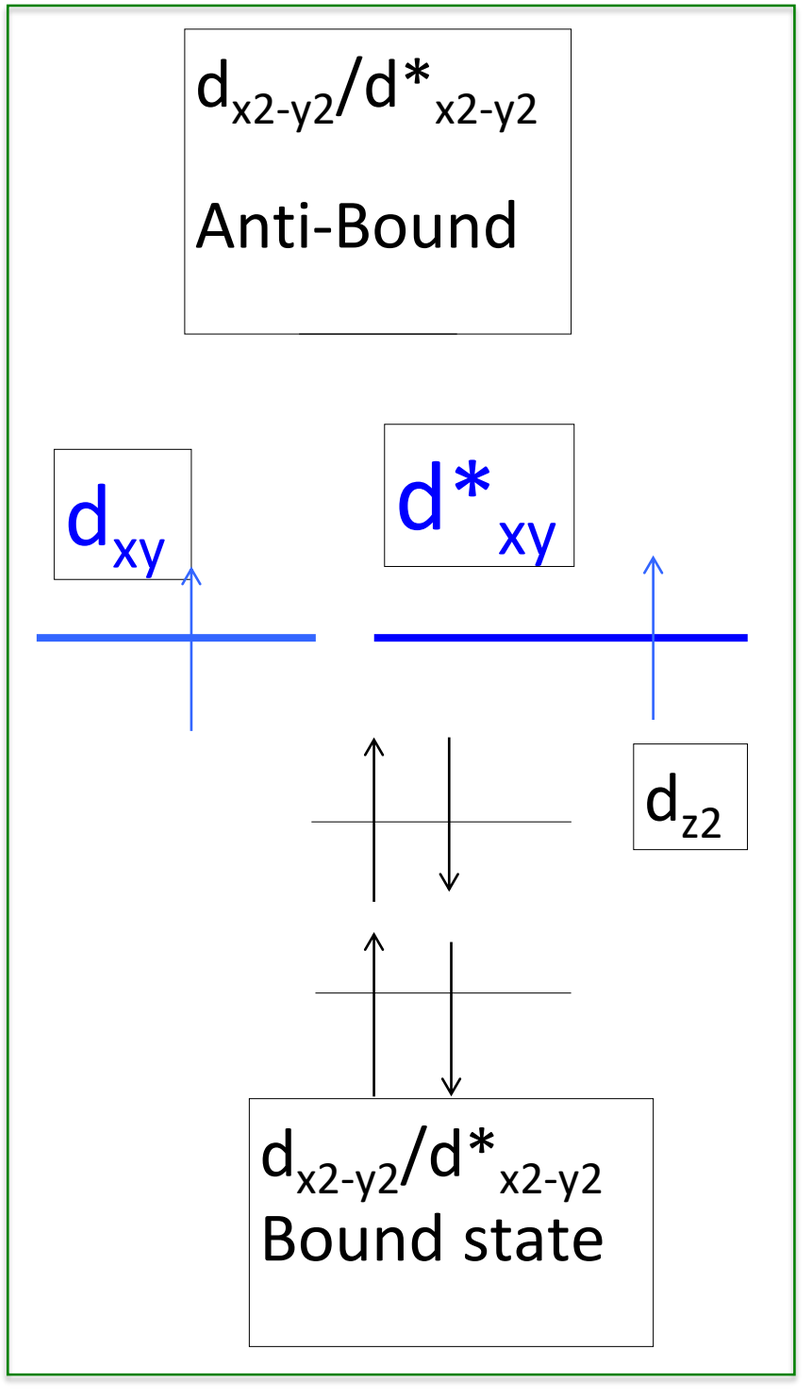
TABLE I. The intraorbital hopping parameters used for the DFT fit of the 5 orbital model.

t_i^{mm}	$i=x$	$i=y$	$i=xx$	$i=xy$	$i=xxy$	$i=xyy$	$i=xxyy$	$i=z$	$i=xz$	$i=xxz$	$i=xyz$
$m=1$	−0.0604	−0.3005	0.0253	0.2388	−0.0414	−0.0237	0.0158		−0.0101	0.0126	
$m=3$	0.3378		0.0011	−0.0947							
$m=4$	0.1965		−0.0528	0.1259	−0.032		0.0045	0.1001	0.0662		0.0421
$m=5$	−0.0656		0.0001		0.01		0.0047	0.0563	−0.0036		

TABLE II. The interorbital hopping parameters used for the DFT fit of the 5 orbital model.

t_i^{mn}	$i=x$	$i=xy$	$i=xxy$	$i=xxyy$	$i=z$	$i=xz$	$i=xyz$	$i=xxyz$
$mn=12$		0.1934	−0.0325	0.0158			−0.0168	
$mn=13$	−0.4224	0.0589	0.0005					
$mn=14$	0.1549	−0.007	−0.0055			0.0524	0.0349	0.0018
$mn=15$	−0.0526	−0.0862					−0.0203	
$mn=24$						0.0566		0.0283
$mn=34$			−0.0108					
$mn=35$	−0.2845		0.0046					
$mn=45$		−0.0475		0.0004	−0.019	−0.0023		

Understanding electronic structure of iron-based superconductors



Local levels at Fe

- **Fe^{2+} is special!**
- Two pure d_{xy}-type orbitals are isolated near Fermi Energy!
- Two d_{xy} orbital models can capture electronic structures near Fermi Energy.

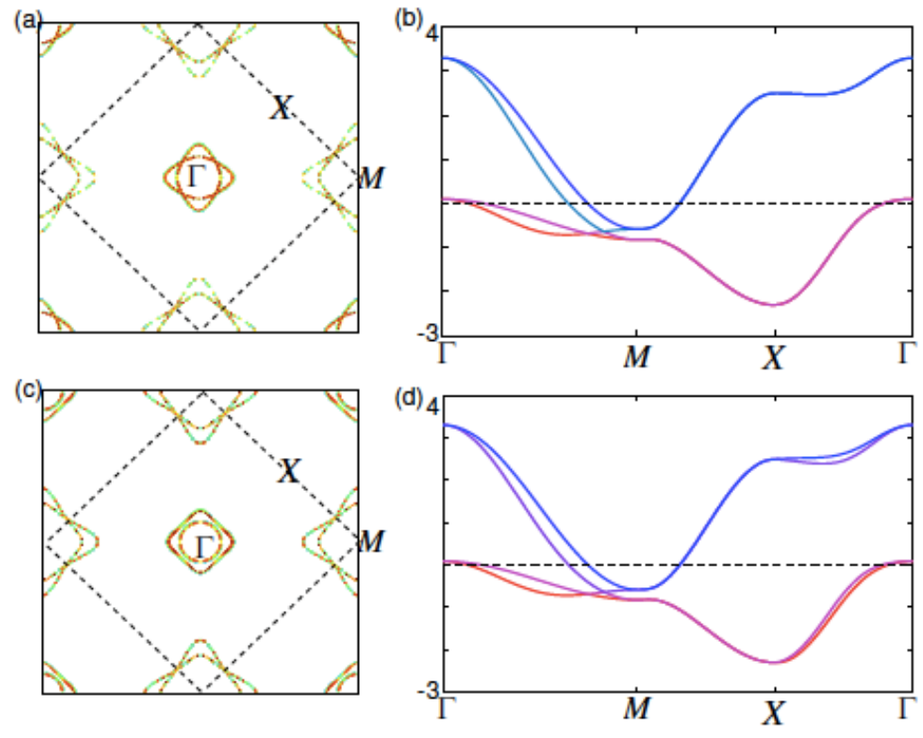


FIG. 1. A typical Fermi surfaces (a), band dispersions (b) resulted from Eq.7 with parameters $t_{1s} = 0.4, t_{1d} = -0.03, t_{2s} = 0.3, t_{2d} = 0.6, t_{3s} = 0.05, t_{3d} = -0.05$ and $\mu = -0.3$. (c) and (d) are corresponding results by adding $t_r = 0.02$ in Eq.17 with the same parameter setting.

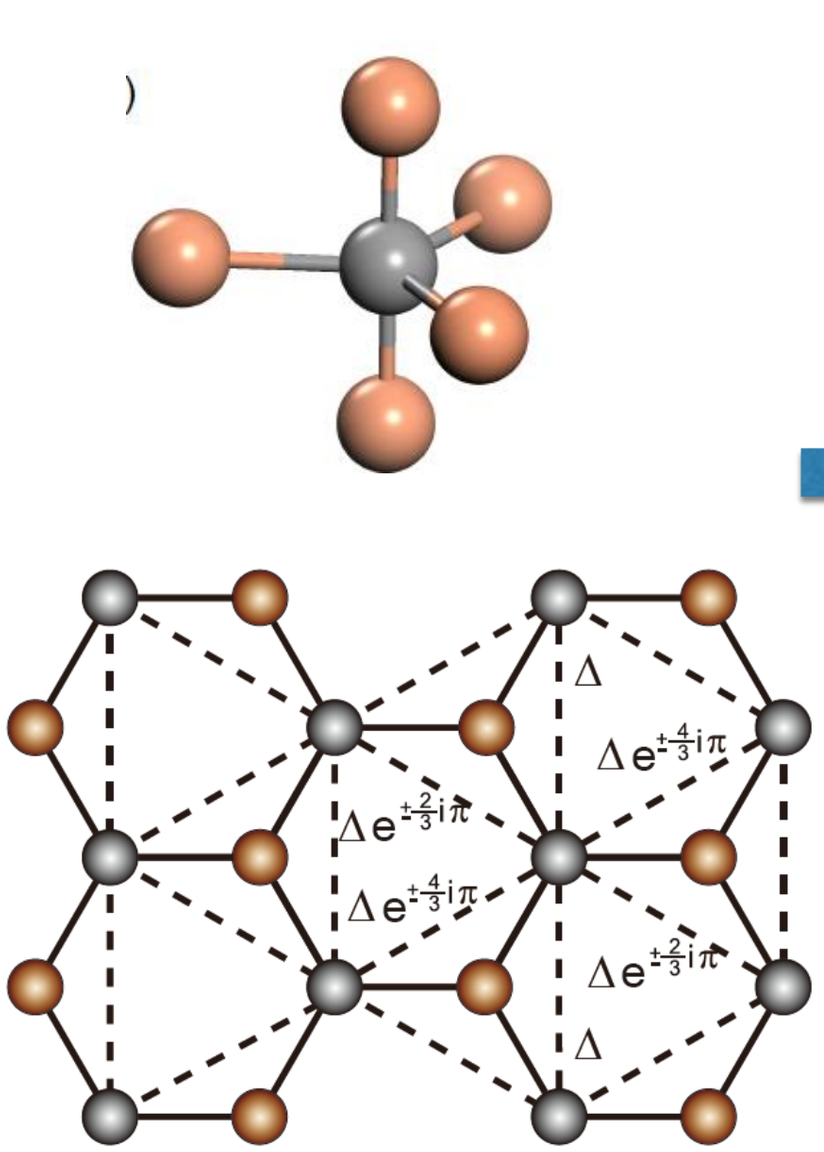
J.Hu and NN Hao, PRX 2, 021009 (2012)

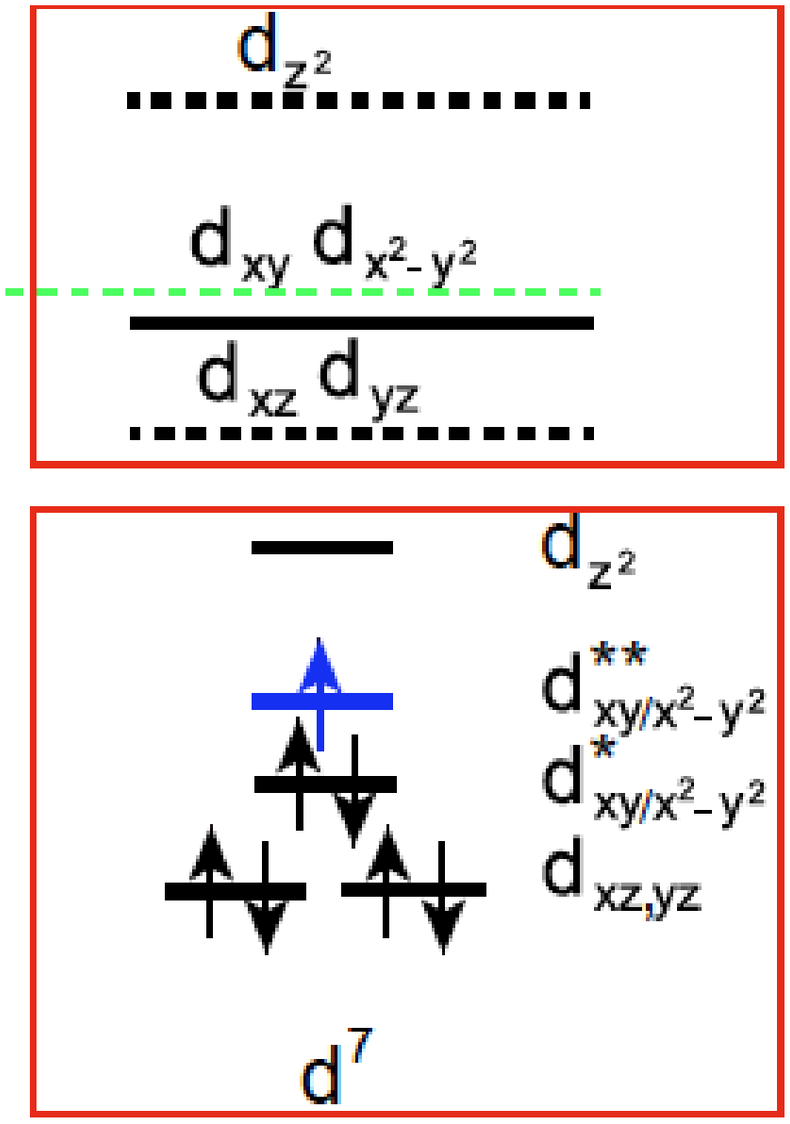
- Rareness: Symmetry matching , collaboration between local cation-anion complexes, global lattice symmetry and doping level !

- Uniqueness: Cu and Fe are irreplaceable in their corresponding families

Can we find or design new families of unconventional high temperature superconductors ?

Prediction: Possible new high Tc Superconductors(I)

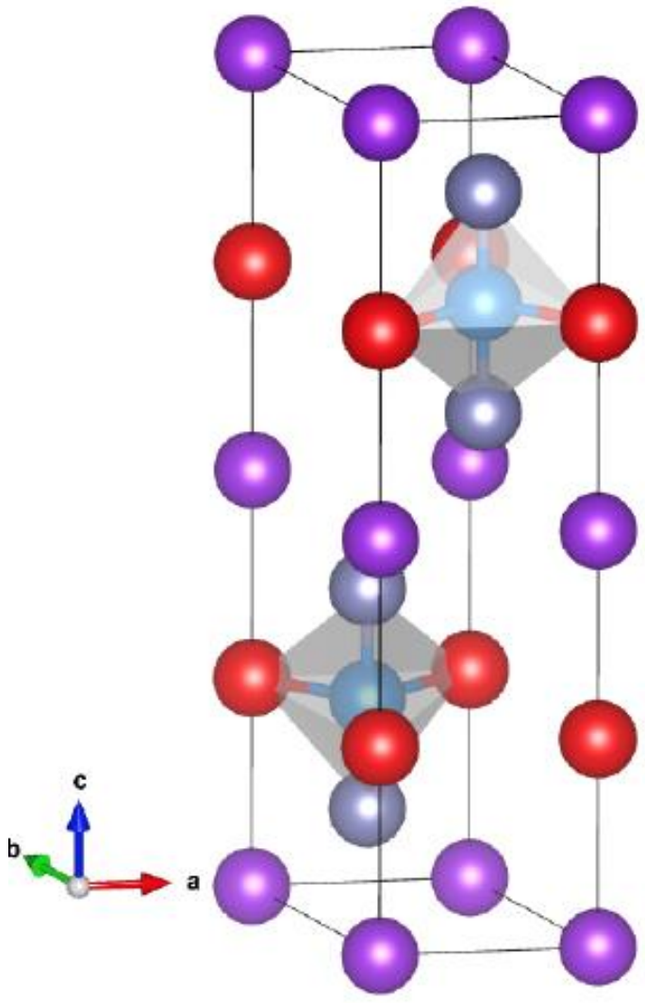




- Triangular Bipyramidal—five coordinations: d7 is unique to achieve high Tc

JP Hu et al, Phys. Rev. X 5, 041012 (2015) Arxiv:1506.03904

Prototype From Triangular Bipyramidal



$YMnO_3$

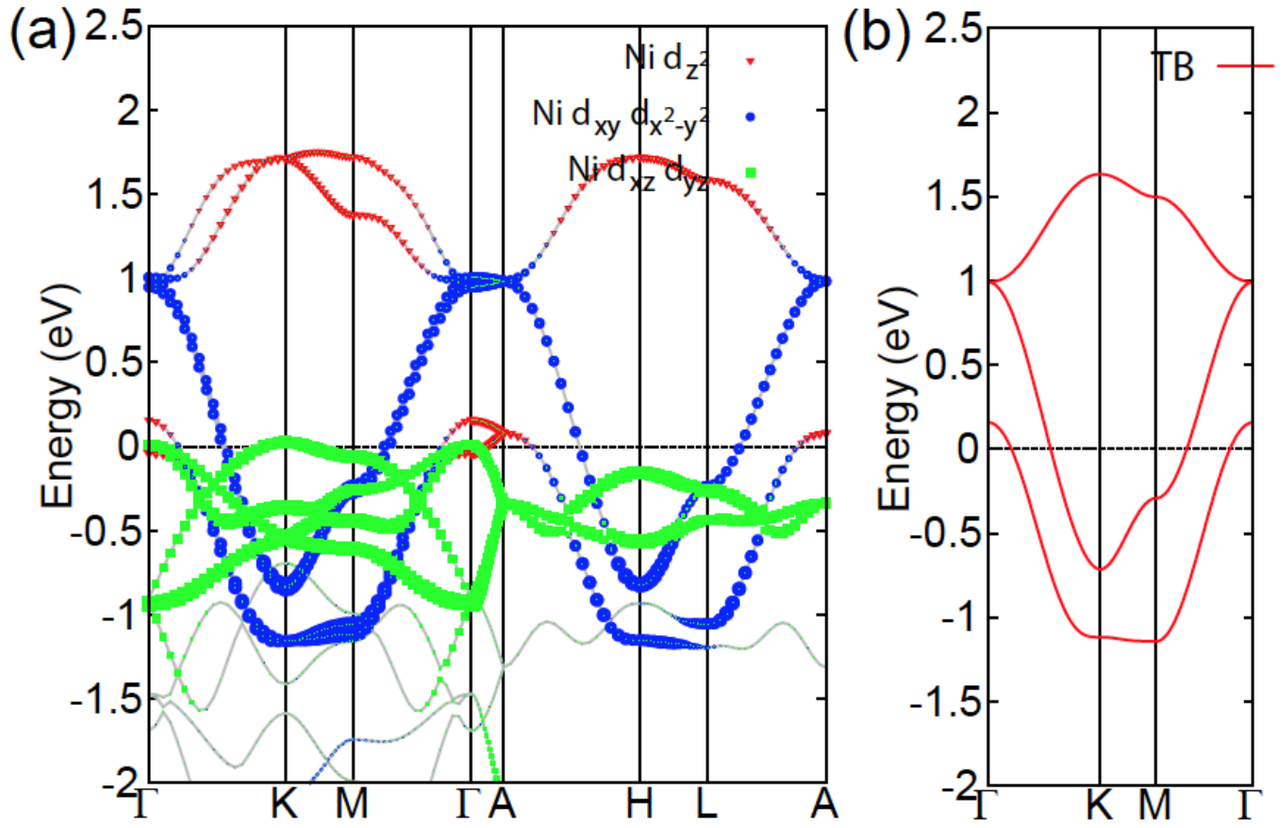
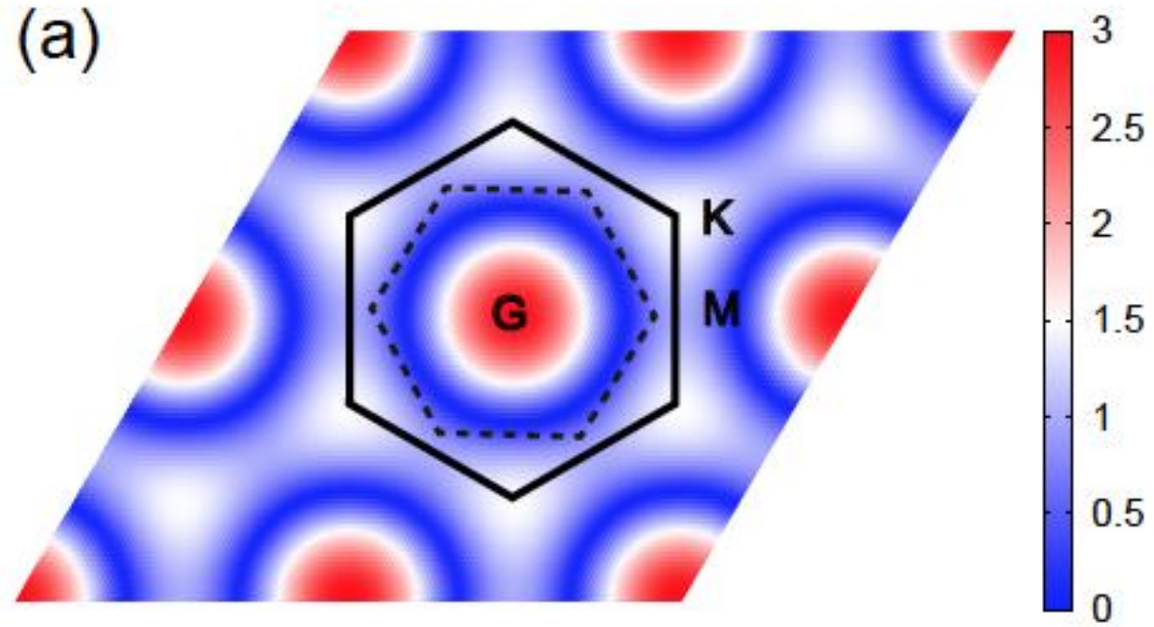


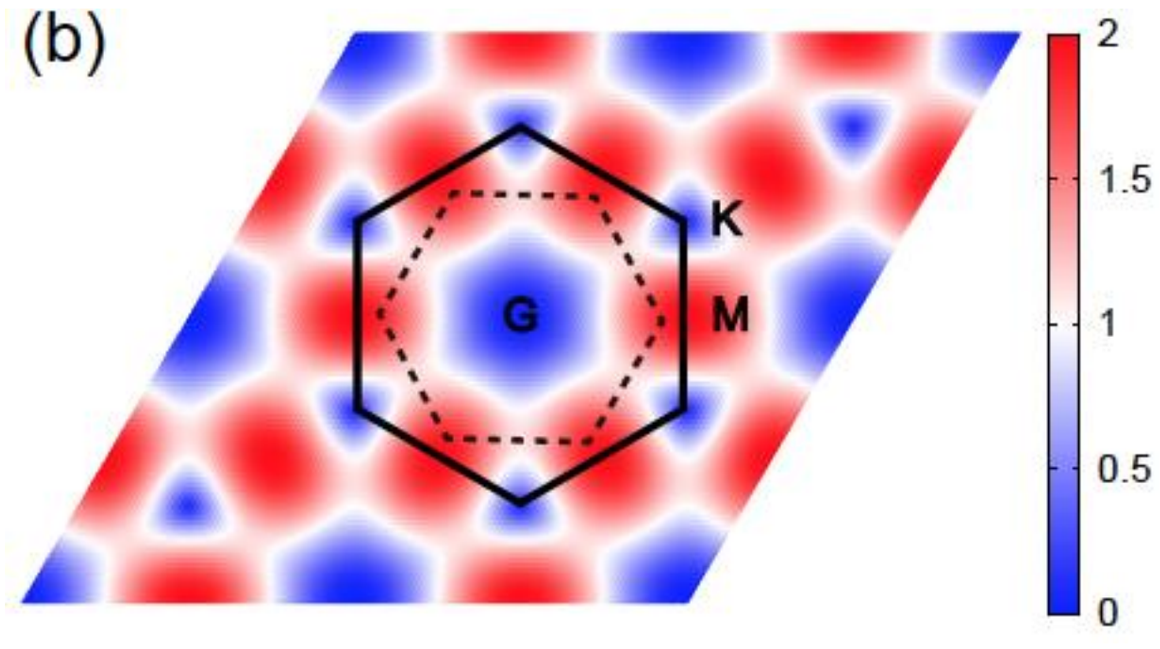
FIG. 3: (a) The band structures of $YNiO_3$ obtained from the first principle calculations and (b) the extracted three bands for the tight binding model. The orbital characters of the bands in (a) are indicated by the different colors specified in the right top corner of the figure.

YNiO3

The isolation of the orbital is protected by symmetry.

Pairing Symmetry and Tc





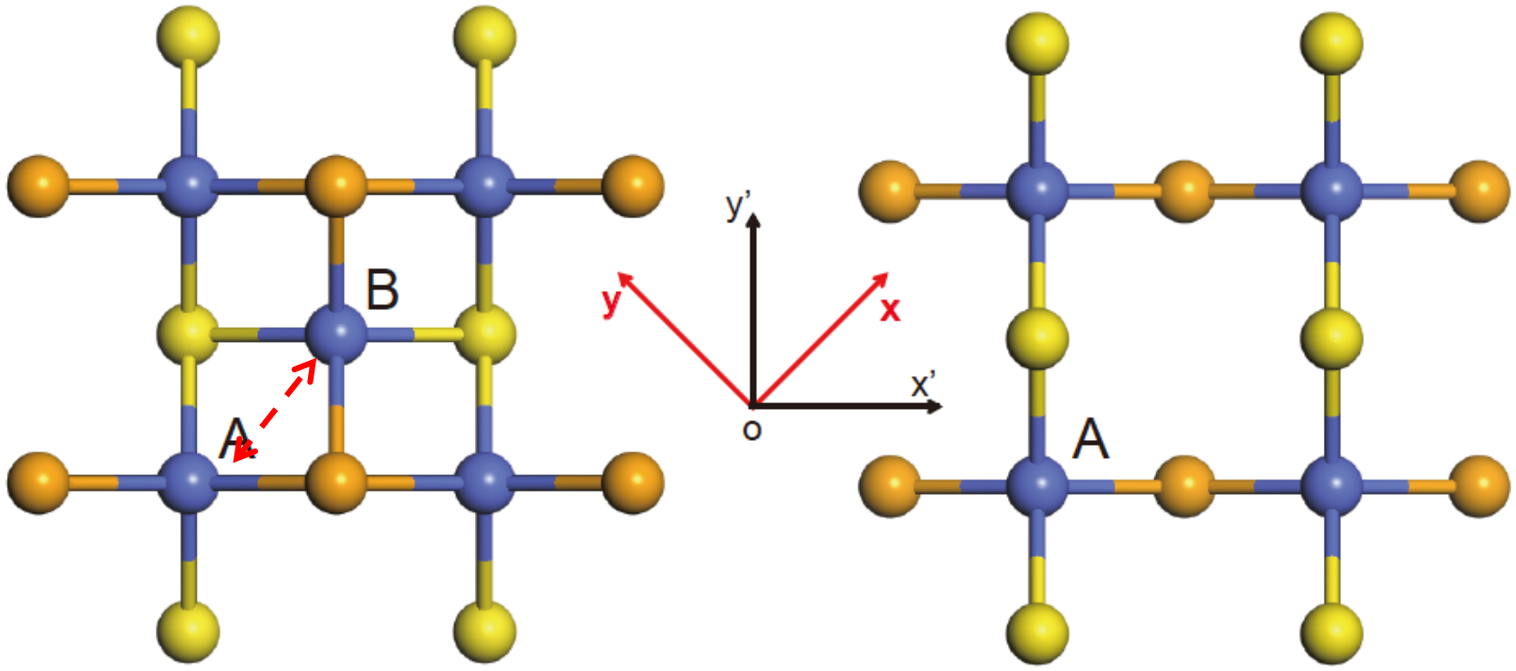
- S-wave has little weight
- d+id has very large weight
- Energy Scale:

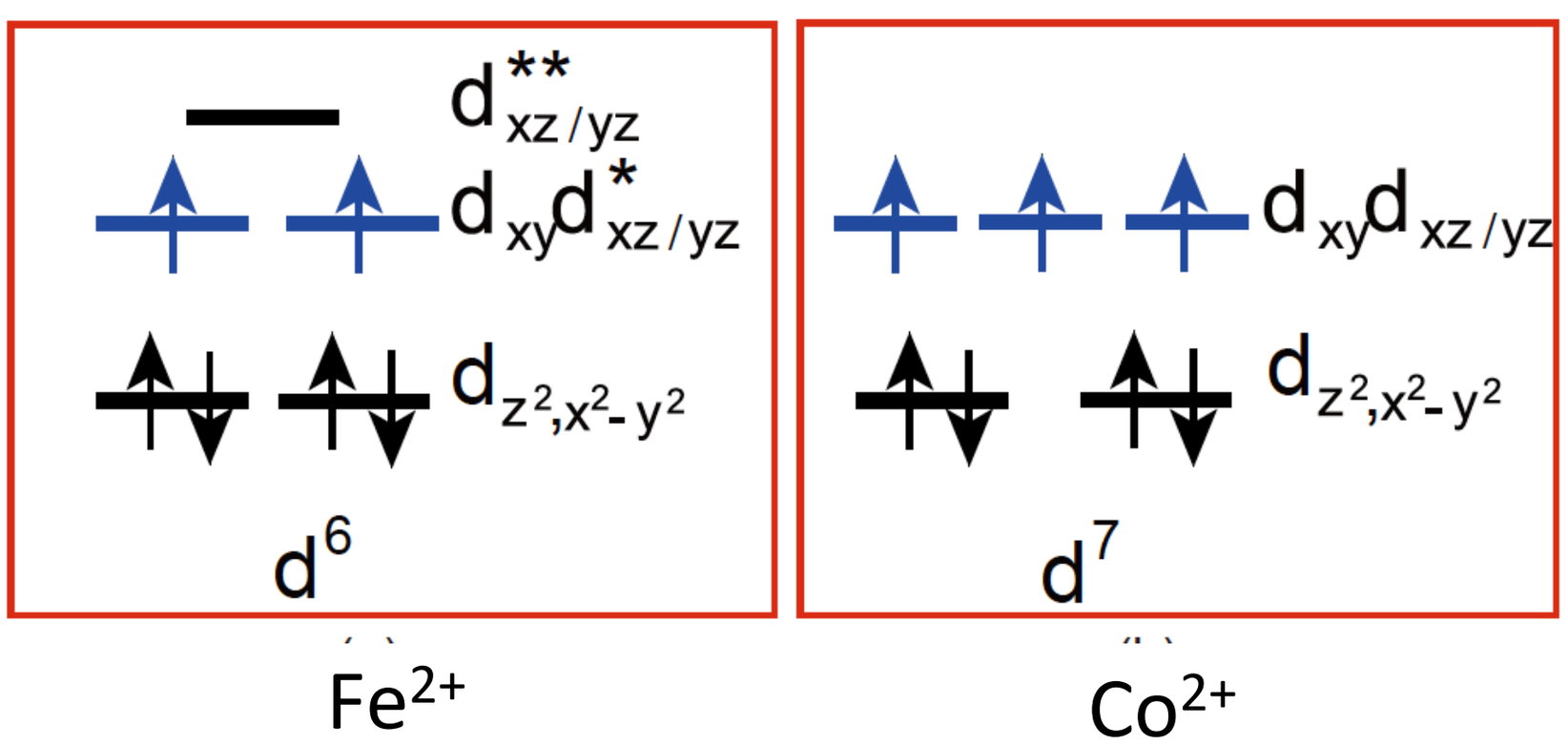
Cuprates

Ni/Co-based

iron-based

Prediction: Possible new high Tc Superconductors(II)

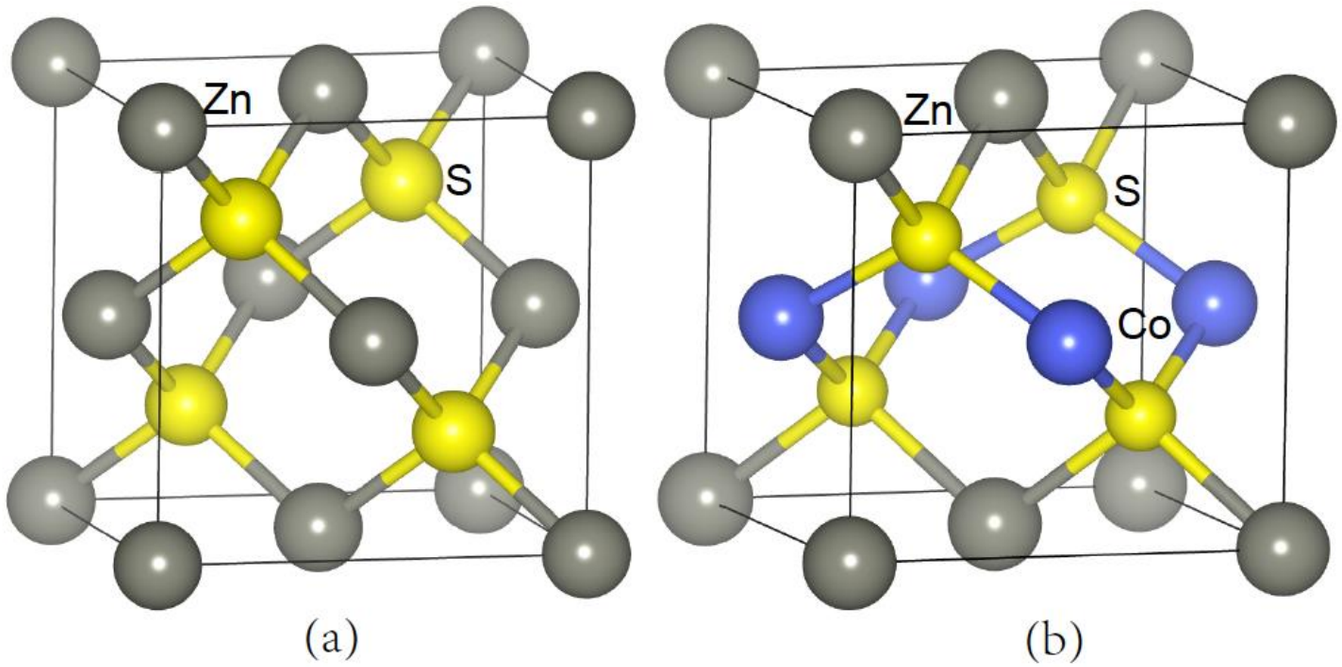




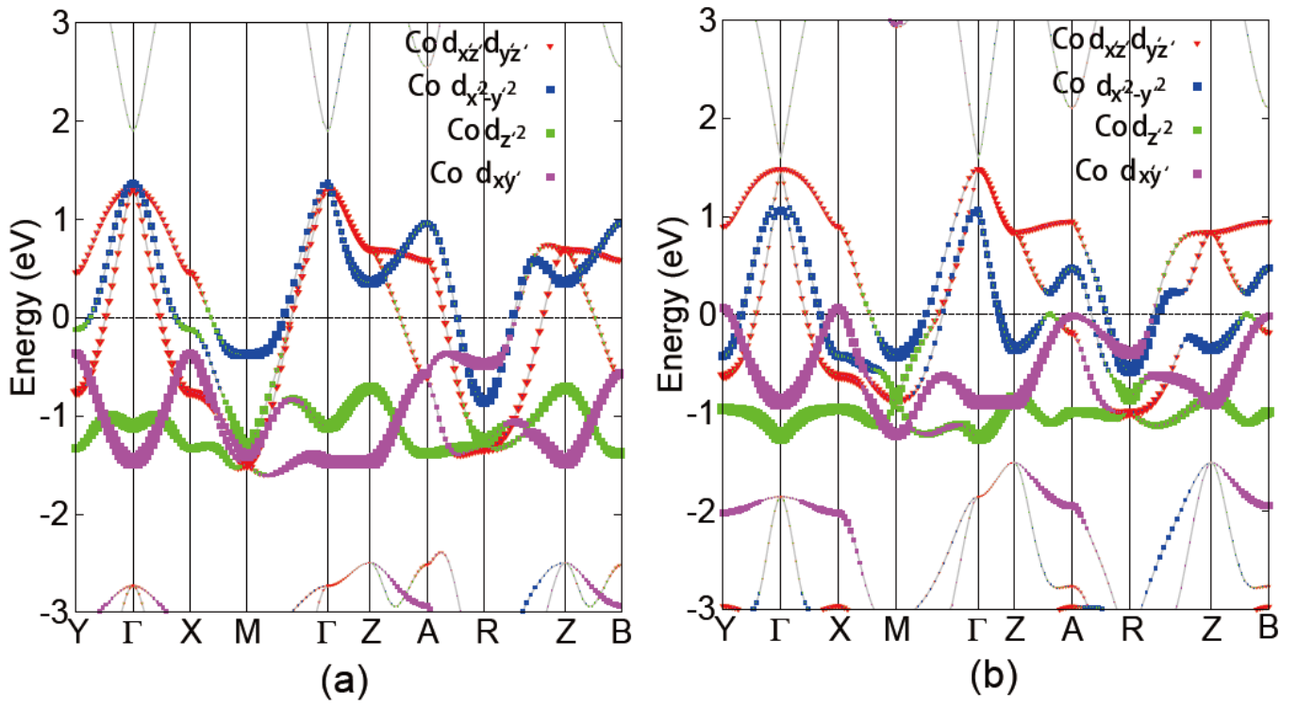
J.Hu and CongCong Le, arxiv: 1611.02835(2016)

Prediction: Possible new high Tc Superconductors(II)

ZnS



$ZnCoS_2$

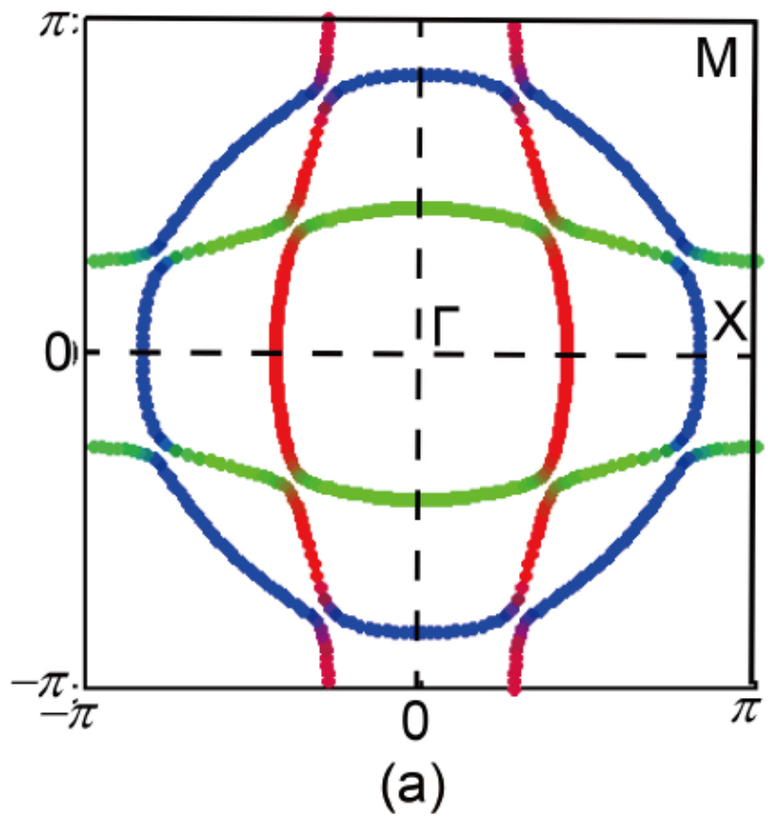


$ZnCo(S,Se)_2$

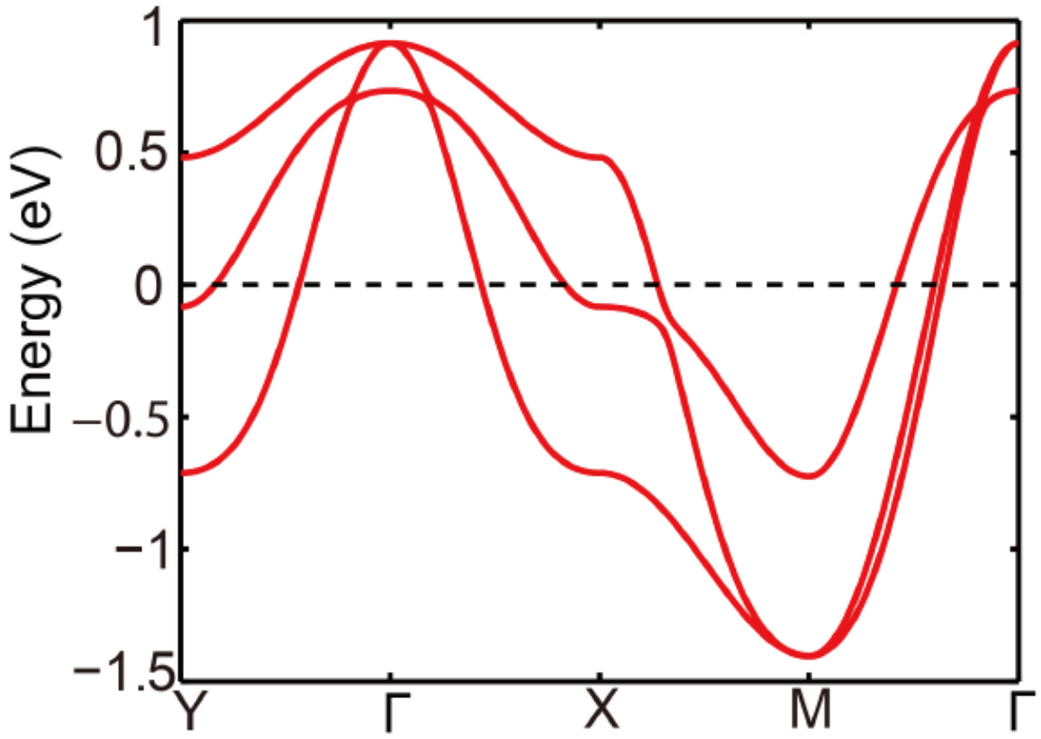
J.Hu and CongCong Le, arxiv: 1611.02835(2016)

Prediction: Possible new high Tc Superconductors(II)

A bridge and unifier of cuprates and iron-based SCs



(a)



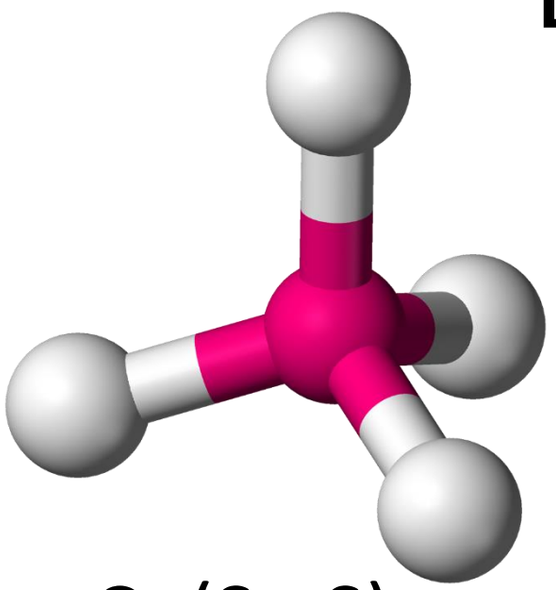
(b)

Prediction:

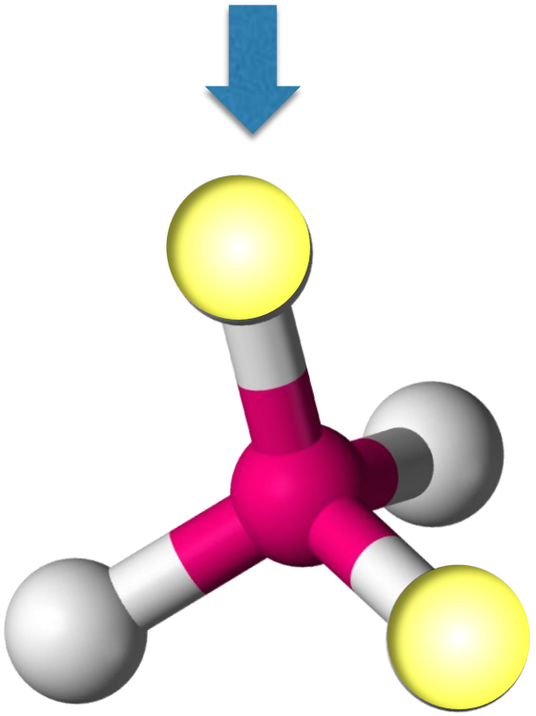
- Similarity to Cuprates: d-wave, Mottness
- Similarity to iron-based superconductors: Multi-orbital, nematicity
- Maximum Tc should be higher than iron-based superconductors

J.Hu and CongCong Le, Sci. Bull. 62 212 (2017)
arxiv: 1611.02835(2016), arXiv:1702.07517

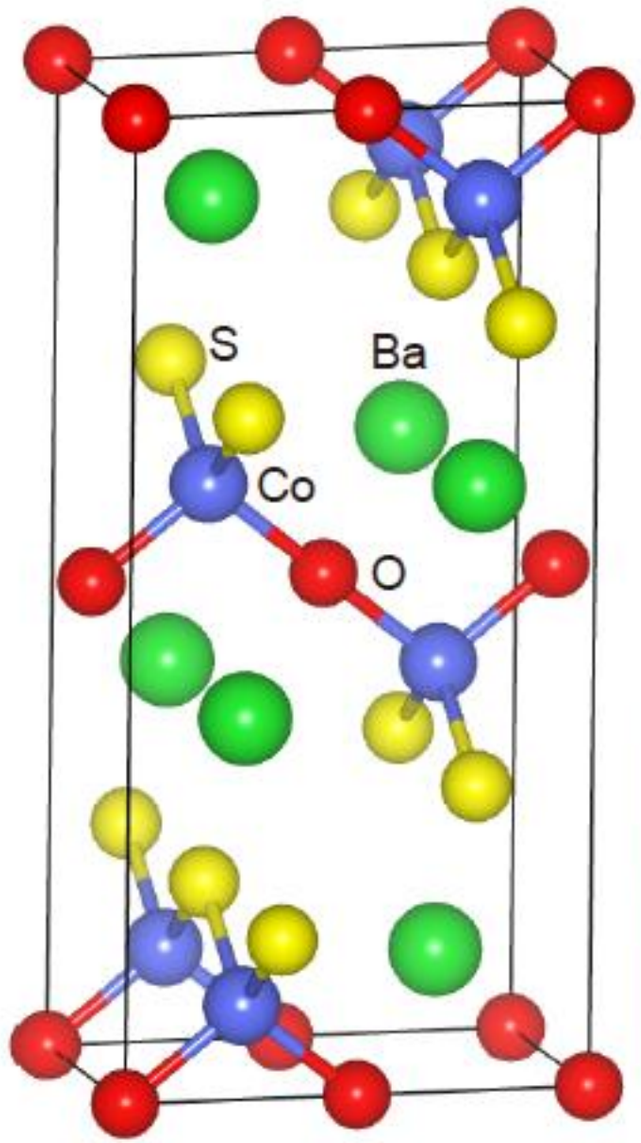
BaCoSO: Oxychalcogenides



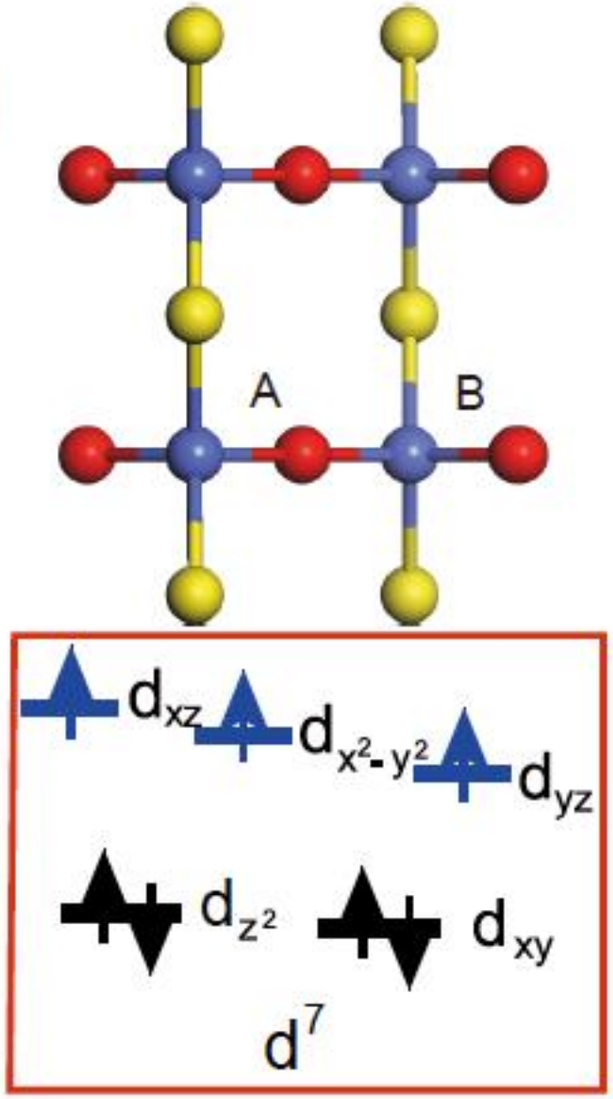
$Co(Se,S)_4$



$Co(Se,S)_2O_2$



(a)

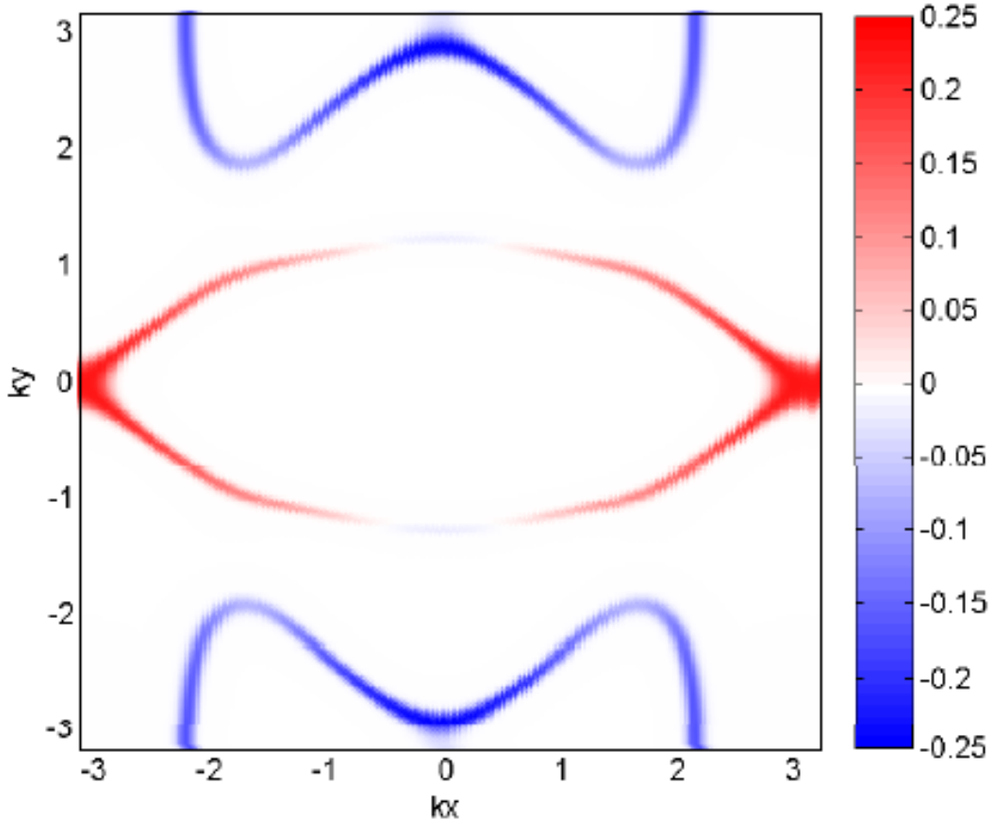


(b)

BaCoSO

CC Le, SS Qin and JP Hu, arxiv:1612.03470 (2016), arXiv:1702.08304(2017)

Co/Ni Oxychalbogenides



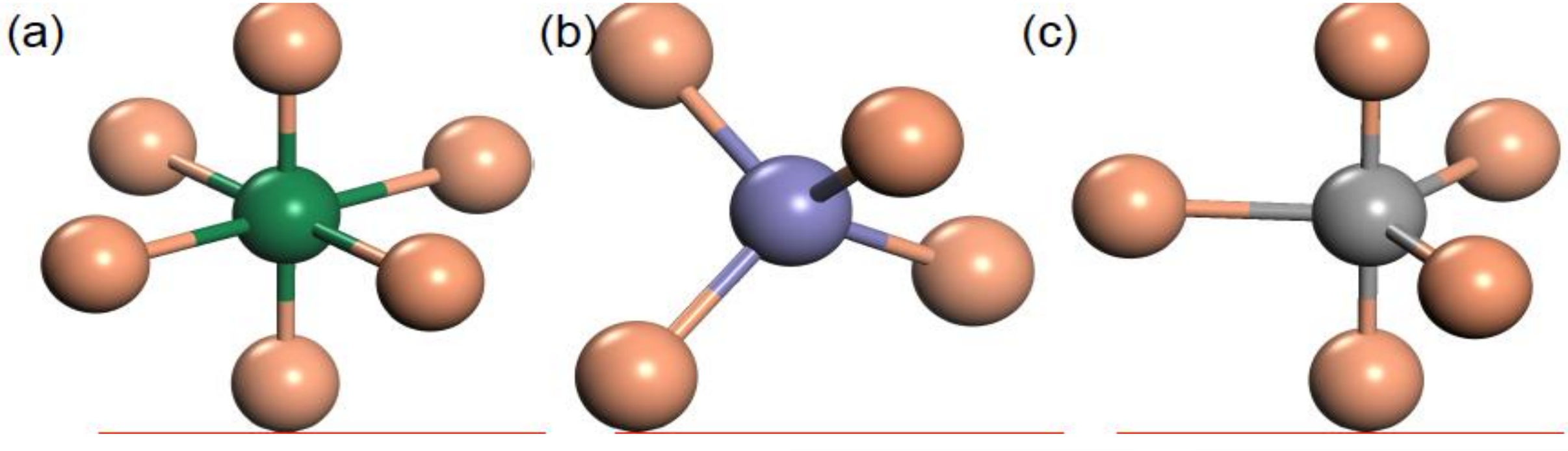
Sign distribution on electron doped Fermi surfaces of BaCoSO

BaCoSO

- Corner shared tetrahedra
- d^7 filling configuration: Mott insulator
- AFM Neel temperature over 200K
- Lacking of D_{4h} symmetry classification, but Pairing symmetry resembles both cuprates and iron-based superconductors (nodes and sign change between two pockets)
- Challenge: introduce doping?

CC Le, SS Qin and JP Hu, arxiv:1612.03470 (2016), arXiv:1702.08304(2017)

Summary for High Tcs



- Octahedral
- Corner share
- Square Lattice
- d^9, dx^2-y^2
- Cu^{2+}
- d-wave pairing

- Tetrahedral
- Edge share
- Square Lattice
- d^6, dxy, dxz/yz
- Fe^{2+}
- s-wave

- Tetrahedral
- Corner share
- Square Lattice
- d^7 dxy, dxz,d yz
- Co^{2+},Ni^{3+}
- d-wave

- TBP
- Corner share
- Trigonal Lattice
- d^7, dxy/x^2-y^2
- Co^{2+},Ni^{3+}
- d+id-wave pairing

bulk / M_{55}^-									
	hcp Sc ico	hcp Ti irico	bcc V ptet	bcc Cr ptet	bcc Mn ptet	bcc Fe ptet	hcp Co ico	fcc Ni ico	fcc Cu ico
	hcp Y	hcp Zr irico	bcc Nb ptet	bcc Mo ptet	hcp Tc	hcp Ru cp	fcc Rh ico/cp	fcc Pd ico	fcc Ag ico

Summary

- Iron-based superconductors are special systems to realize extended-S wave

- Only AFM couplings induced through anions are important in providing pairing.

- Orbital distillation rule (Scalapino): Isolating the d-orbitals that strongly participate superexchange is the key to realize high Tc

- Special high Tc environments: realized by the collaboration between local cation-anion complexes, global lattice symmetry and doping level

- Two high Tc environments to realize possible Co/Ni-based high Tc

JP Hu et al, Phys. Rev. X 5, 041012 (2015)
JP Hu and J. Yuan, Front. of Phys., arXiv:1506.03904
JP Hu, Sci. Bull., 61, 561 (2016) arXiv:1512.09190
J.Hu and CongCong Le, Sci. Bull. 62 212 (2017) arxiv: 1611.02835, arXiv:1702.07517
CC Le, SS Qin and JP Hu, arxiv:1612.03470 (2016), arXiv:1702.08304(2017)

Acknowledgements

- Students & Postdoctor: XX Wu, CongCong Le, J. Yuan, YinXiang Li, Qiang Zhang, Xinloong Han

- X.H Chen , H. Ding, X. J. Zhou, D. L. Feng

- Q.K Xue, X. Chen, H.H. Wen, S.H. Pan, N.L. Wang

- Theory: S.A. Kivelson, T. Xiang, Z.Y. Lu, Lu Yu, D.H. Lee