Possible New Families of Unconventional High Temperature Superconductors

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Theory of electron nematic order in LaFeAsO

Chen Fang, Hong Yao, Wei-Feng Tsai, JiangPing Hu, and Steven A. Kivelson

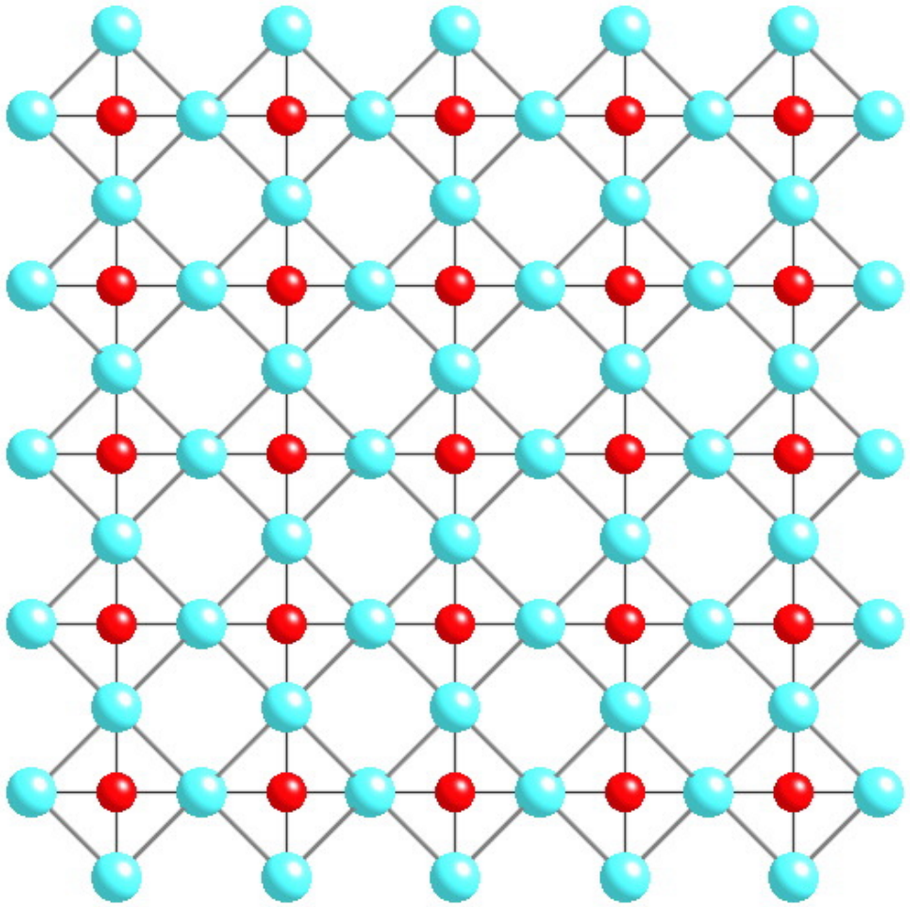
Phys. Rev. B 77, 224509 – Published 20 June 2008

Of course, the big issue of the day is whether the physics of high temperature superconductivity in the rare-earth oxypnictides is related to that in the cuprates.

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

Why are Fe and Cu special ?

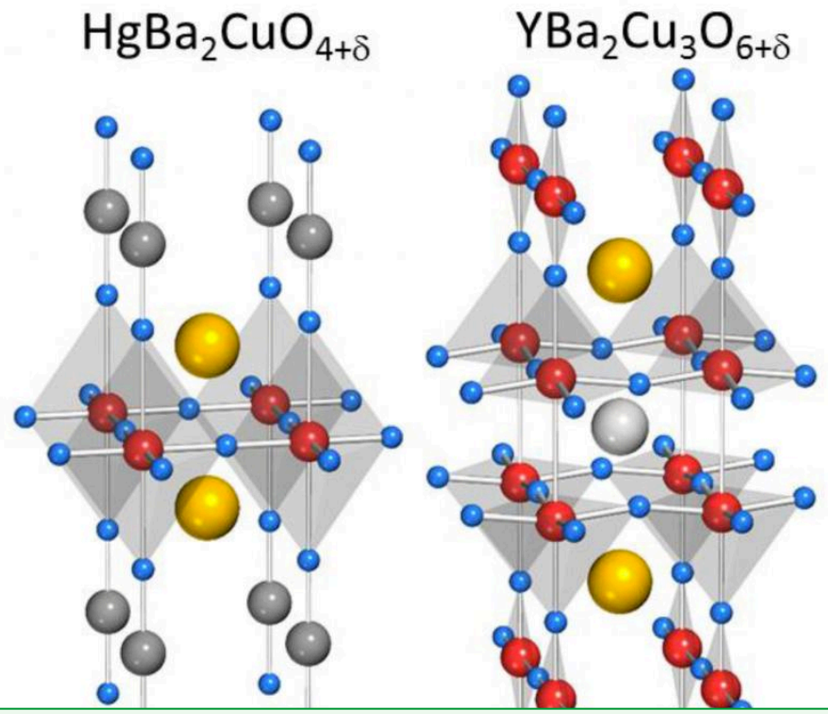
Cuprates



- Why is CuO_2 layer so special?

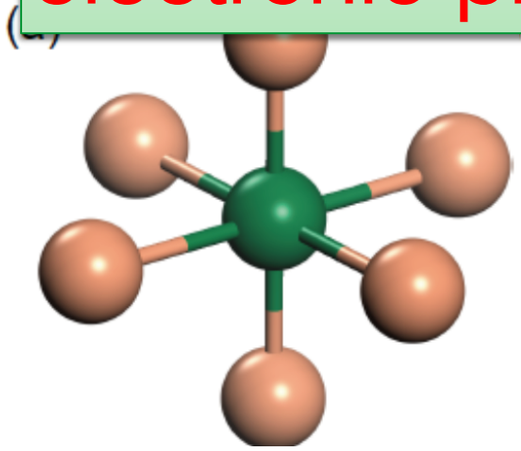
Both Cu and O seem to be irreplaceable!

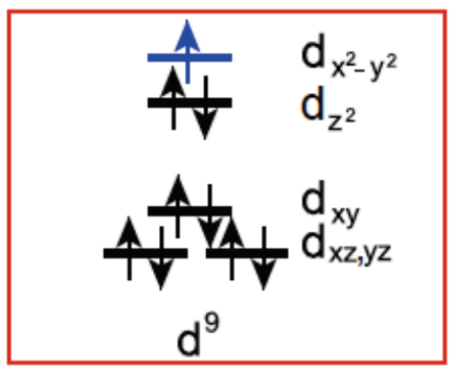
Octahedron, Perovskite structure and Cuprates



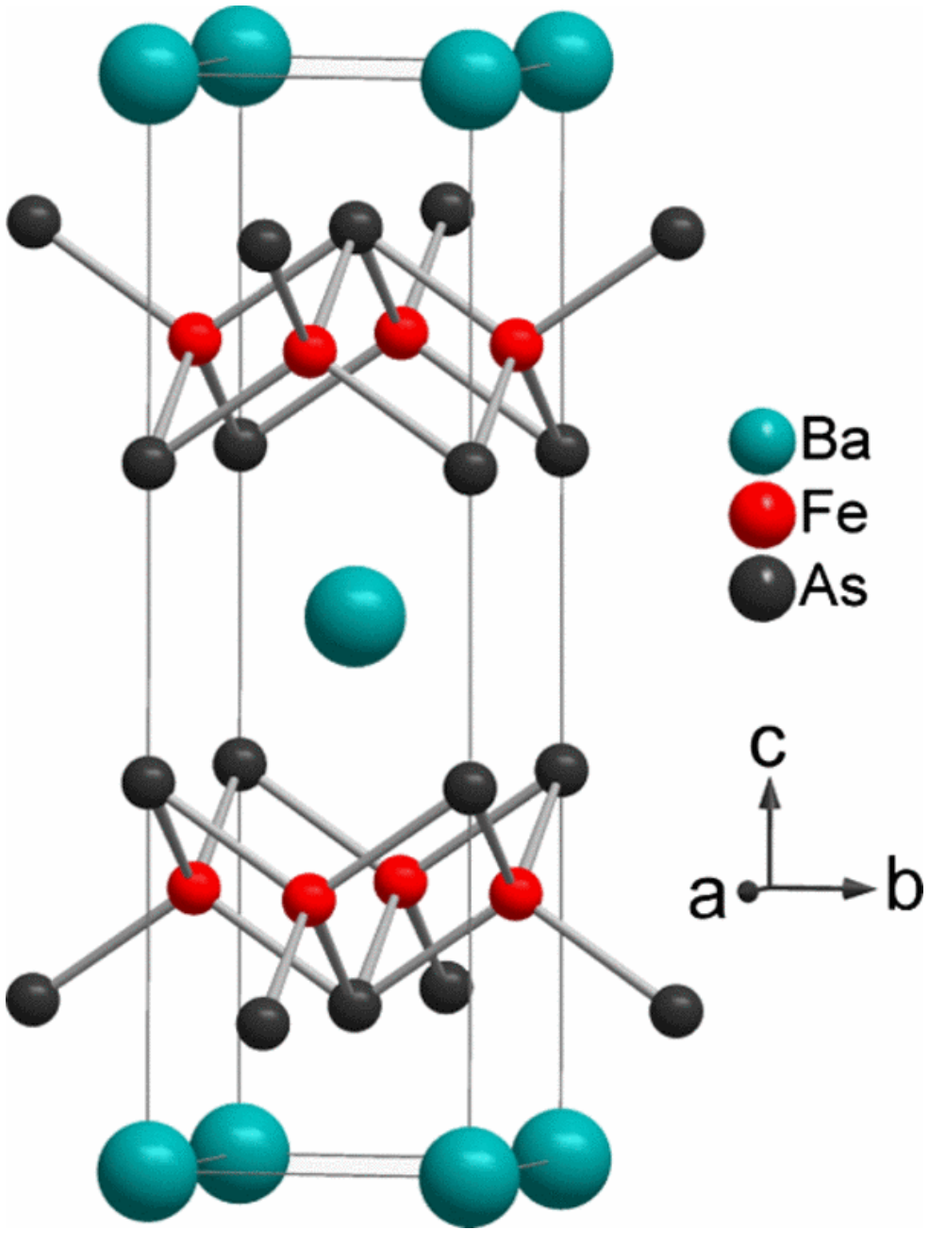
- Single d-orbital: d_{x2-y2}
- The d_{x2-y2} orbital has the highest energy in the d shell
- Separation between t_{2g} (c>a=b) lows d_{z^2}
- d^9 is unique to achieve high Tc

d_{x2-y2} orbital, which is responsible for the largest superexchange AFM interaction, is isolated to carry the electronic physics !!



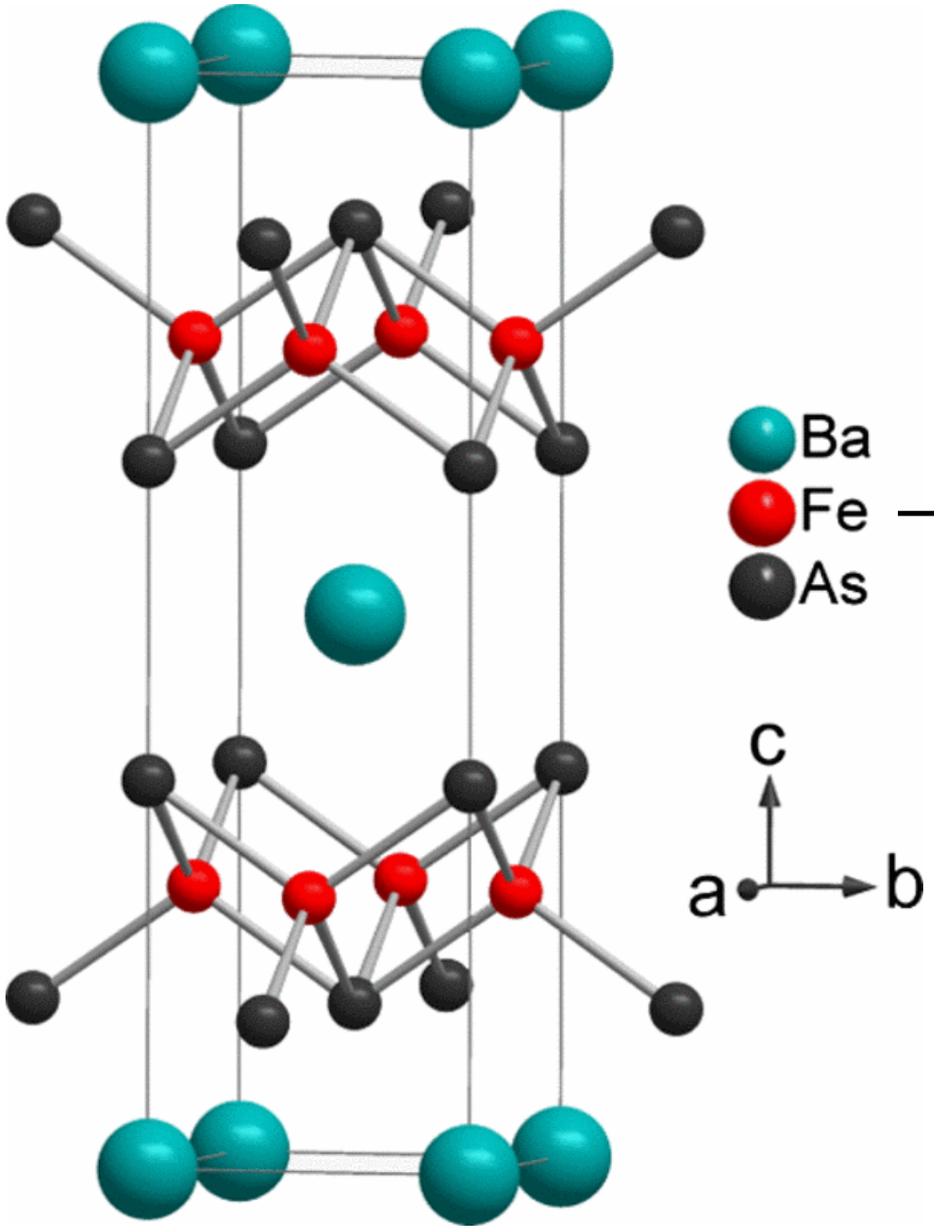


Challenge in the quest of the special part of iron-based superconductors



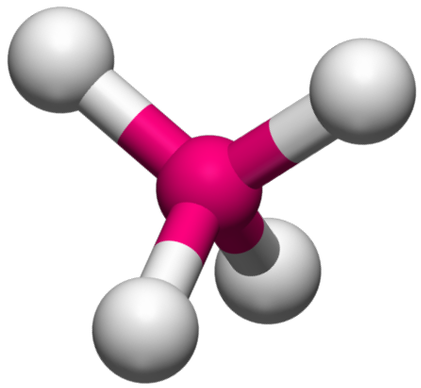
- Multi-orbital systems
- Fe is in the middle of the periodic table for the 3d transition metal elements
- Anion is replaceable:
  S, Se, As, P,Te
- complex interactions

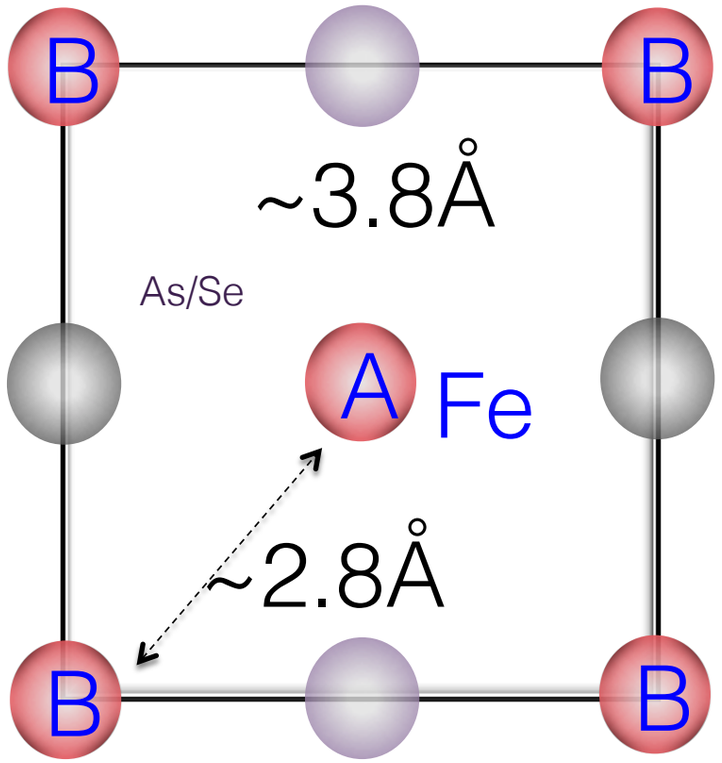
Fe is very special!

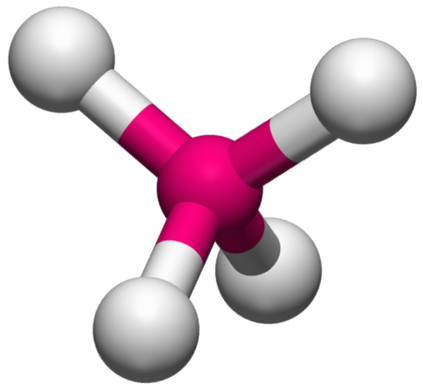


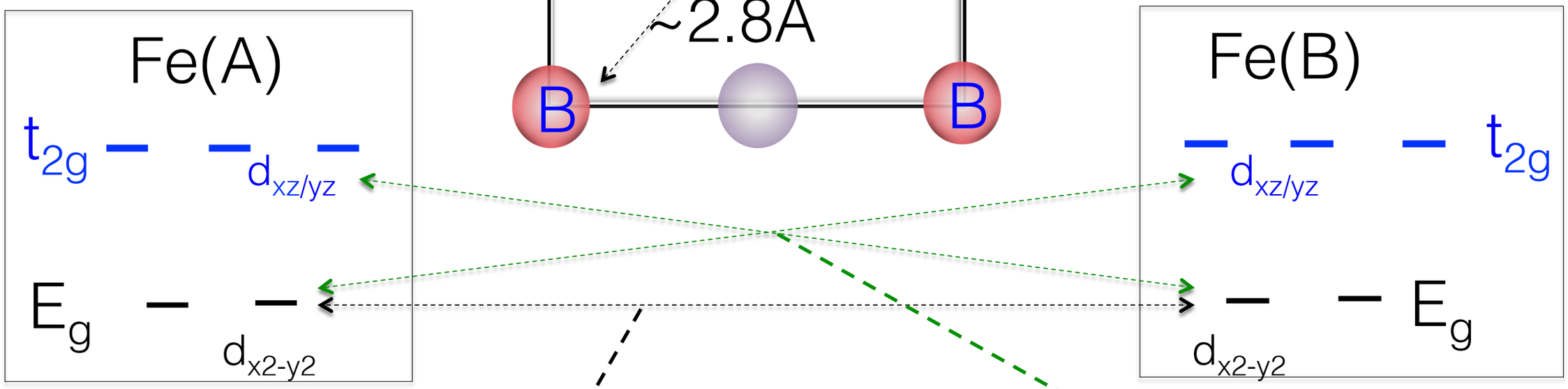
→ Cr, Mn, Co, Ni, Cu

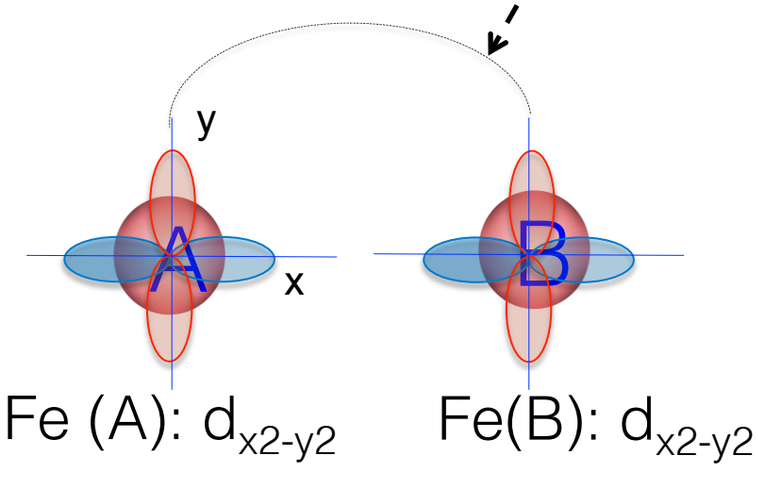
Tetrahedron and iron-based superconductors

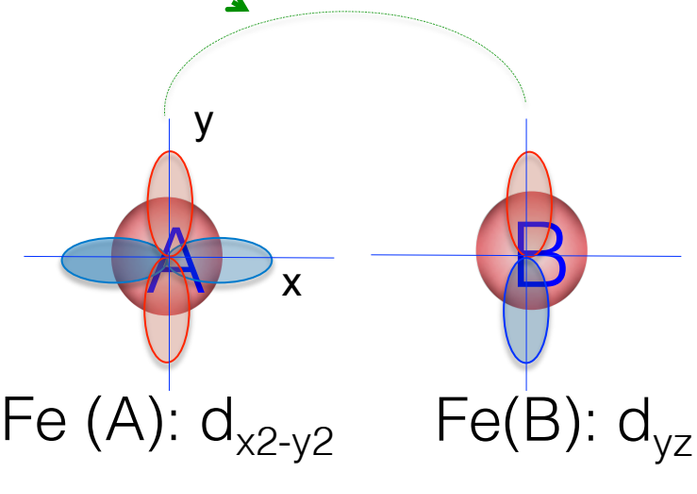












Local electronic structure in iron-based superconductors

- 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

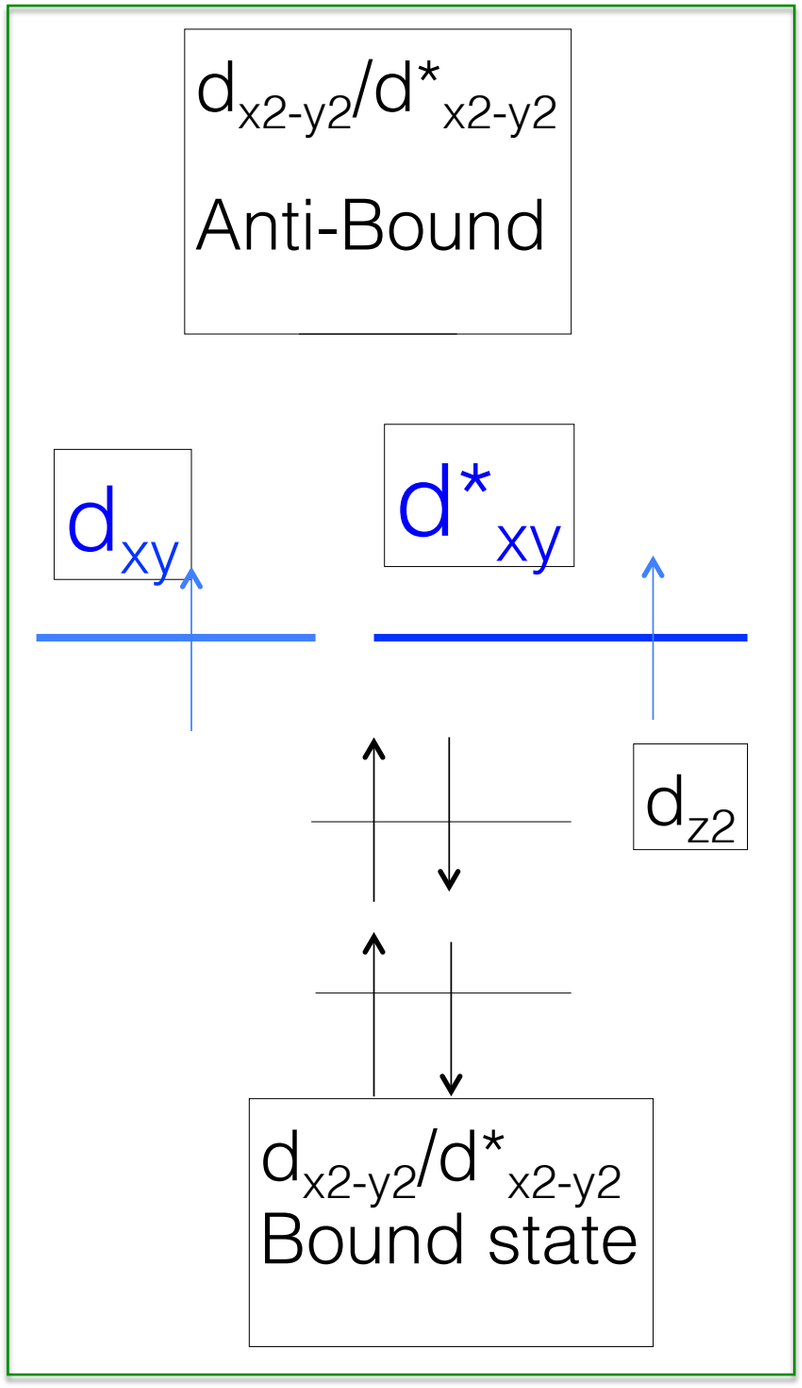
TABLE I. The intraorbital hopping parameters used for the DFT fit of the 5 orbital model.

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!
- Strong t_{2g} and E_g orbital hybridization
- Two pure d_{xy}-type orbitals are isolated near Fermi Energy!
- Two d_{xy} orbital models can capture electronic structures near Fermi Energy.

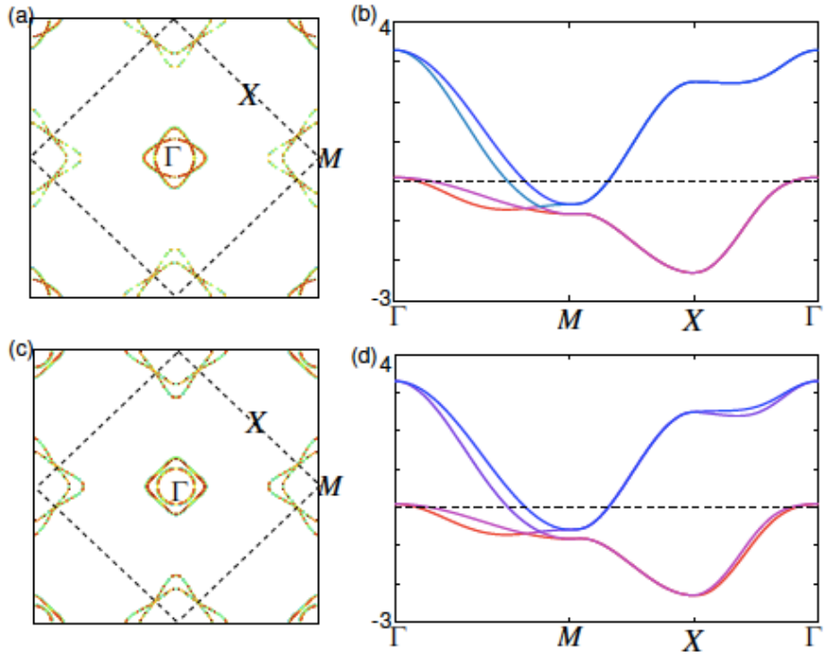
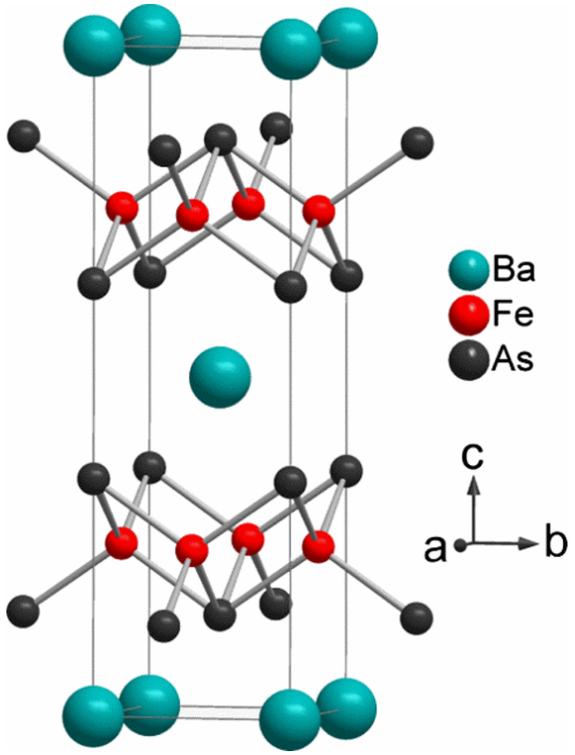
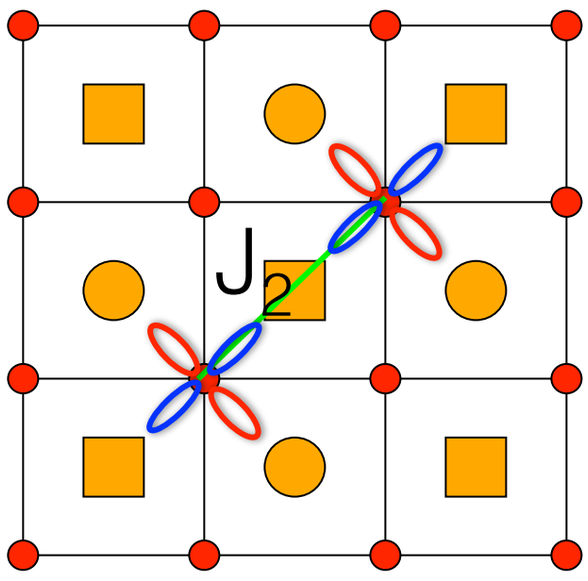


FIG. 1. A typical Fermi surfaces (a), band dispersions (b) resulted from Eq.7 with parameters $t_{1s} = 0.4, t_{1d} = -0.03, t_{2s} = 0.3, t_{2d} = 0.6, t_{3s} = 0.05, t_{3d} = -0.05$ and $\mu = -0.3$. (c) and (d) are corresponding results by adding $t_r = 0.02$ in Eq.17 with the same parameter setting.

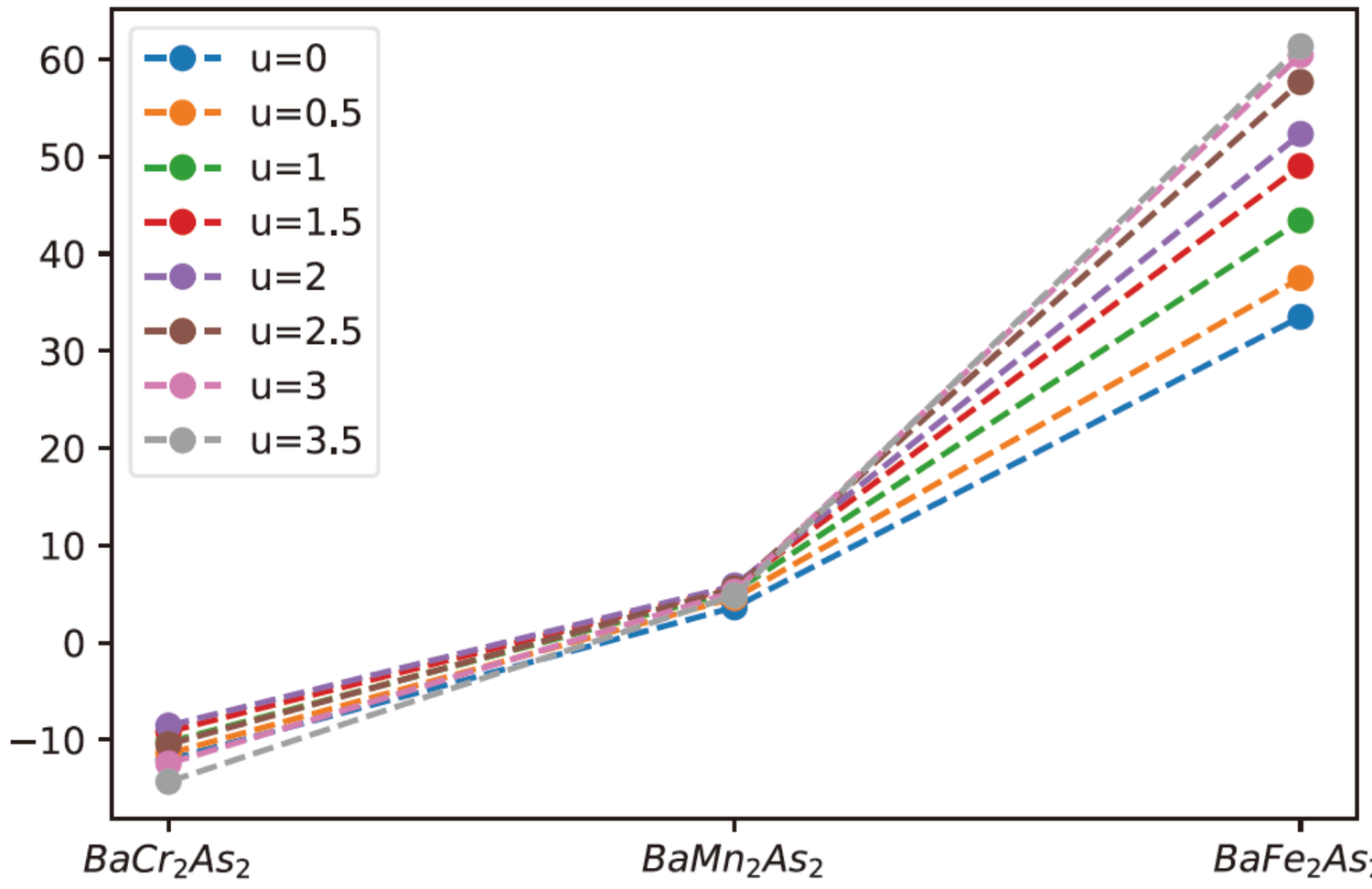
J.Hu and NN Hao, PRX 2, 021009 (2012)

Why Fe is special?





Cr, Mn, Co, Ni, Cu



- Next nearest neighbor(NNN) AFM coupling reaches maximum with Fe
- Stripe AFM order for Fe
- Checkerboard AFM for Cr and Mn, but do not support superconductivity
- Co, Ni, Cu: nonmagnetic or weak ferromagnetic

Those d-orbitals with the strongest in-plane d-p couplings have to be isolated near Fermi energy!

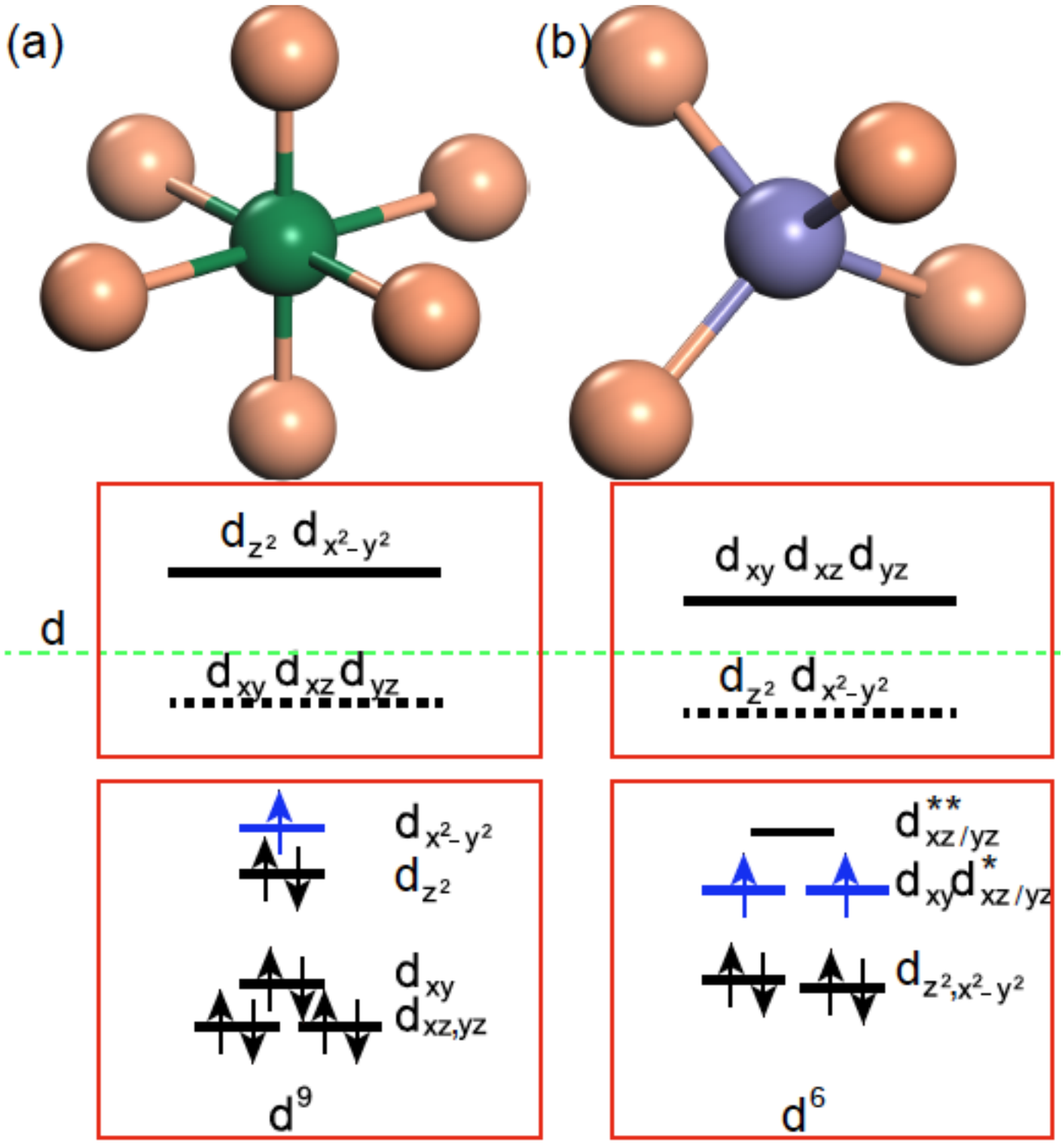
- Rareness:

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

  b. Chemistry limitation: atom sizes, limited cation-anion complexes

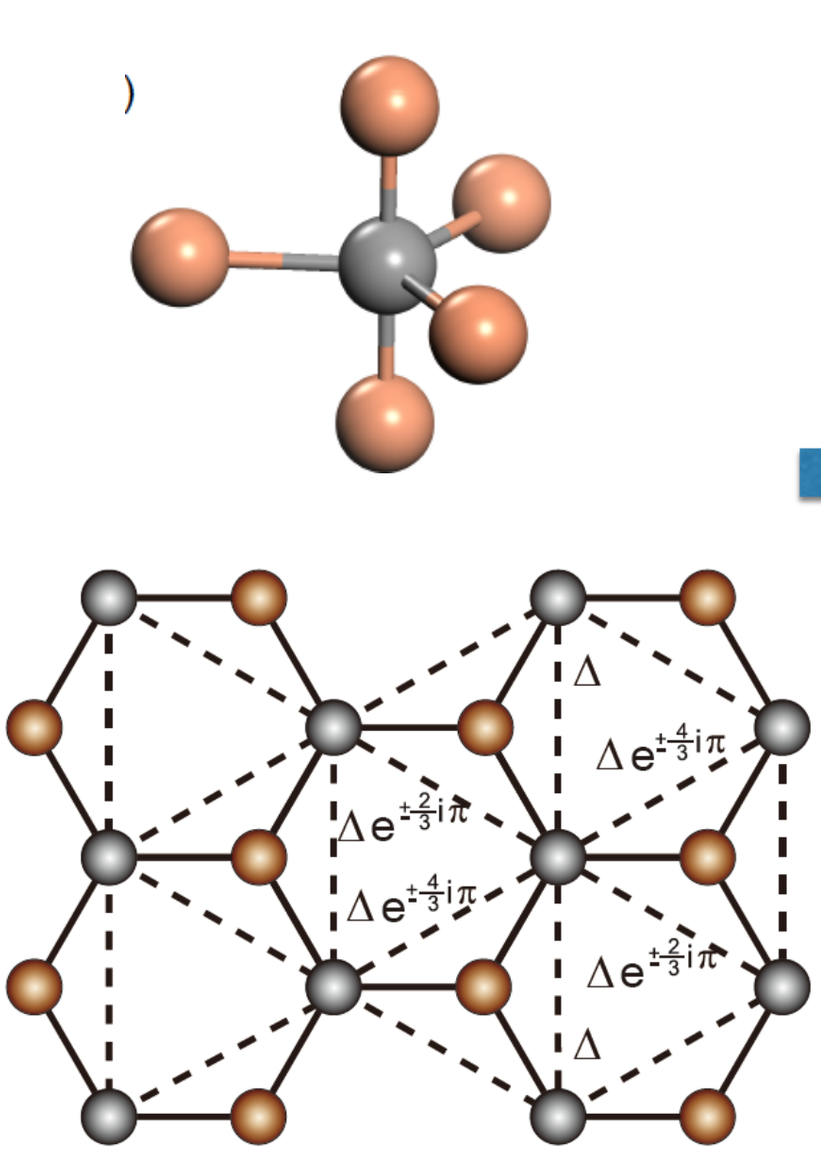
- Uniqueness: Cu and Fe are irreplaceable in their corresponding families

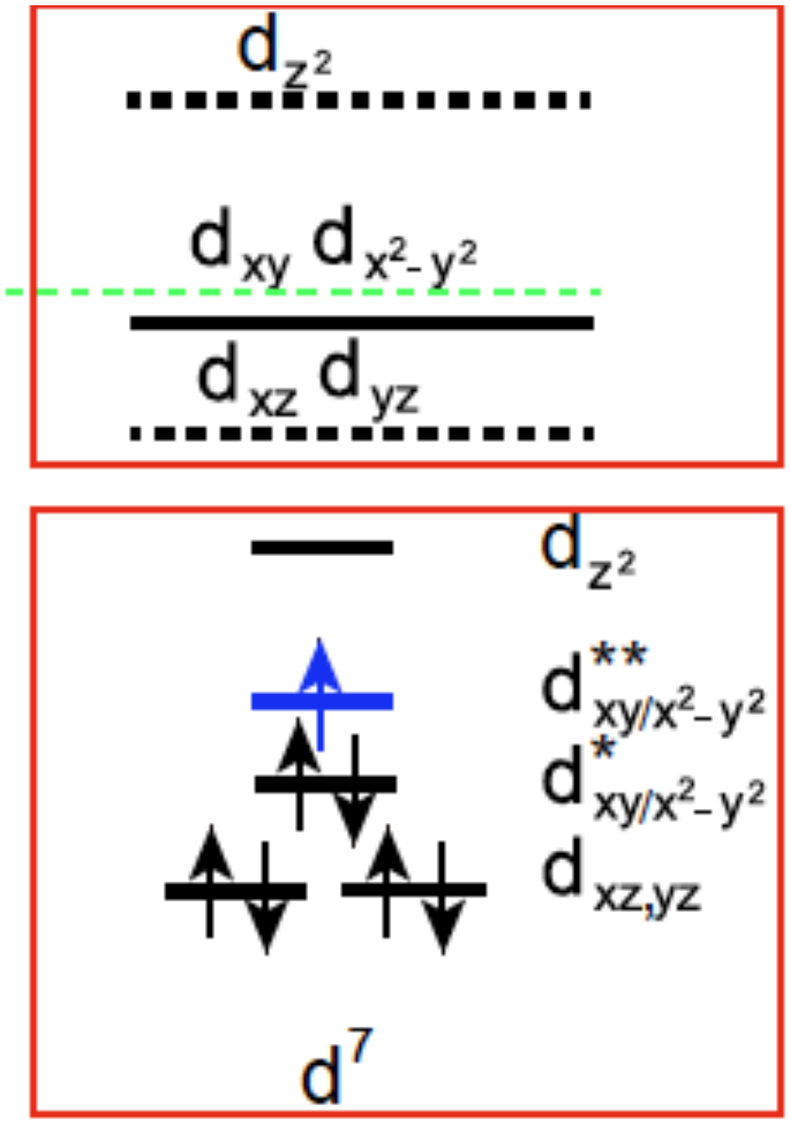
Cuprates vs iron-based superconductors



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

Prediction: Possible new high Tc Superconductors(I)

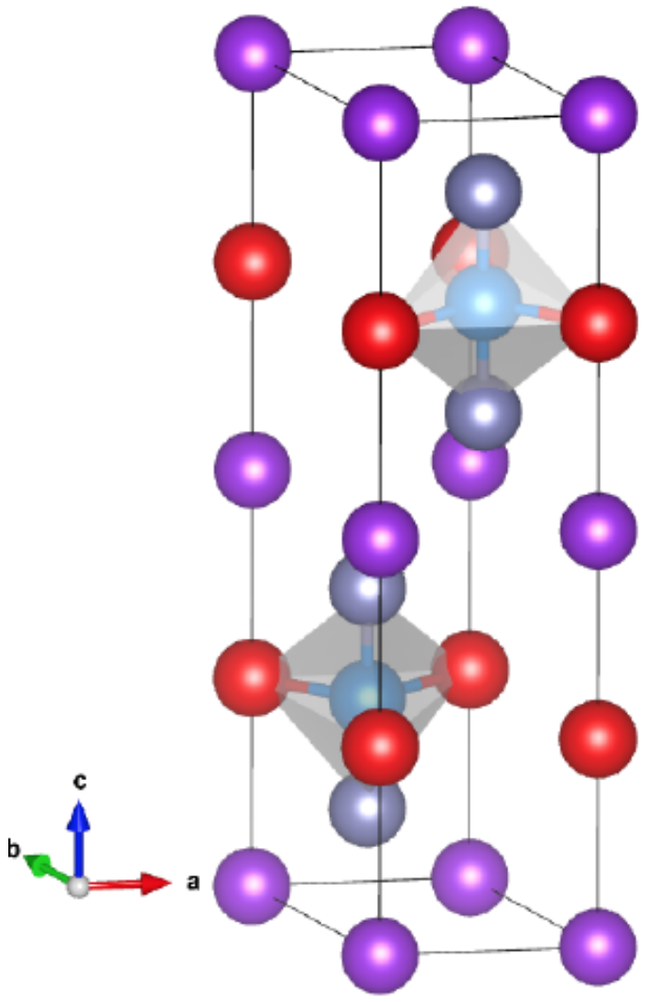




- Triangular Bipyramidal—five coordinations: d7 is unique to achieve high Tc

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

Prototype From Triangular Bipyramidal



$YMnO_3$

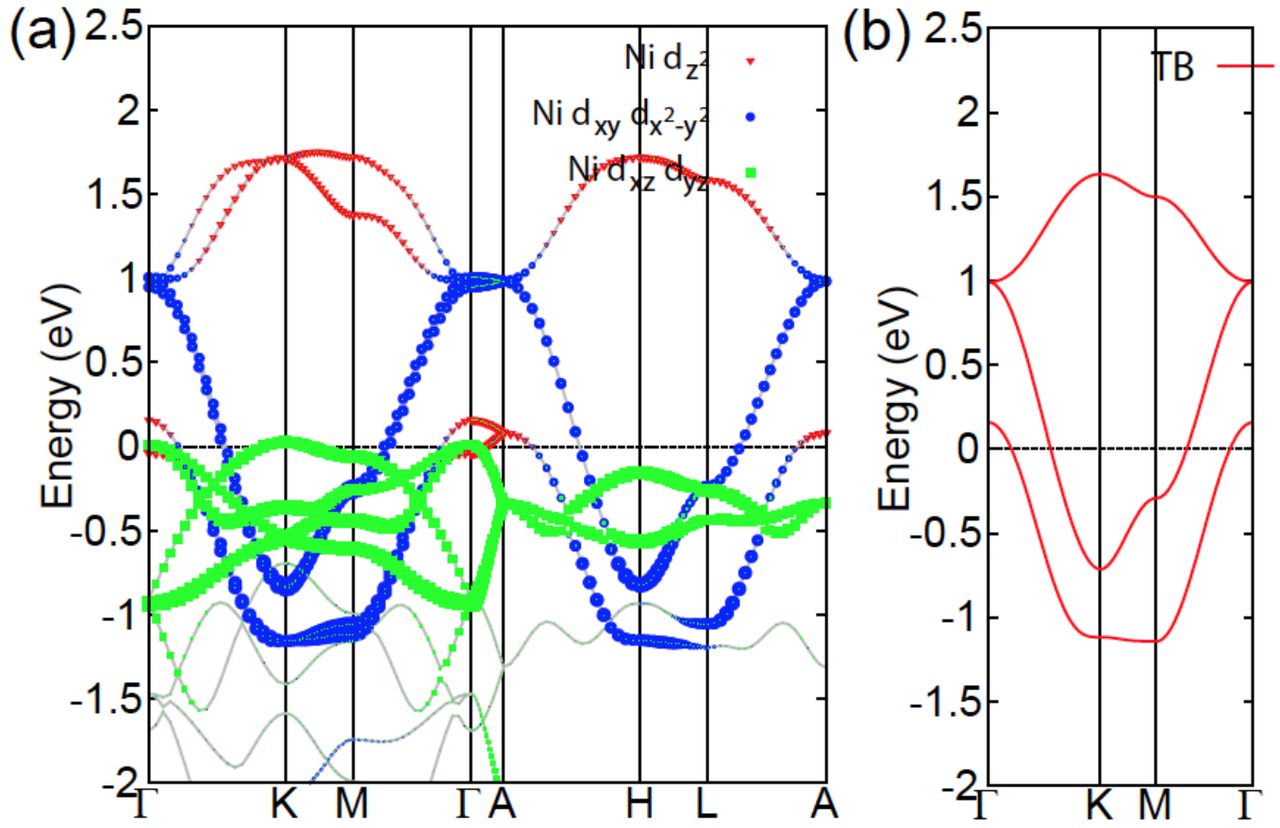
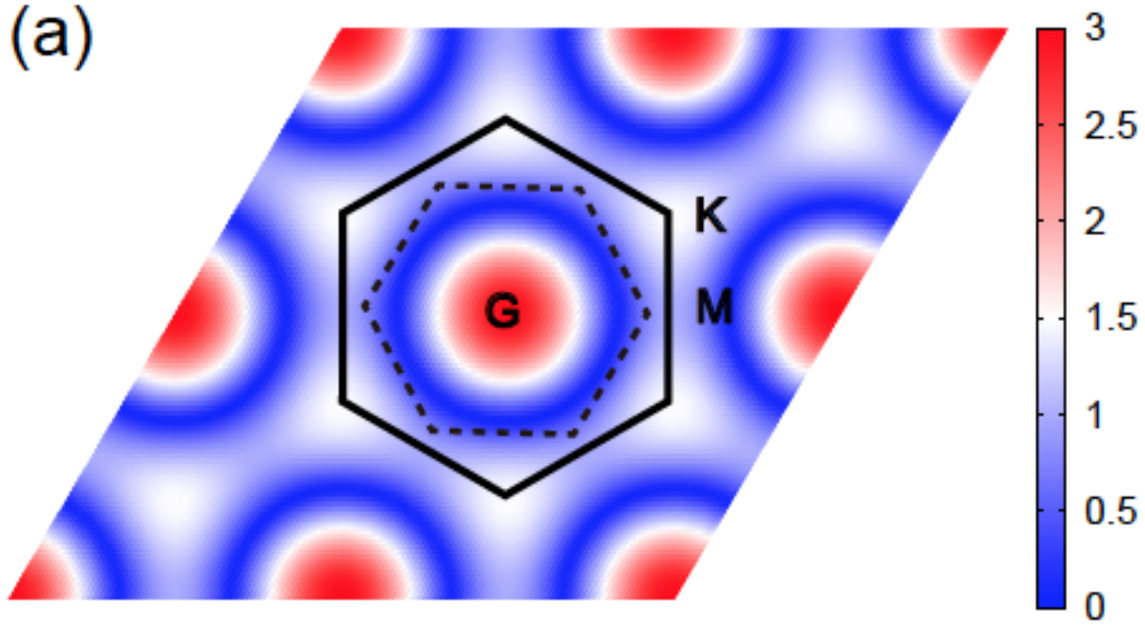


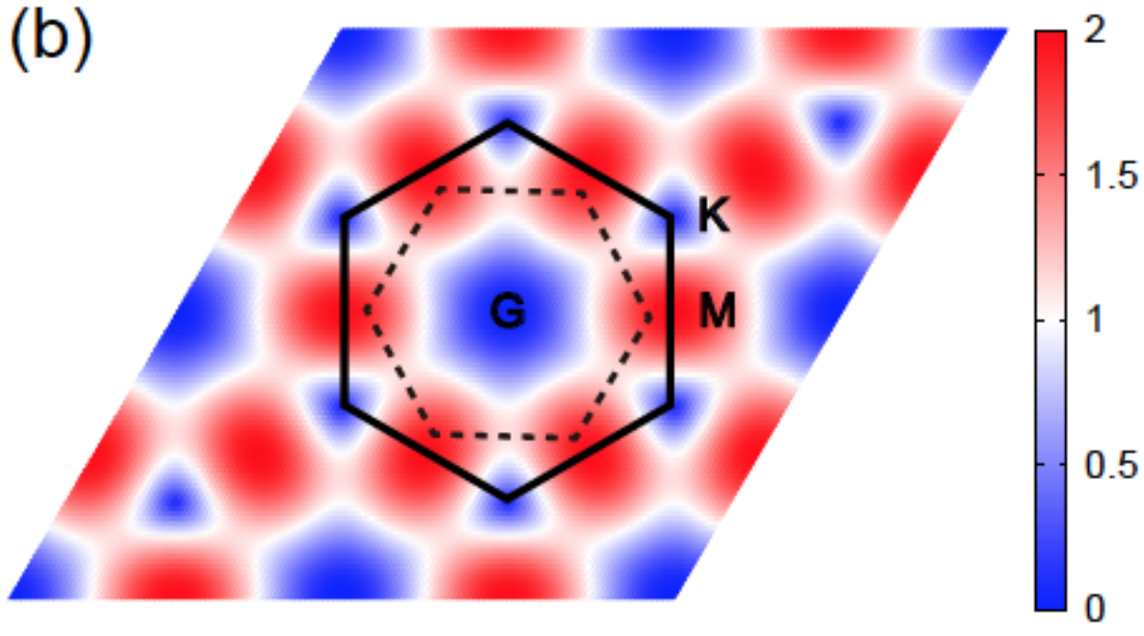
FIG. 3: (a) The band structures of $YNiO_3$ obtained from the first principle calculations and (b) the extracted three bands for the tight binding model. The orbital characters of the bands in (a) are indicated by the different colors specified in the right top corner of the figure.

YNiO3

The isolation of the orbital is protected by symmetry.

Pairing Symmetry and Tc





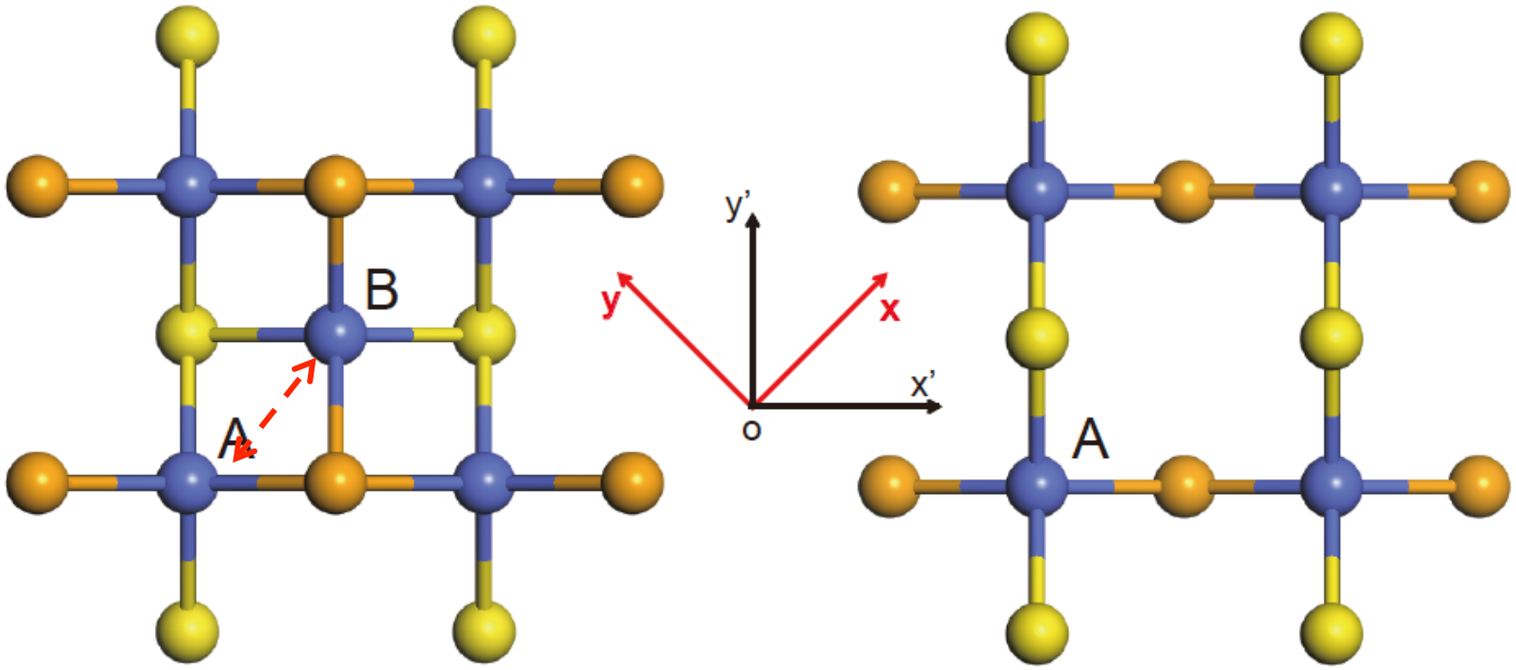
- S-wave has little weight
- d+id has very large weight
- Energy Scale:

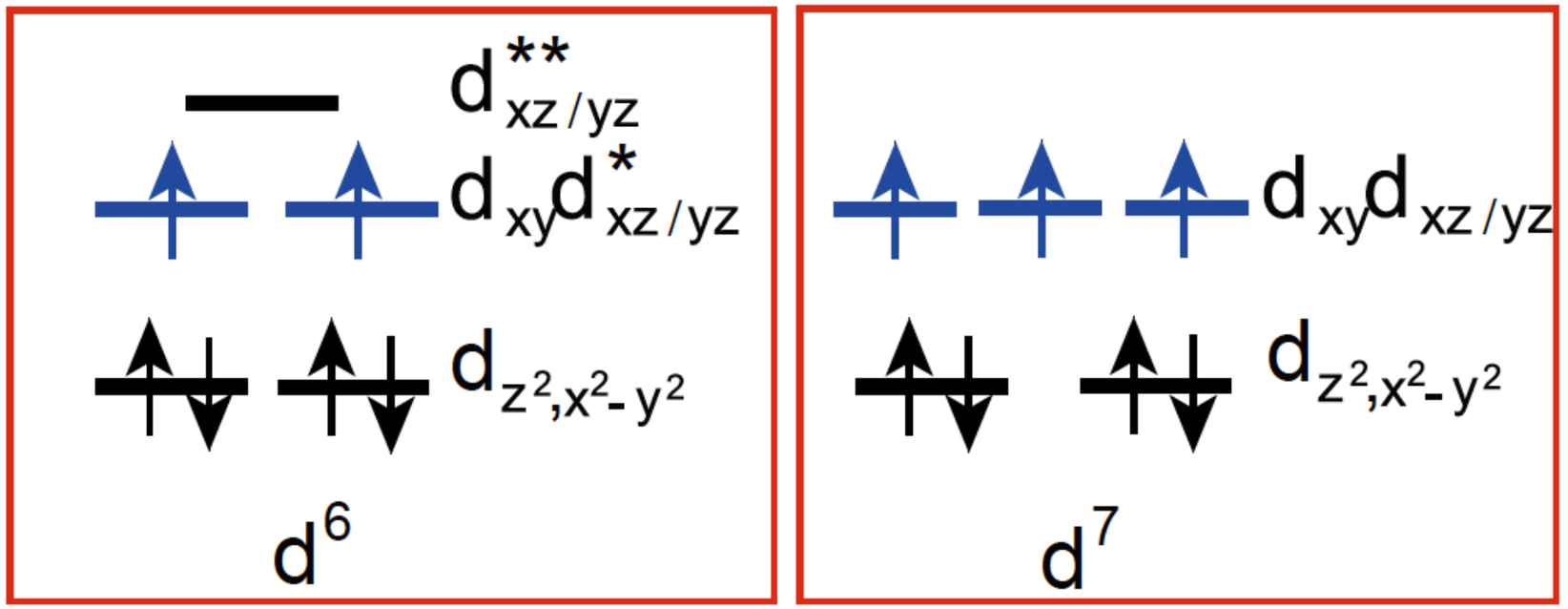
Cuprates

Ni/Co-based

iron-based

Prediction: Possible new high Tc Superconductors(II)



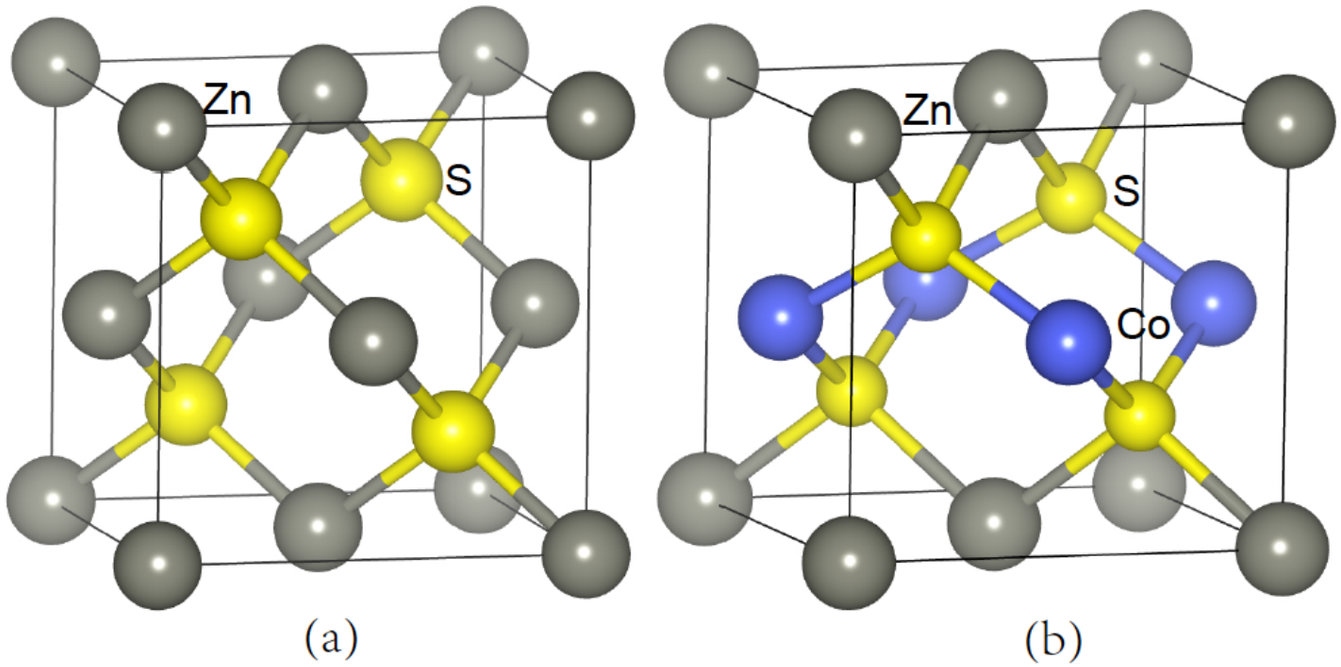


Fe^{2+} Co^{2+}

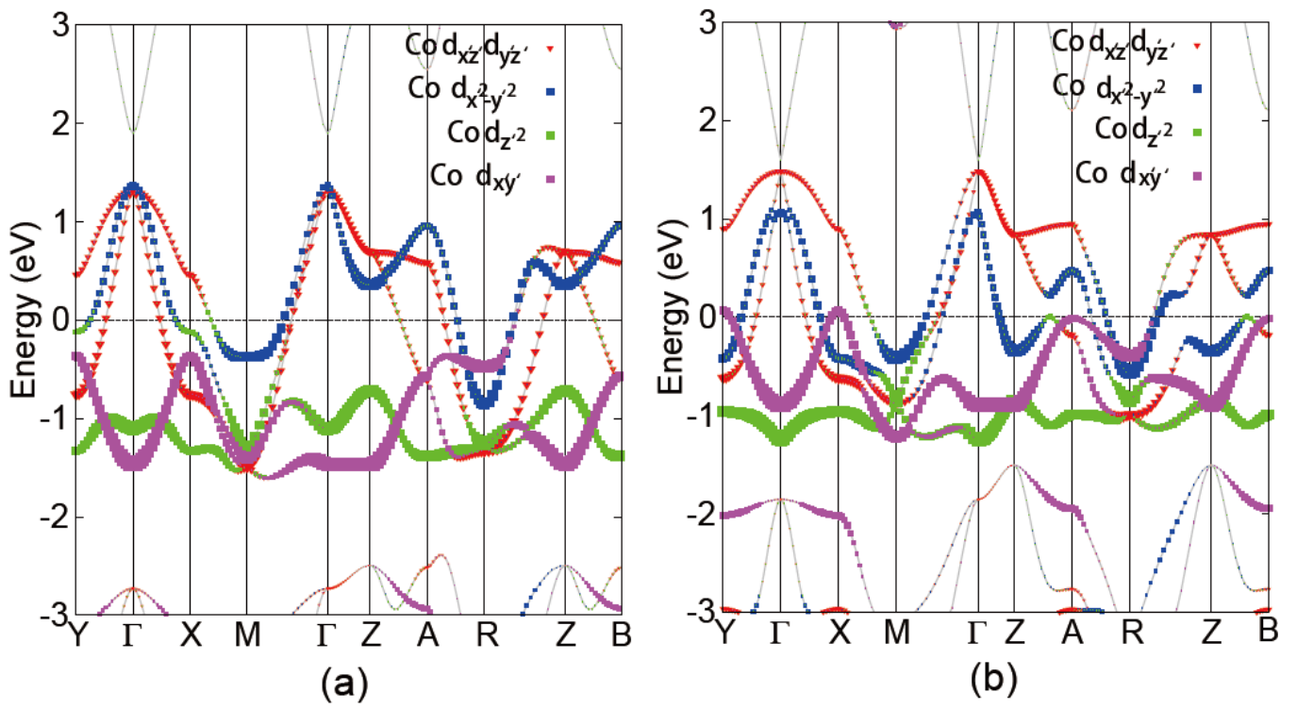
J.Hu and CongCong Le, arxiv: 1611.02835(2016)

Prediction: Possible new high Tc Superconductors(II)

Zn



$ZnCoS_2$

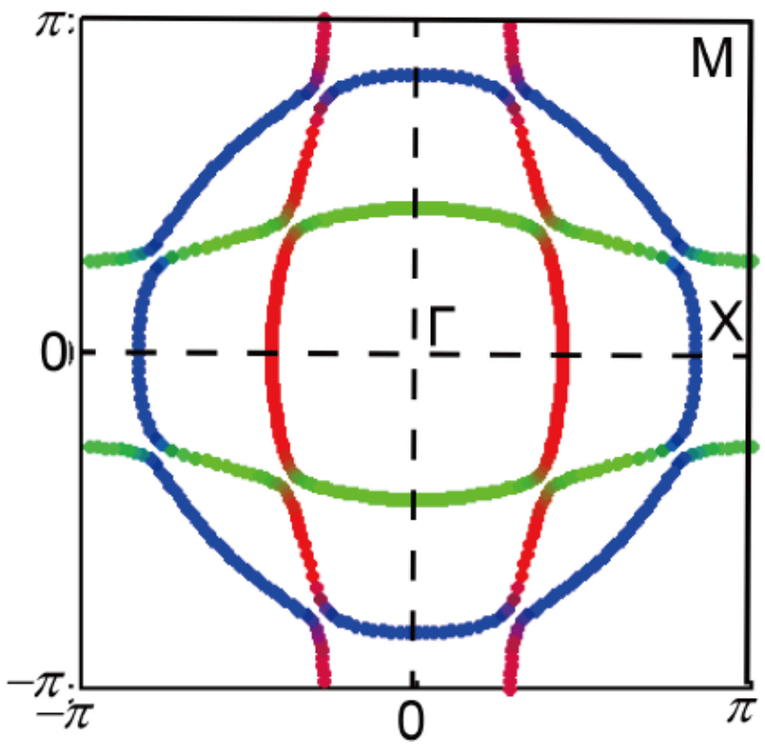


$ZnCo(S,Se)_2$

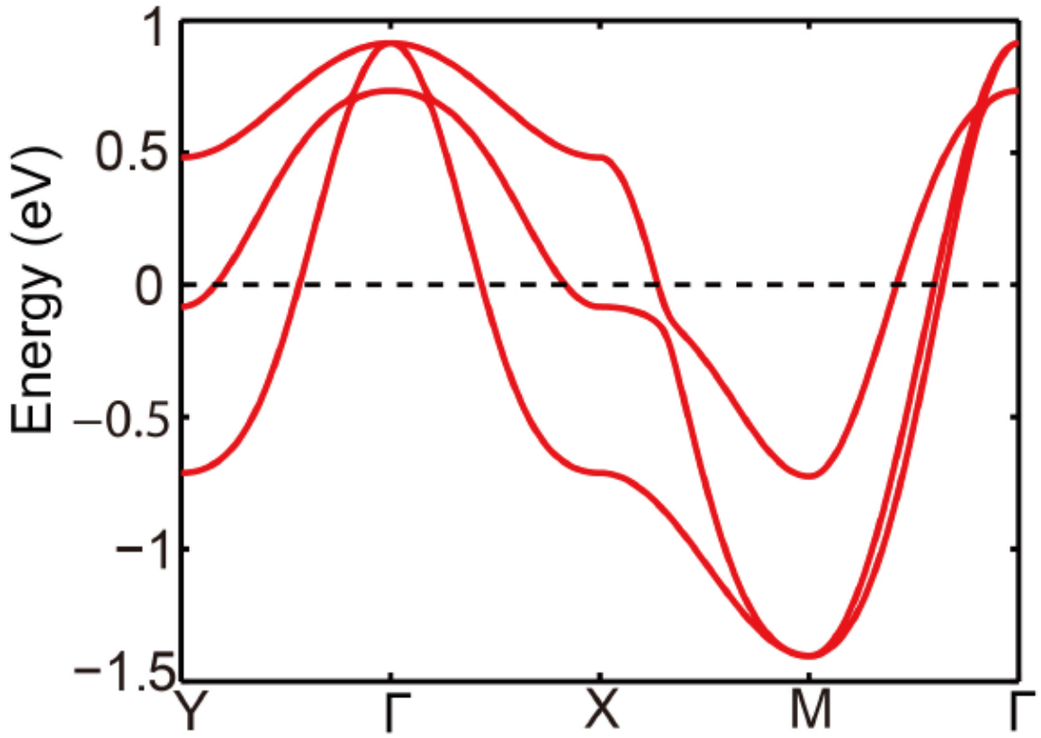
J.Hu and CongCong Le, Sci. Bull. 62 212 (2017)

Prediction: Possible new high Tc Superconductors(II)

A bridge and unifier of cuprates and iron-based SCs



(a)



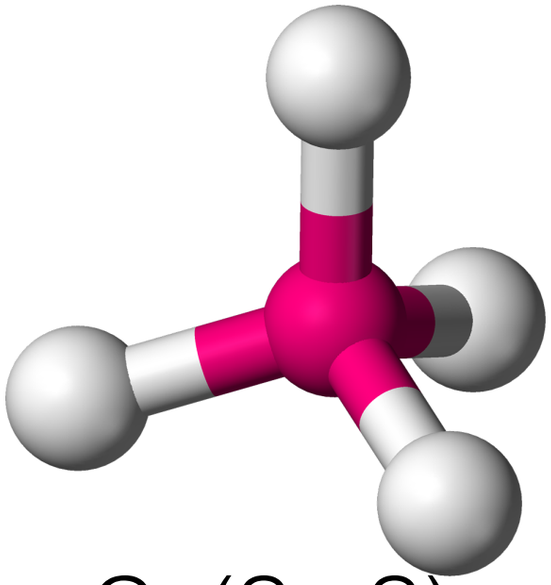
(b)

Prediction:

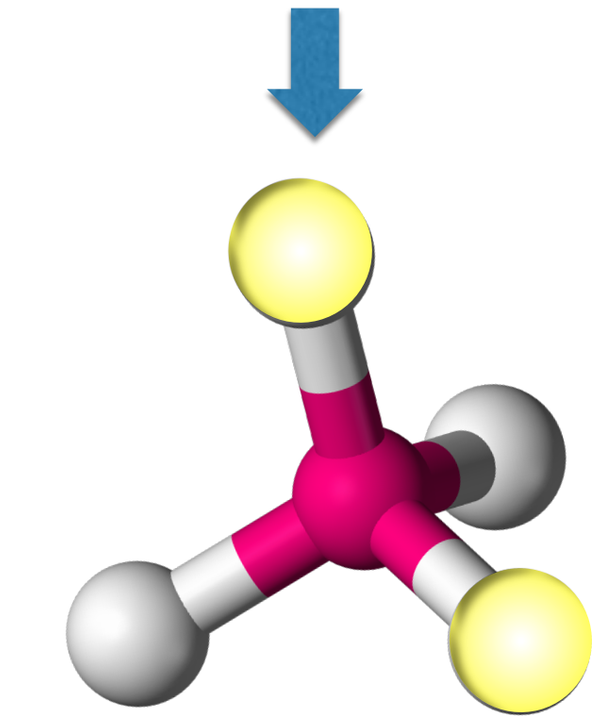
- Similarity to Cuprates: d-wave, Mottness
- Similarity to iron-based superconductors: Multi-orbital, nematicity
- Maximum Tc should be higher than iron-based superconductors

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

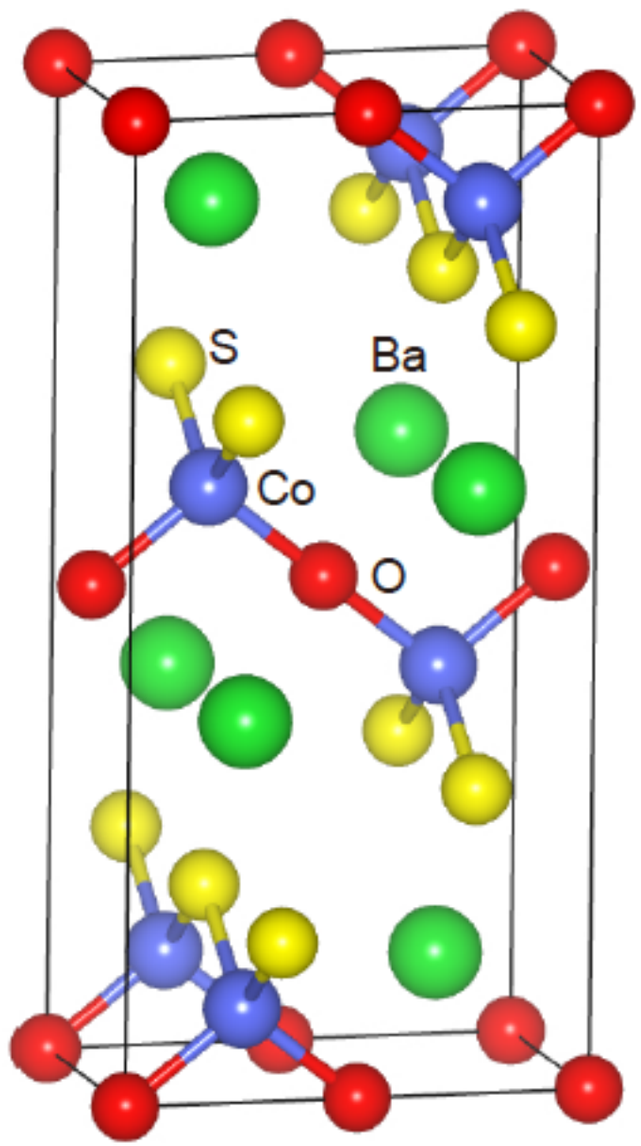
Possible candidates: BaCoSO(Oxychalcogenides)



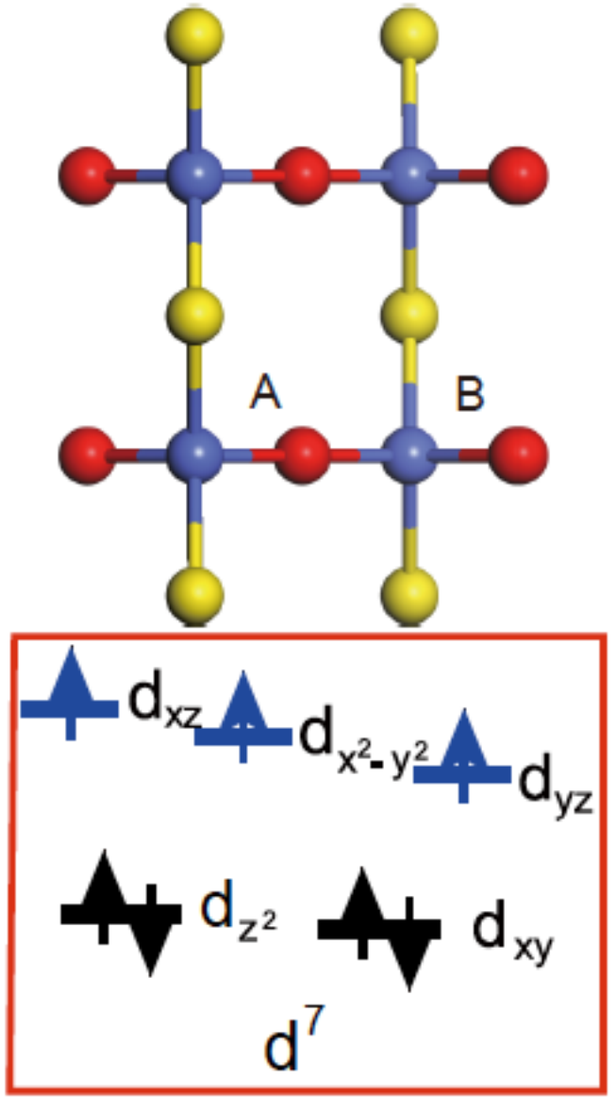
$Co(Se,S)_4$



$Co(Se,S)_2O_2$



(a)

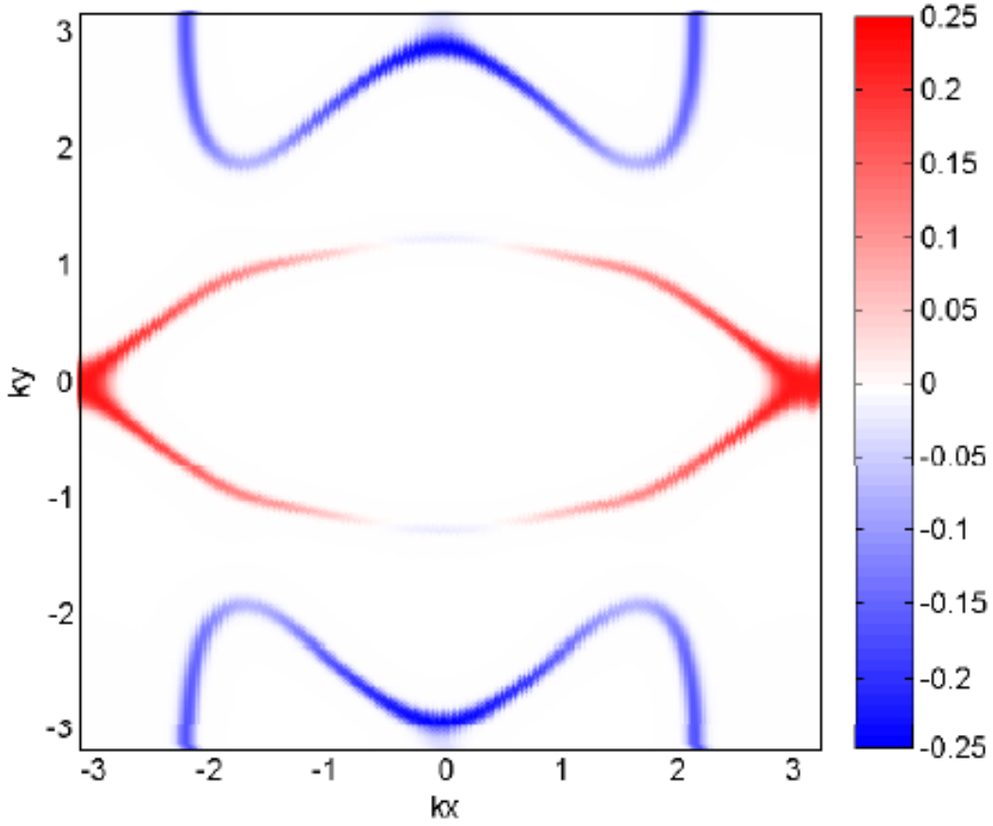


(b)

BaCoSO

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

Co/Ni Oxychalbogenides



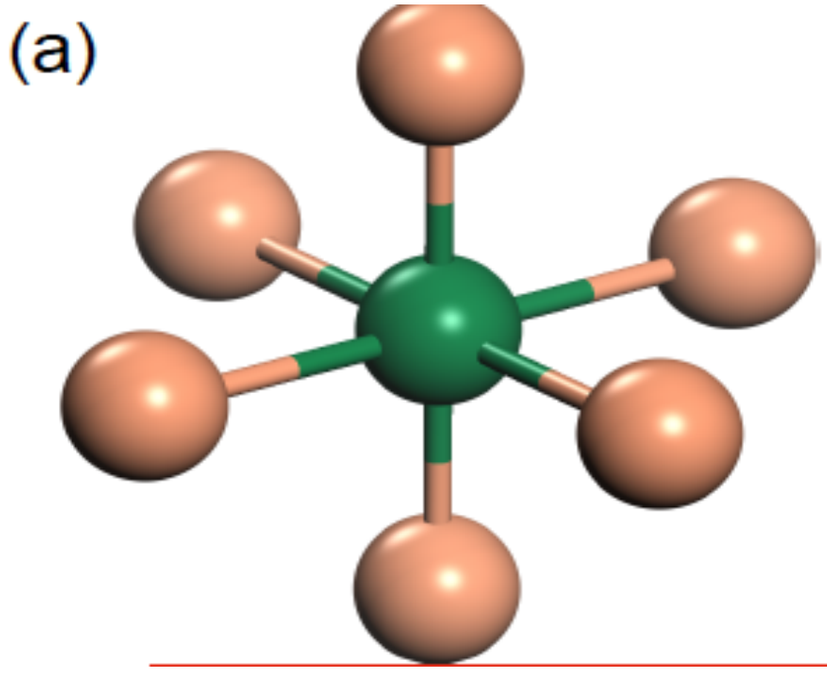
Sign distribution on electron doped Fermi surfaces of BaCoSO

BaCoSO

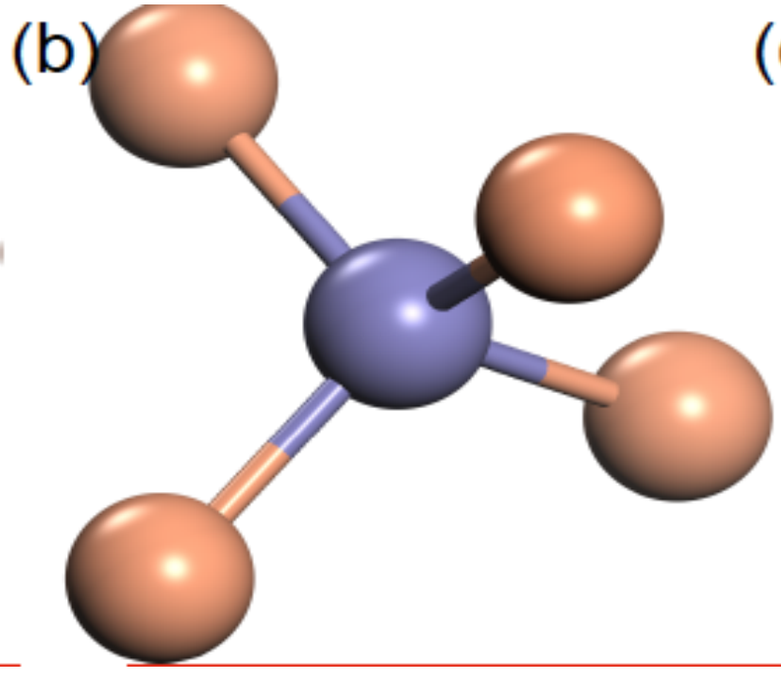
- Corner shared tetrahedra
- d^7 filling configuration: Mott insulator
- AFM Neel temperature over 200K
- Lacking of D_{4h} symmetry classification, but Pairing symmetry resembles both cuprates and iron-based superconductors (nodes and sign change between two pockets)
- Challenge: introduce doping?

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

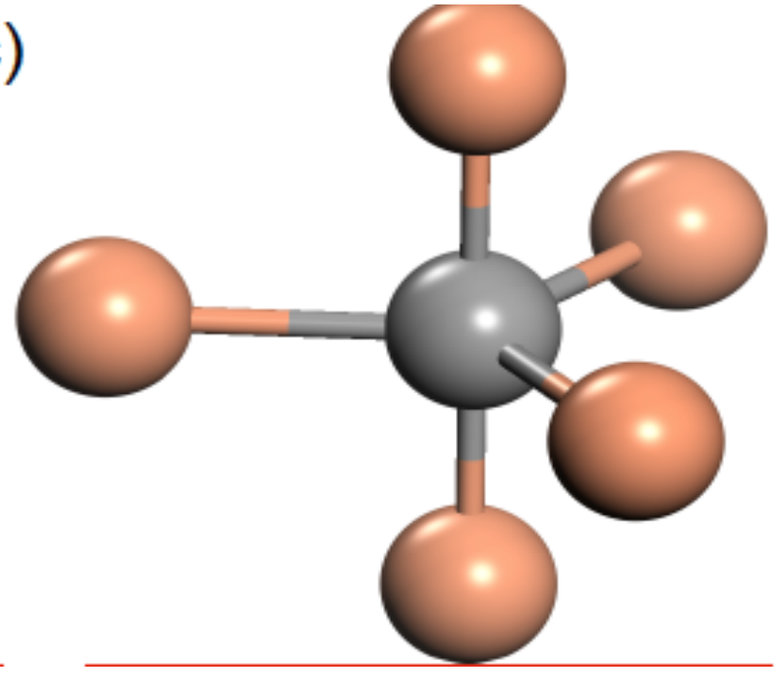
Summary for High Tcs



- 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
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