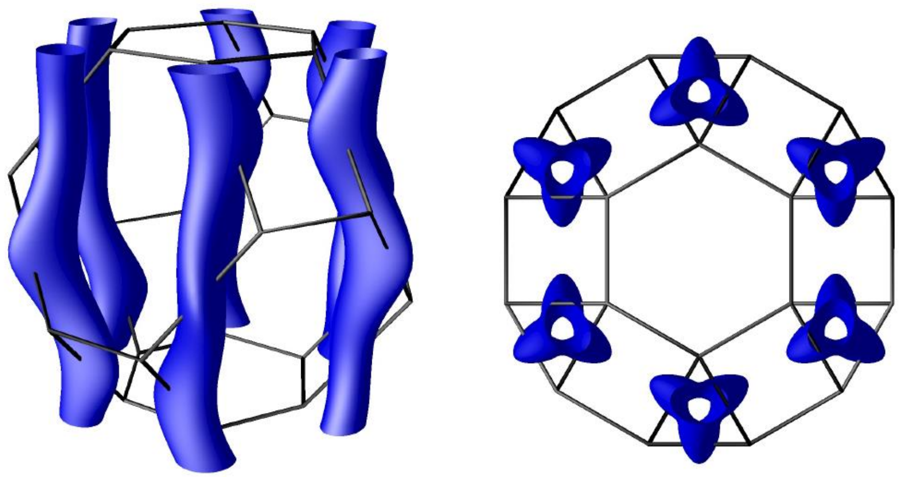
Possible *new* unconventional superconductors?



Roser Valentí
Institute of Theoretical Physics
University of Frankfurt
Germany

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Novel States in Spin-Orbit Coupled Quantum Matter: from Models to Materials

KITP, Santa Barbara July 27-31 2015

Theory:

(Frankfurt)

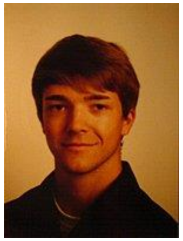
Cesc Salvat-Pujol

Harald Jeschke

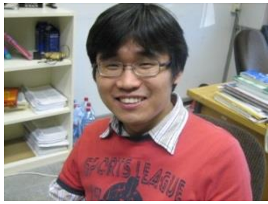
Igor Mazin (Washington DC)

Frank Lechermann (Hamburg)

Ronny Thomale (Wuerzburg)



Mario Fink (Wuerzburg)



Hunpyo Lee (Seoul)

Daniel Guterding

Steffen Backes

Experiment:

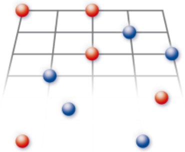
Paul Canfield (Ames Lab)

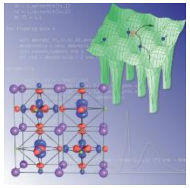
Jochen Mannhart (MPI Stuttgart)

Michael Lang (Frankfurt)

Cornelius Krellner (Frankfurt)

Financial support: German Science Foundation DFG
SFB/TR 49, FOR1346, SPP 1458
A. von Humboldt Foundation

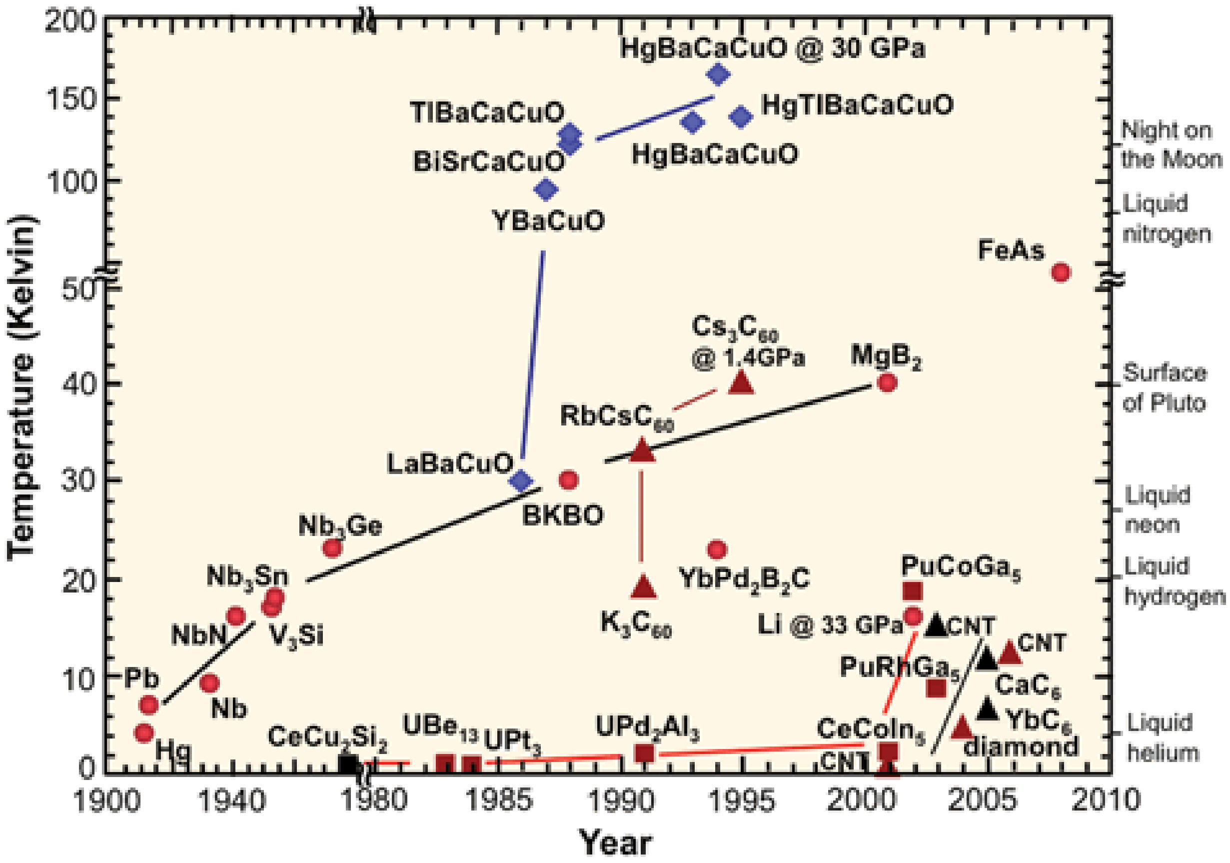




- ***Can we predict new materials with unconventional superconducting properties?***

- ***Theoretical tools?***

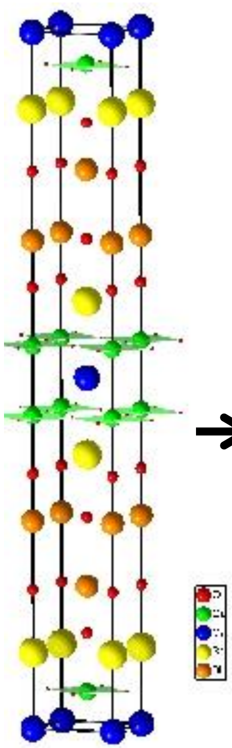
Superconductor families since 1911



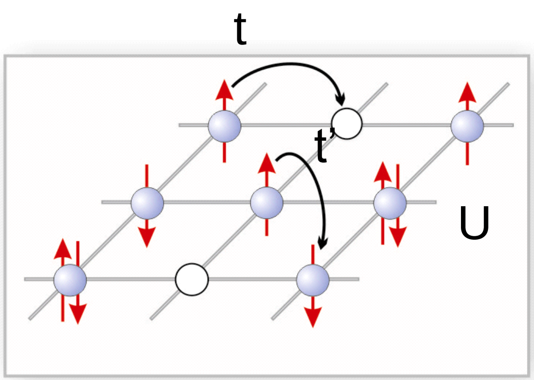
Source: U.S. Department of Energy

high-Tc Cu-based superconductors

- Complex phase diagrams: **High-Tc superconductors**

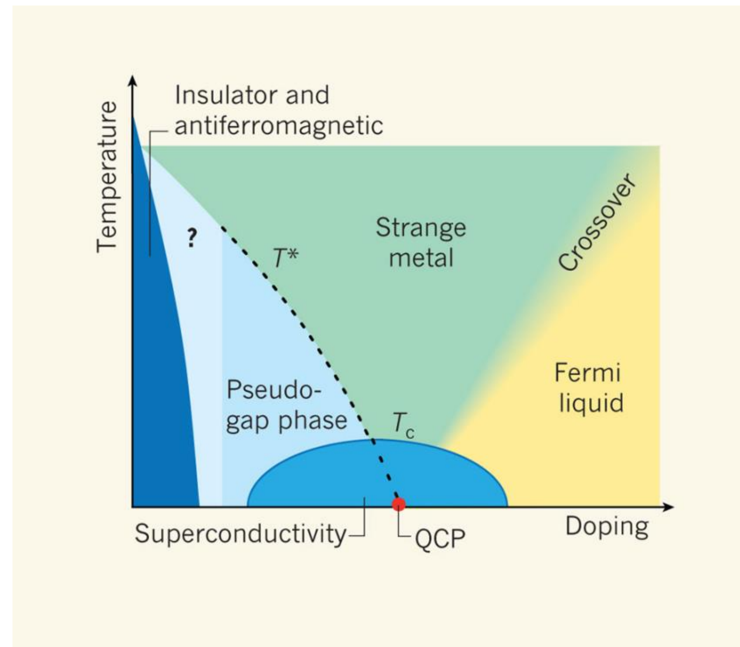


$Bi_2Sr_2CaCu_2O_8$



Hubbard model

$$H_{\text{Hubbard}} = t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



*C. Varma Nature **468**, 184 (2010)*

Competing ordered phases

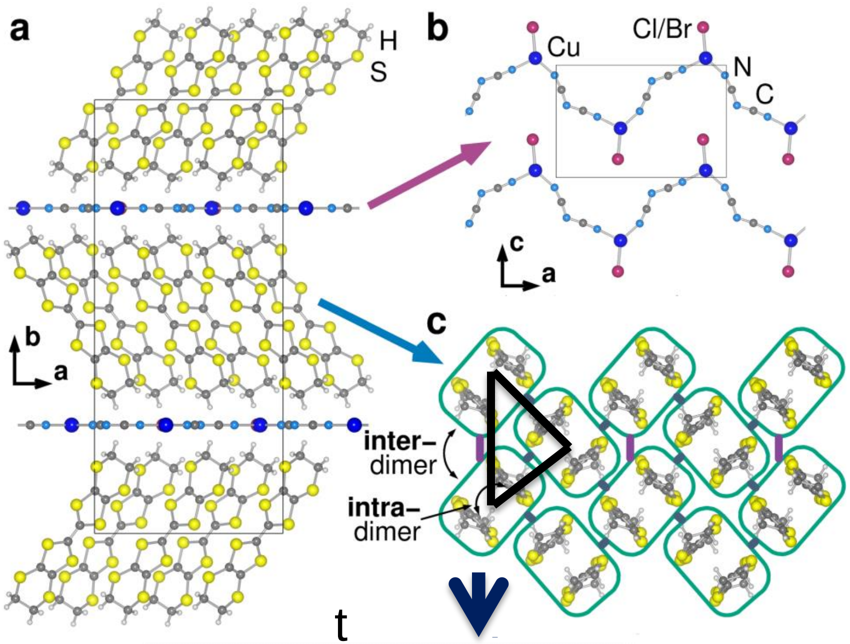
Correlation:

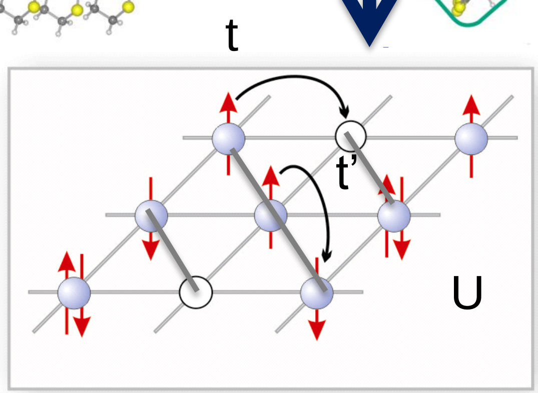
- Mott transition: metal - insulator

Organic superconductors

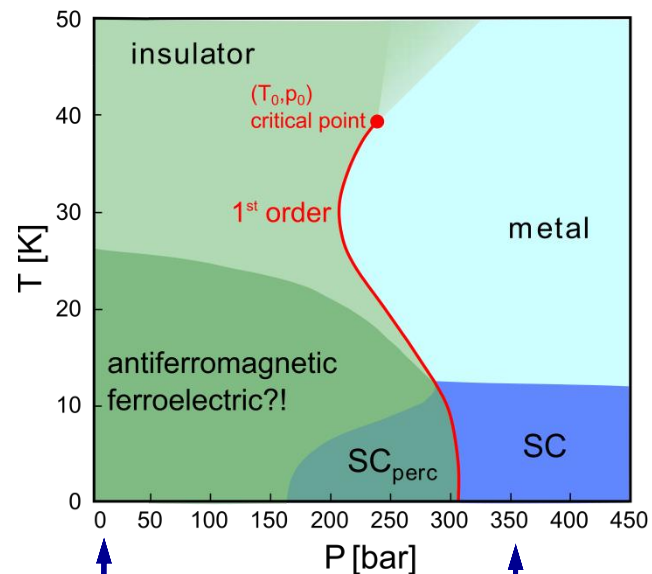
κ-$(BEDT\text{-}TTF)_2X$

X^-





$[(BEDT\text{-}TTF)_2]^+$



X = $Cu[N(CN)_2]Cl$ $Cu[N(CN)_2]Br$

*Shimizu et al. PRL **91,** 107001 (2003)*

*Lunkenheimer et al. Nat. Mat. **11**, 755 (2012)*

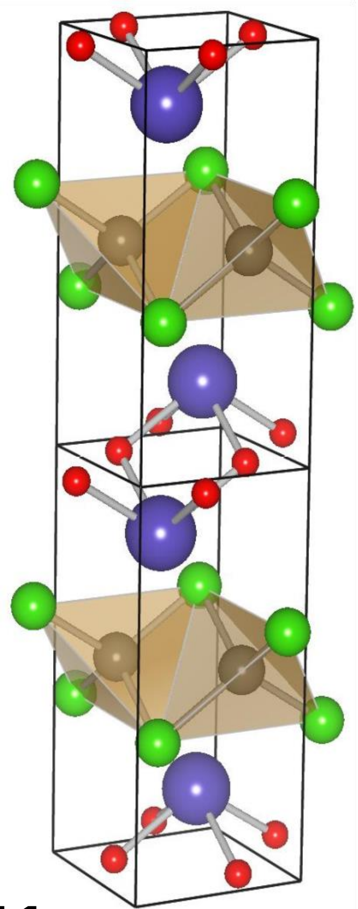
Competing ordered phases

Correlation:

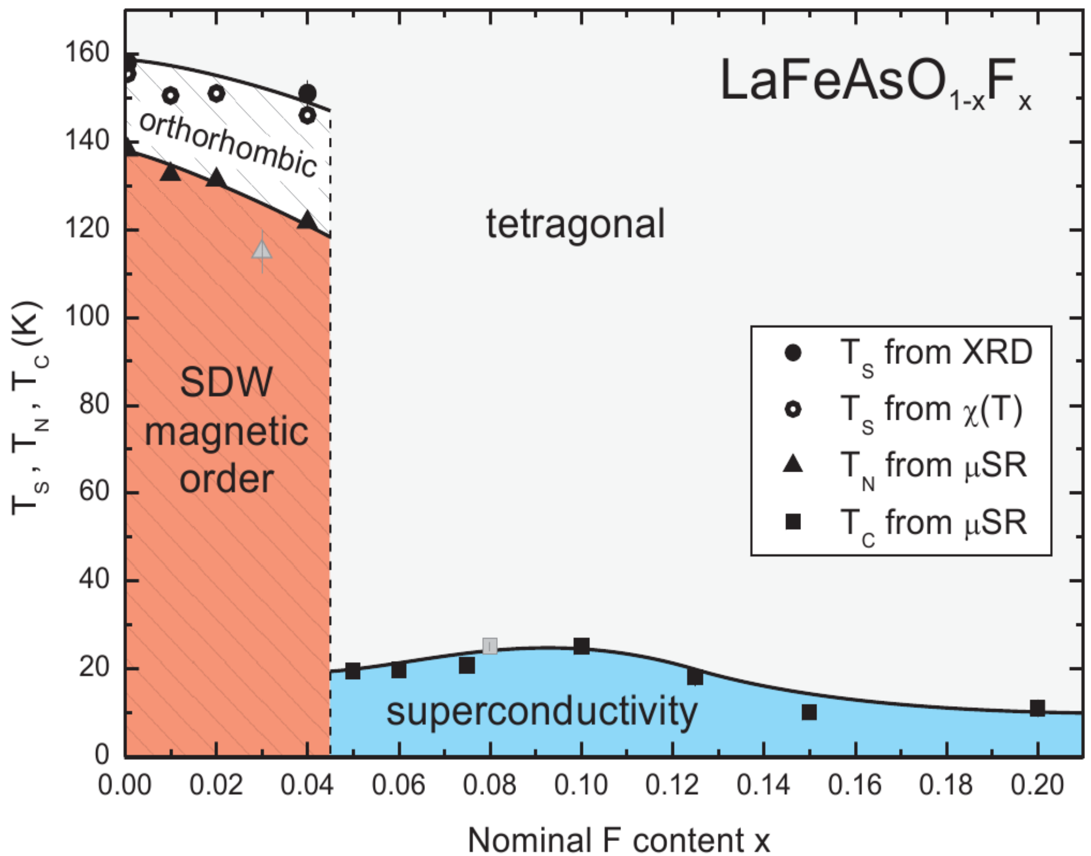
- Mott transition:
  metal - insulator

2008: Fe-based superconductors

- T_c= 26K



1111



*Kamihara et al. JACS **130**, 3296 (2008)*
*Luetkens et al. Nat. Mat. **8**, 305 (2009)*

Competing ordered phases

- Families:

pnictides

1111 *RE*O(F)FeAs (T_{cmax}=55K SmOFeAs)

122 *AE*Fe_2As_2 (T_{cmax}=38K BaFe2As2 upon doping)

111 *AM*FeAs (T_{cmax}= 18K LiFeAs)

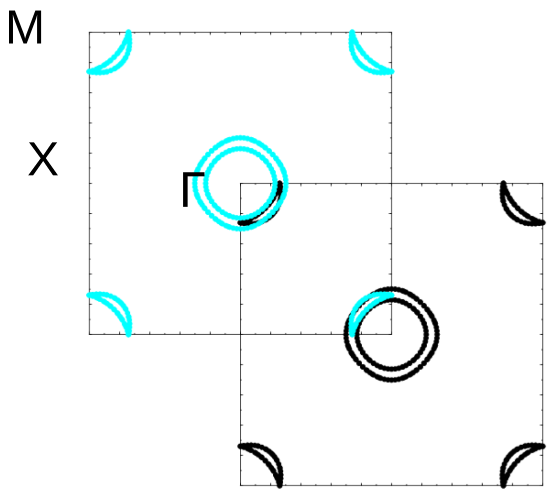
chalcogenides

11 FeSe (T_{cmax}= 8K)

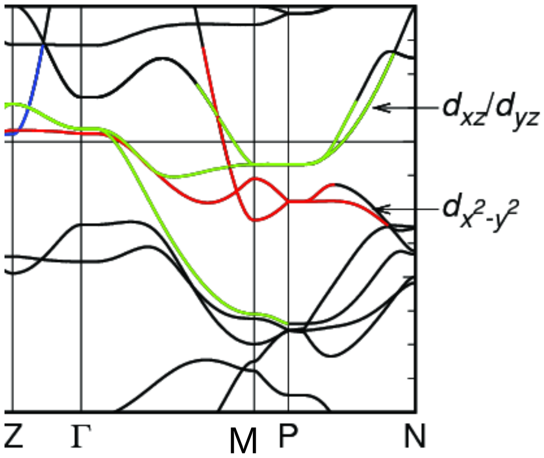
$A_xFe_{2-z}Se_2$ (A=K, Cs,Rb) T_{cmax}=30K → Under P Tc ↑

- FeSe under pressure (T_{cmax} =37K)
- FeSe with molecular intercalation (T_{cmax}=44K)
- FeSe monolayer on $SrTiO_3$ (T_{cmax} ~ 100K?)

- nesting-driven magnetism:

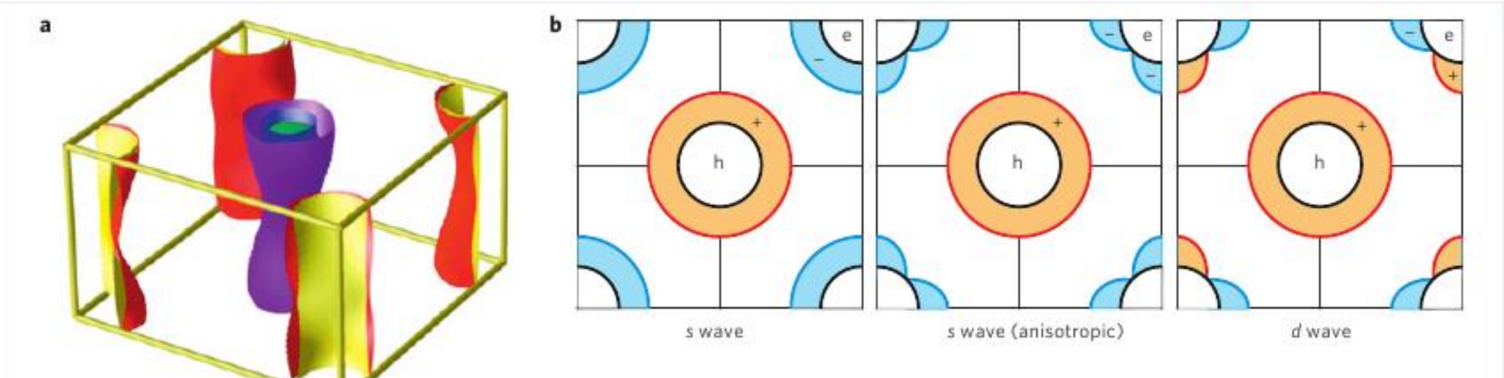


- multiorbital systems:



Fink et al. PRB (2009) ARPES
Ruillier-Alberque et al. PRL (2012) Transport

- superconducting order parameter:

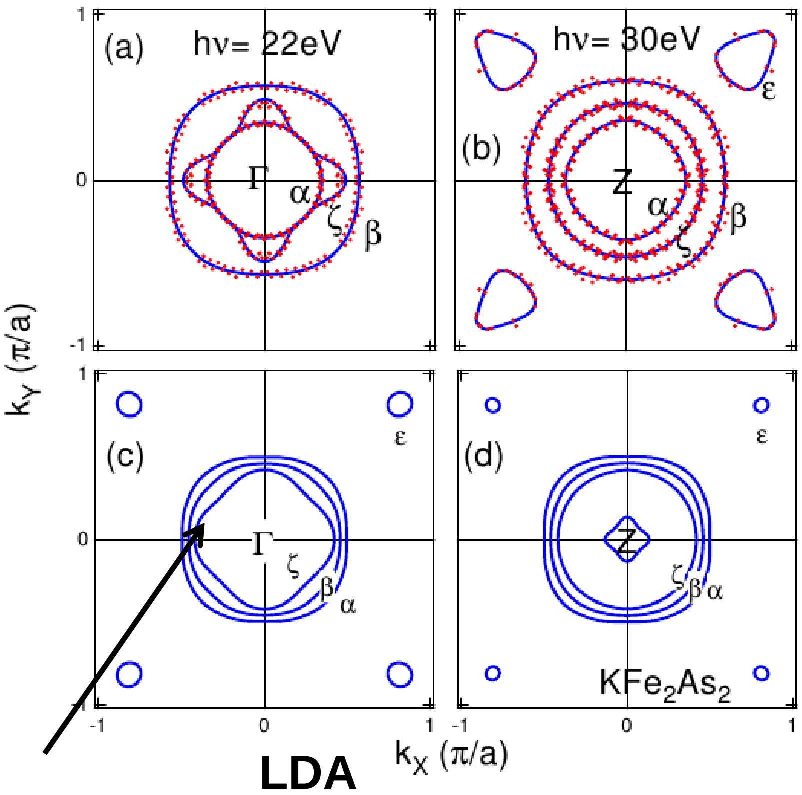


Correlation effects?

Paglione, Greene Nat. Phys. ***6****, 645 (2010)*
Hirschfeld, Korshunov, Mazin Rep. Prog. Phys. ***74****, 124508 (2011)*

Traces in experiment:

- ARPES: renormalization of bands



High sensitivity to structural details

KFe_2As_2

ARPES: Yoshida et al. arXiv:1205.6911
*Okazaki et al. Science **337**, 1304 (2012)*
*dHvA: Terashima et al. PRB **87**, 224512 (2013)*

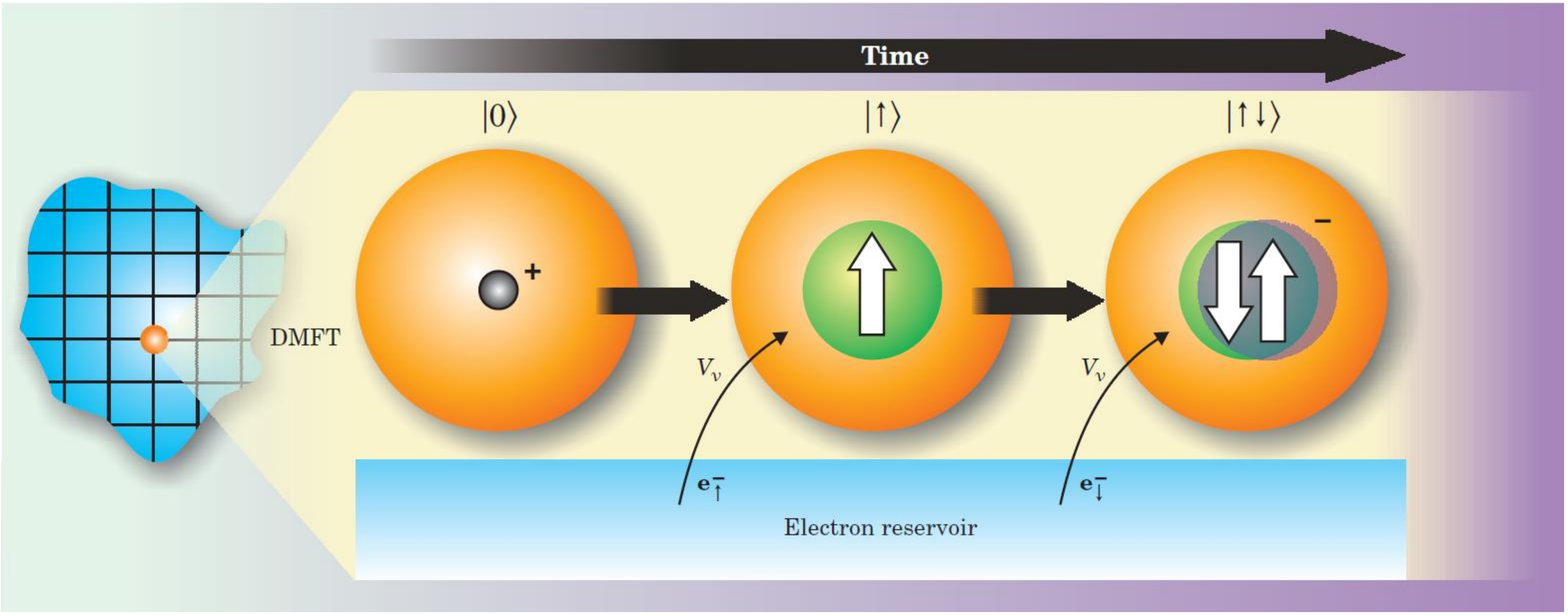
ARPES, de Haas van Alphen, optical conductivity, thermodynamics,…

microscopic description correlated systems

Ab initio DFT + Many-body methods

One-electron approximation

Density Functional theory + **Dynamical Mean Field Theory (DMFT)**



Extensions:
Dynamical Cluster Approximation (DCA), Cluster DMFT (CDMFT)

*G. Kotliar, D. Vollhardt Phys. Today **57**, 53 (2004)*

*A. Georges, G. Kotliar PRB **45**, 6479 (1992)*

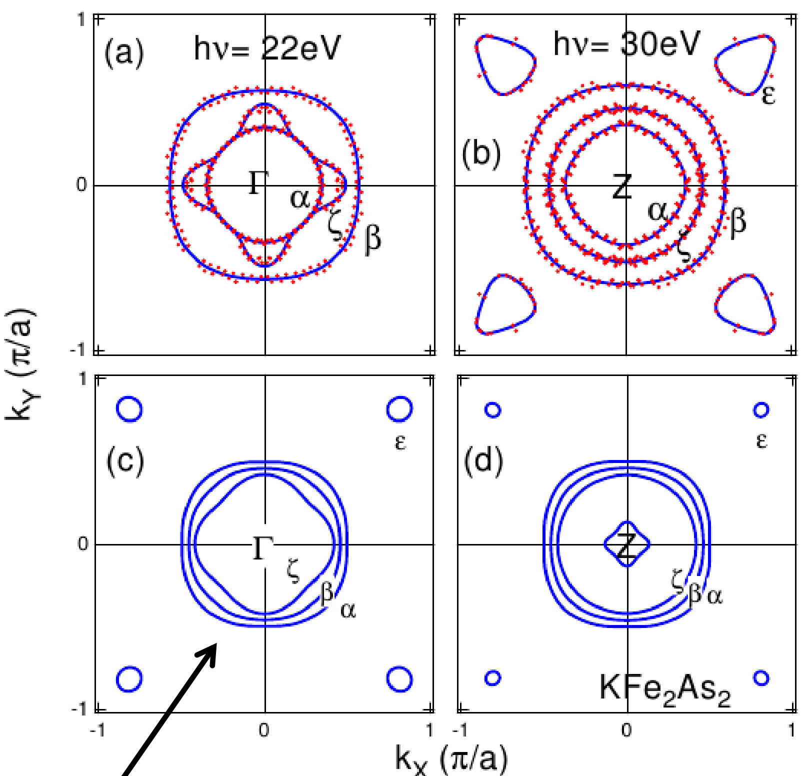
*W. Metzner, D. Vollhardt PRL **62**, 324 (1989)*

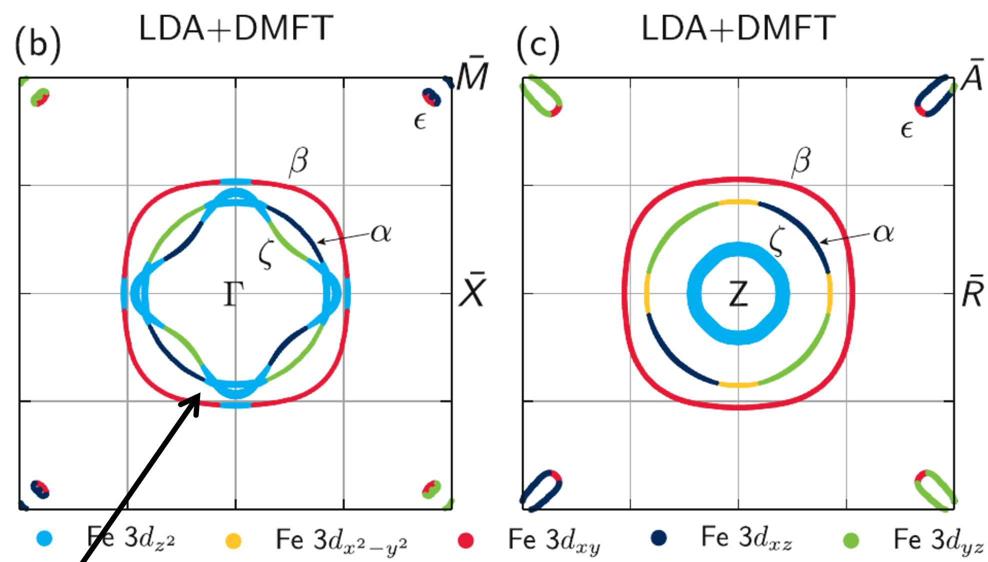
*T. Maier, M. Jarrell, T. Pruschke, H. Hettler RMP **77**, 1027 (2006)*

Extreme hole-doped case KFe2As2 DFT ←→ LDA+DMFT

U= 4 eV J= 0.8 eV T=290K

ARPES





(change of topology)

Backes, Guterding, Jeschke, RV NJP ***16****, 083025 (2014)*

Guterding, Backes, Jeschke, RV PRB ***91****, 140503(R) (2015)*

ARPES: Yoshida et al. arXiv:1205.6911

Okazaki et al. Science ***337****, 1304 (2012)*

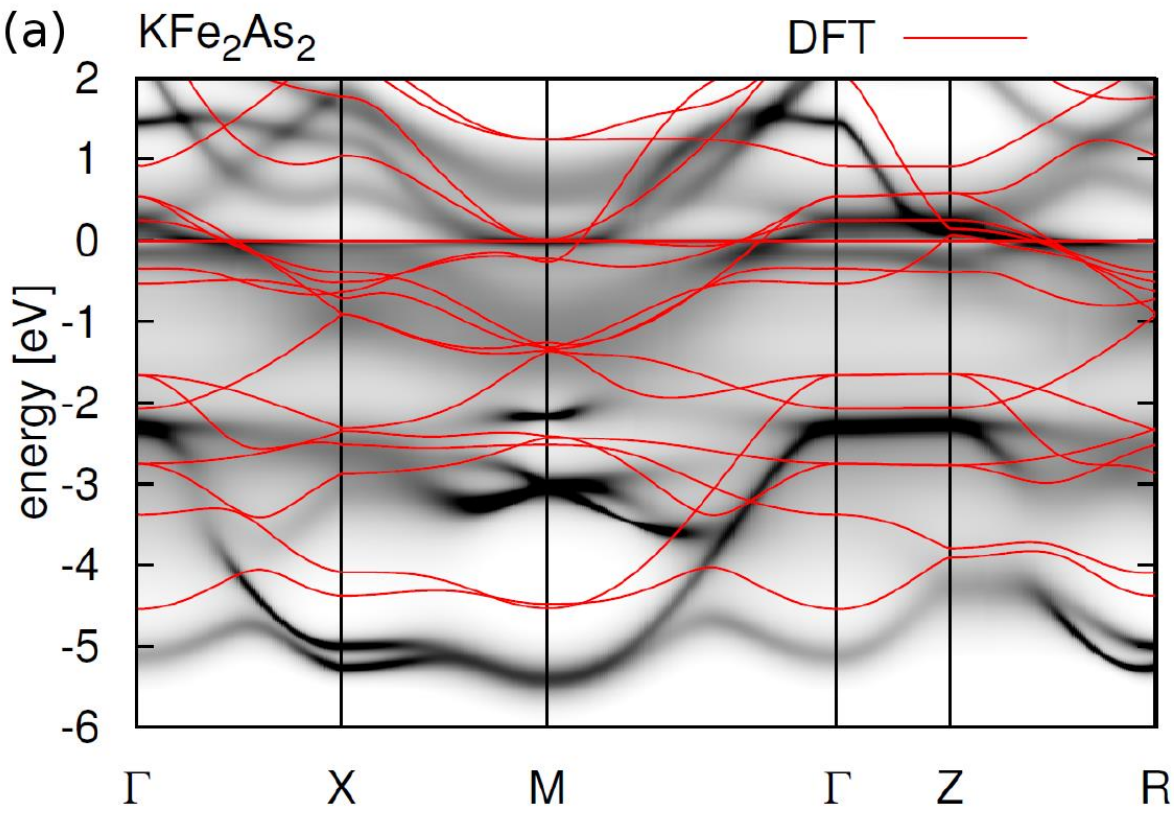
dHvA: Terashima et al. PRB ***87****, 224512 (2013)*

LDA

High sensitivity to structural details

Extreme hole-doped case **KFe2As2** **DFT ←→ LDA+DMFT**

LDA+DMFT: shaded region



LDA+DMFT:

main features of correlated metals

Multiorbital physics

Hund's ←→ Mott's physics

*Yin, Haule, Kotliar Nat. Mater. **10**, 932 (2011)*
*Medici, Mravlje, Georges PRL **107**, 256401 (2011)*
*Hung et al. PRB **91,** 195149 (2015)*
Fanfarillo, Bascones arXiv:1501.04607
Backes, Jeschke, RV arXiv:1507. 07914

New high-Tc superconductors?

- **where to look?**

→ **Nb_3Sn, MgB_2** : robust superconductivity in stochiometric compounds

↑

search easy

→ **Cu-based, FeAs-based** : only superconducting when modified (selective doping, pressure)

↑ (near competing phases: **magnetism**)

search harder

P. C. Canfield Nat. Mat. ***10****, 259 (2011)*

- **where to look?**

→ **Nb_3Sn, MgB_2** : robust superconductivity in stochiometric compounds

↑

search easy

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↑ (near competing phases: **magnetism**)

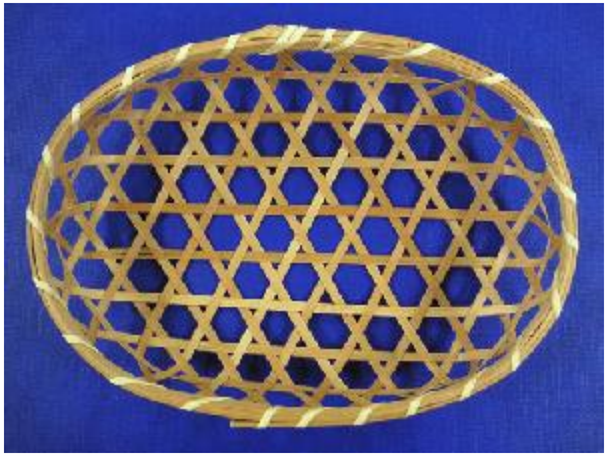
search harder

Prediction of a new unconventional superconductor (using graphene physics)

Prediction of a correlated Dirac metal: f-wave superconductivity ?

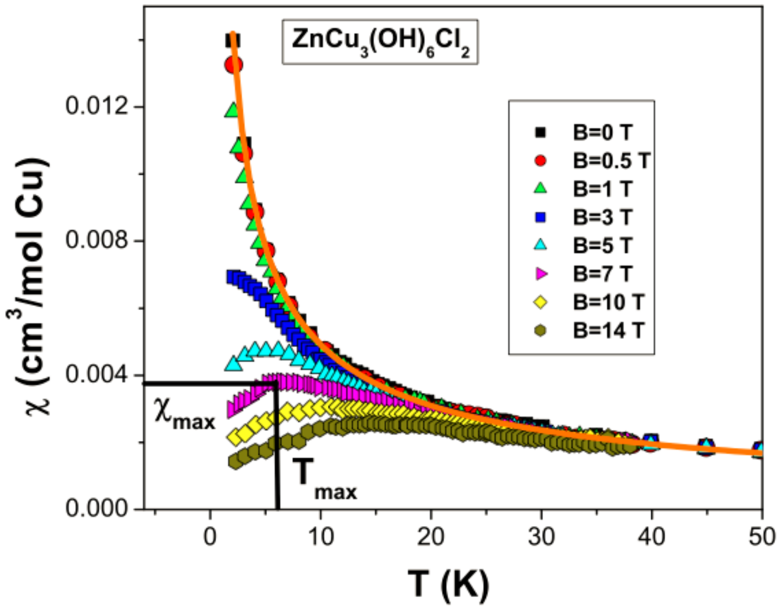
Starting system: **Herbertsmithite**
$ZnCu_3(OH)_6Cl_2$

Kagome lattice of spin ½ Cu



F. Bert, P. Mendels JPSJ ***79****, 011001 (2010)*

J.S. Helton et al. PRL ***104****, 147201 (2010)*



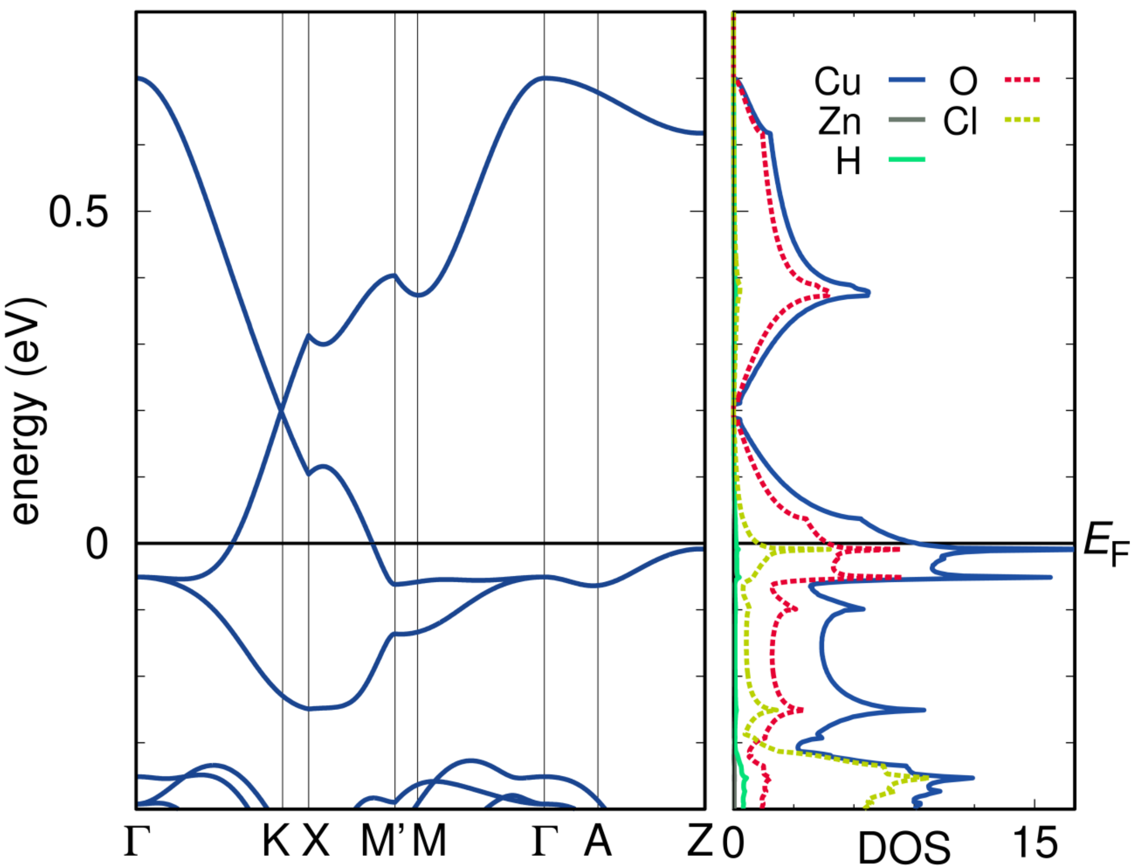
spin liquid!

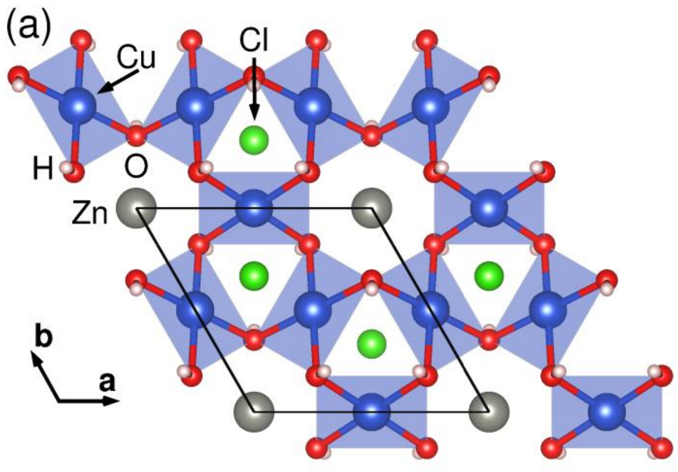
Starting system: **Herbertsmithite**
$ZnCu_3(OH)_6Cl_2$

Kagome lattice of spin ½ Cu

n=1

DFT-GGA calculation/FPLO basis





J_1 = 182 K
J_3 = 3 K
J_5 = -0.4 K

Mott insulator

spin liquid

in a LDA+U calculation a gap opens at Ef

Salvat-Pujol, Jeschke, RV PRB ***88****, 075106 (2013)*

Herbertsmithite

Starting system: **Herbertsmithite**
$ZnCu_3(OH)_6Cl_2$

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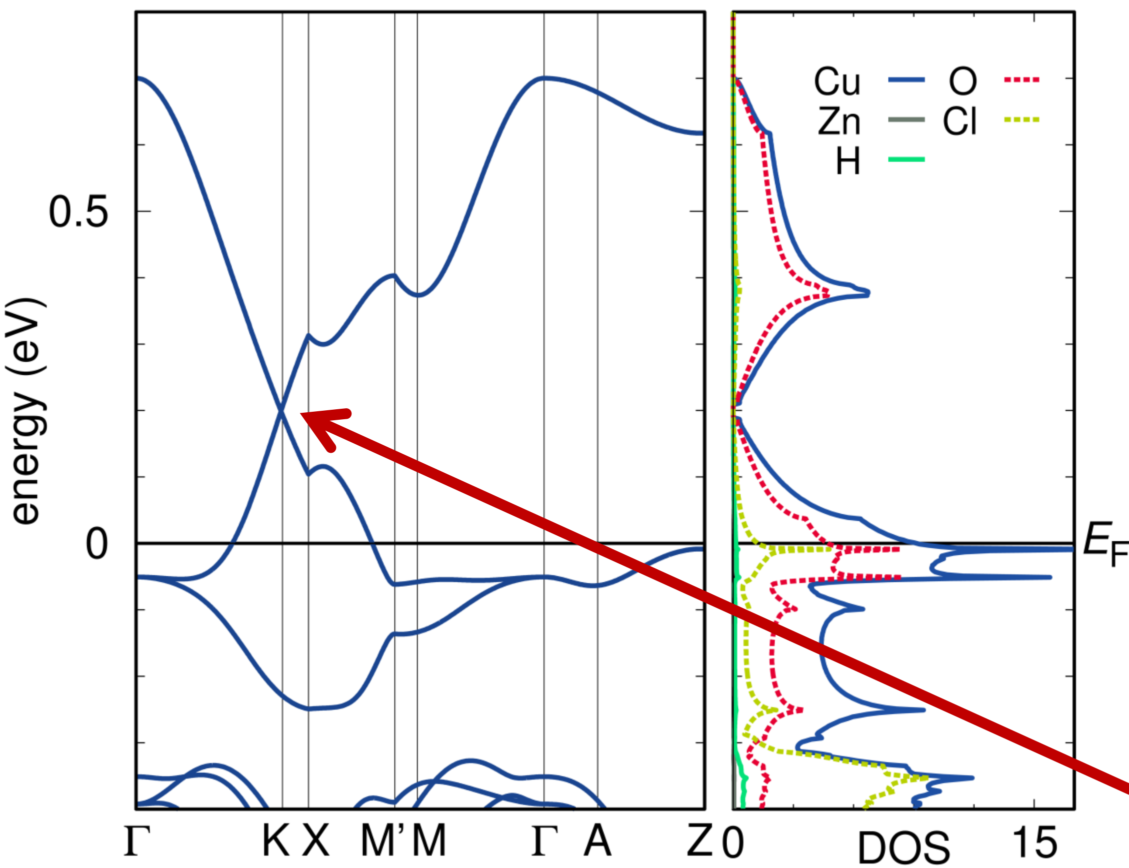
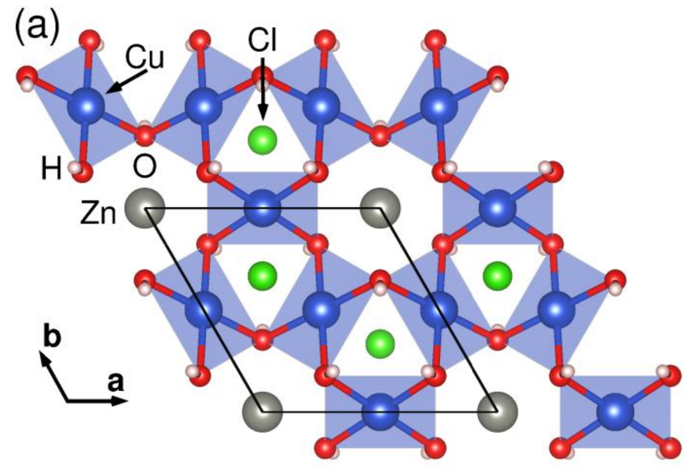
n=1

DFT-GGA calculation/FPLO basis





J_1 = 182 K
J_3 = 3 K
J_5 = -0.4 K

Dirac point

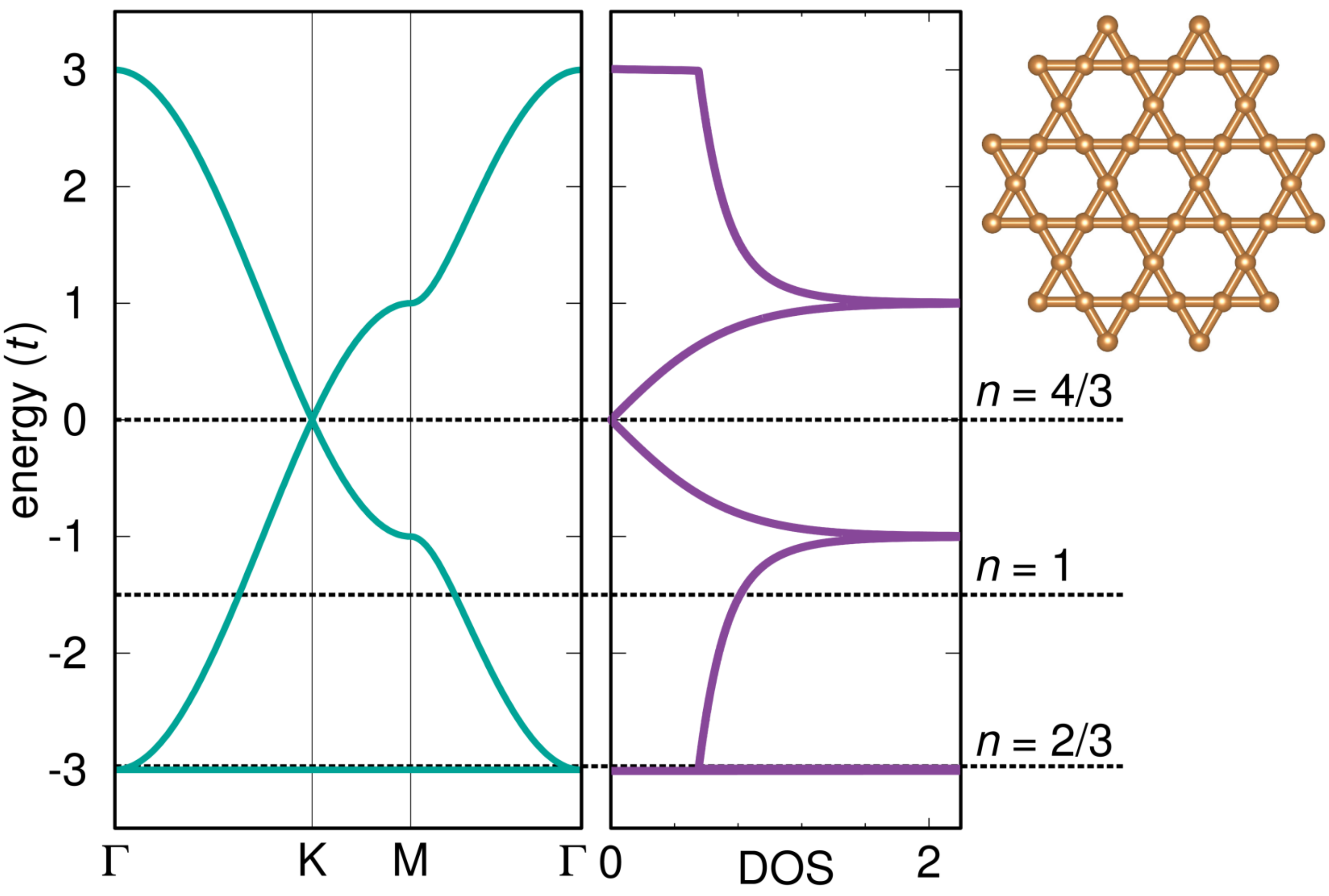
Mott insulator

spin liquid

in a LDA+U calculation a gap opens at Ef

Salvat-Pujol, Jeschke, RV PRB ***88****, 075106 (2013)*

2D nearest-neighbor tight-binding Kagome



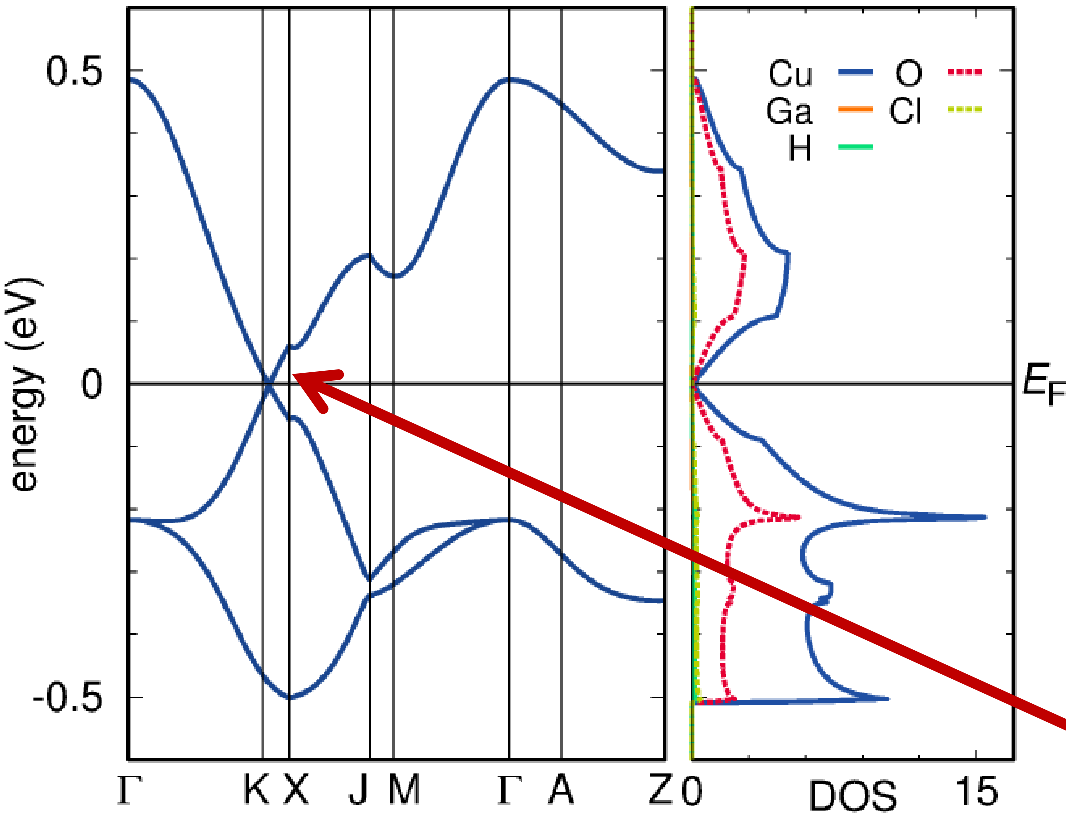
Ga-doped Herbertsmithite

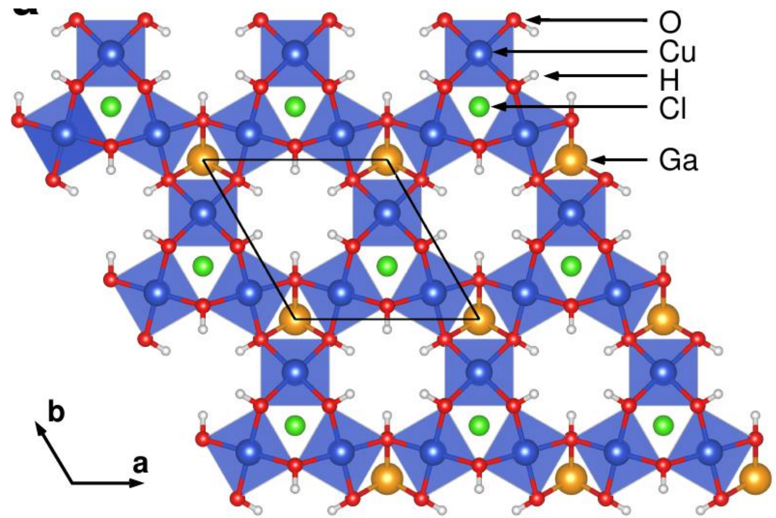
Proposal: **Ga-doped Herbertsmithite**
$GaCu_3(OH)_6Cl_2$

Kagome lattice of spin ½ Cu

n=4/3

DFT-GGA calculation/FPLO basis





Correlated Dirac metal

Dirac point

(protected by hexagonal symmetry)

properties?

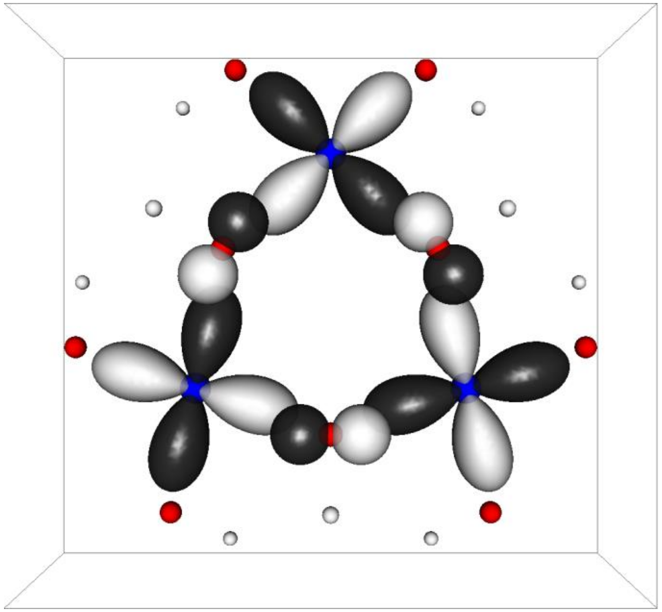
Mazin,Jeschke,Lechermann,Lee,Fink,Thomale,RV Nat. Comm. ***5****, 261 (2014)*

Proposal: **Ga-doped Herbertsmithite**

$GaCu_3(OH)_6Cl_2$

Kagome lattice of spin ½ Cu

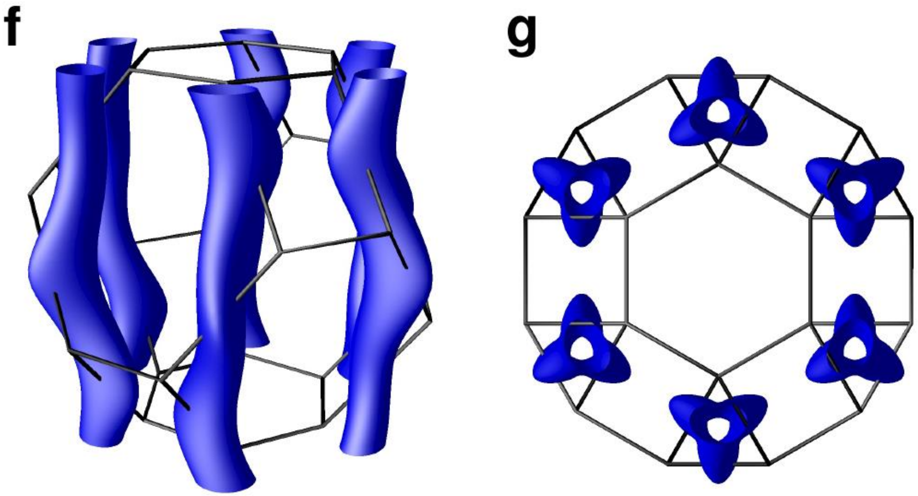
n=4/3



- states at the Fermi level formed by strongly correlated Cu dx^2-y^2 orbitals

effect of correlations?

Fermi surface at E=-60meV



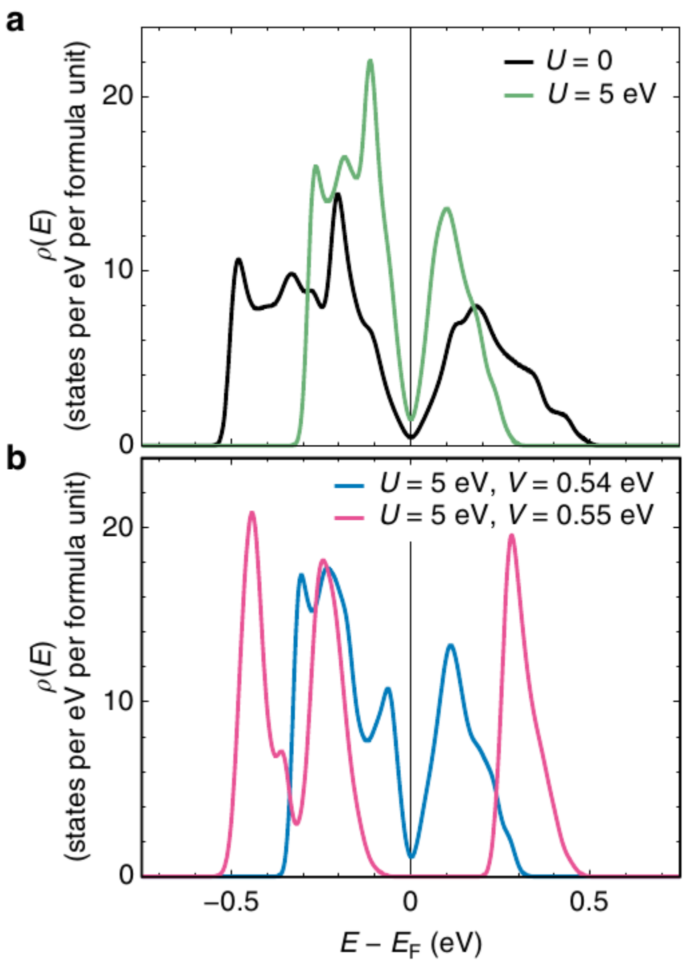
Mazin,Jeschke,Lechermann,Lee,Fink,Thomale,RV Nat. Comm. ***5****, 261 (2014)*

Ga-doped Herbertsmithite: possible instabilities?

Kagome lattice of spin ½ Cu n=4/3

Mott-Hubbard instability?

Dynamical cluster approximation *on the* ***DFT-derived*** *extended Hubbard model*



- U is insufficient to drive the system insulator.

Charge-ordering instability?

- only for V> 2t the system charge orders

(beyond the regime for Ga-doped Herbertsmithite)

→ the system remains metallic !

Mazin,Jeschke,Lechermann,Lee,Fink,Thomale,RV Nat. Comm. ***5****, 261 (2014)*

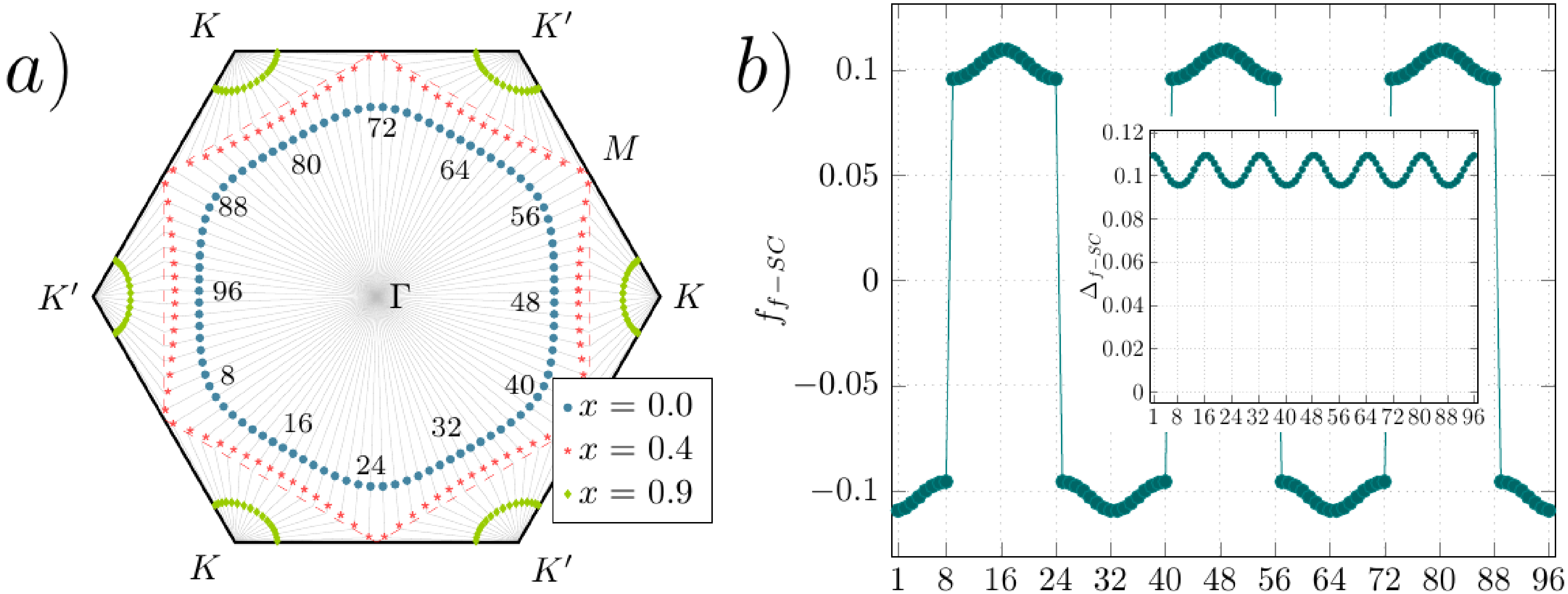
Prediction of a correlated Dirac metal: f-wave superconductivity ?

Proposal: **Ga-doped Herbertsmithite** $Zn_{1-x}Ga_xCu_3(OH)_6Cl_2$

Kagome lattice of spin ½ Cu

n=4/3

If Ga substitution is incomplete→ may expect sizable coupling to spin fluctuations

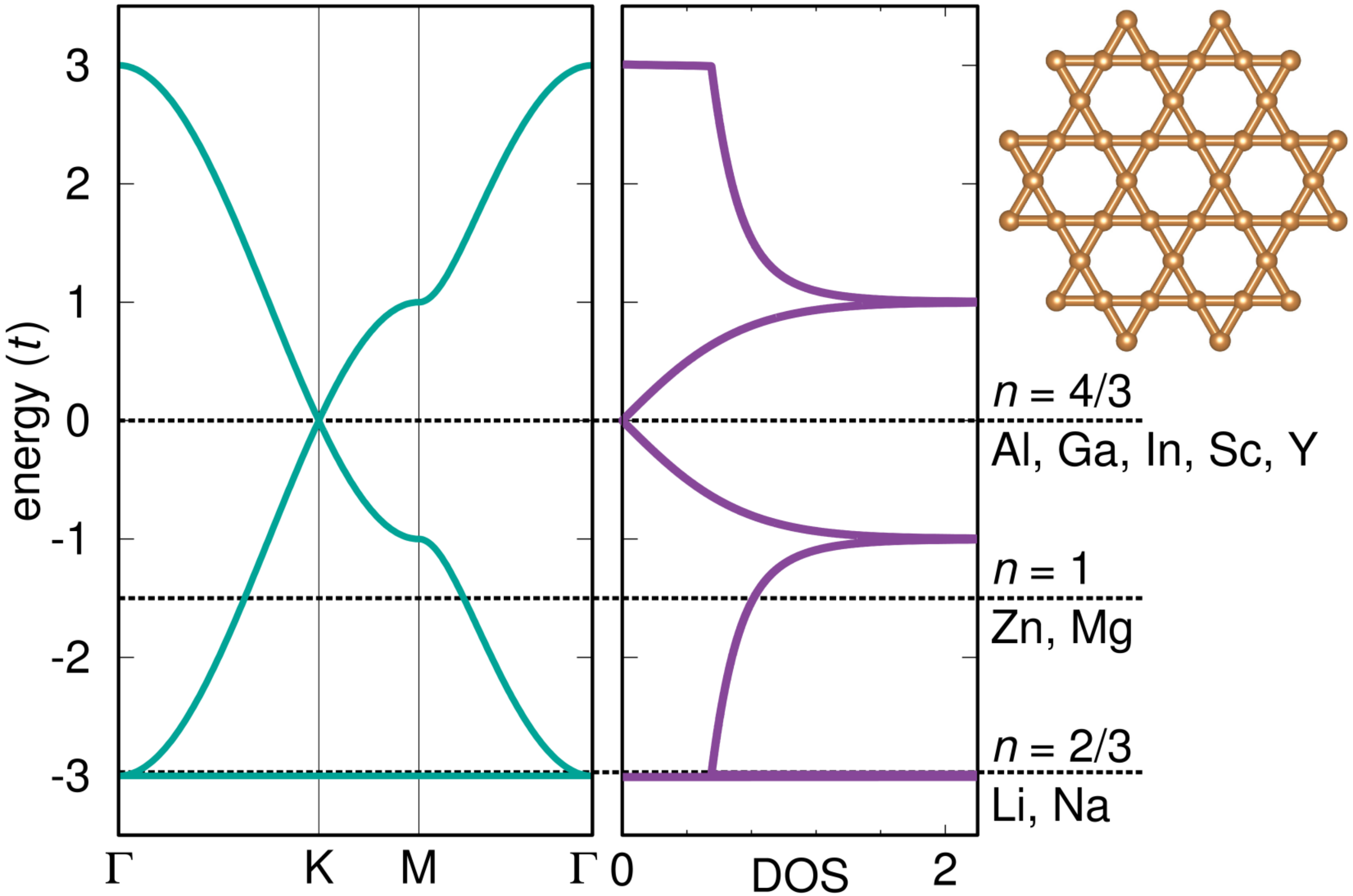


Multisublattice fRG.
Around n=4/3→ nodeless f-wave superconductivity

Estimate Tc=30K-60K

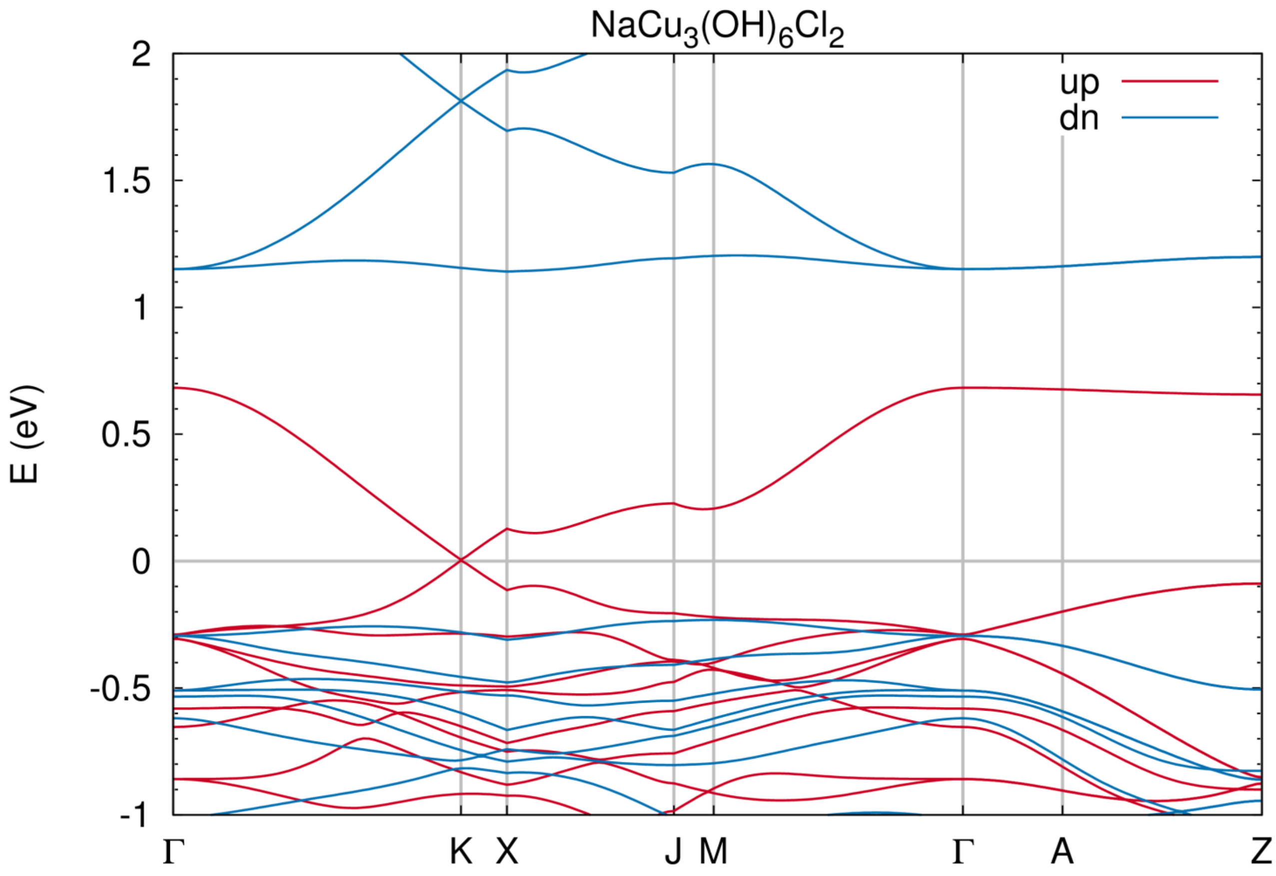
*Mazin,Jeschke,Lechermann,Lee,Fink,Thomale,RV Nat. Comm. **5**, 261 (2014)*

Other fillings than 3/4



Guterding, Jeschke, RV in preparation

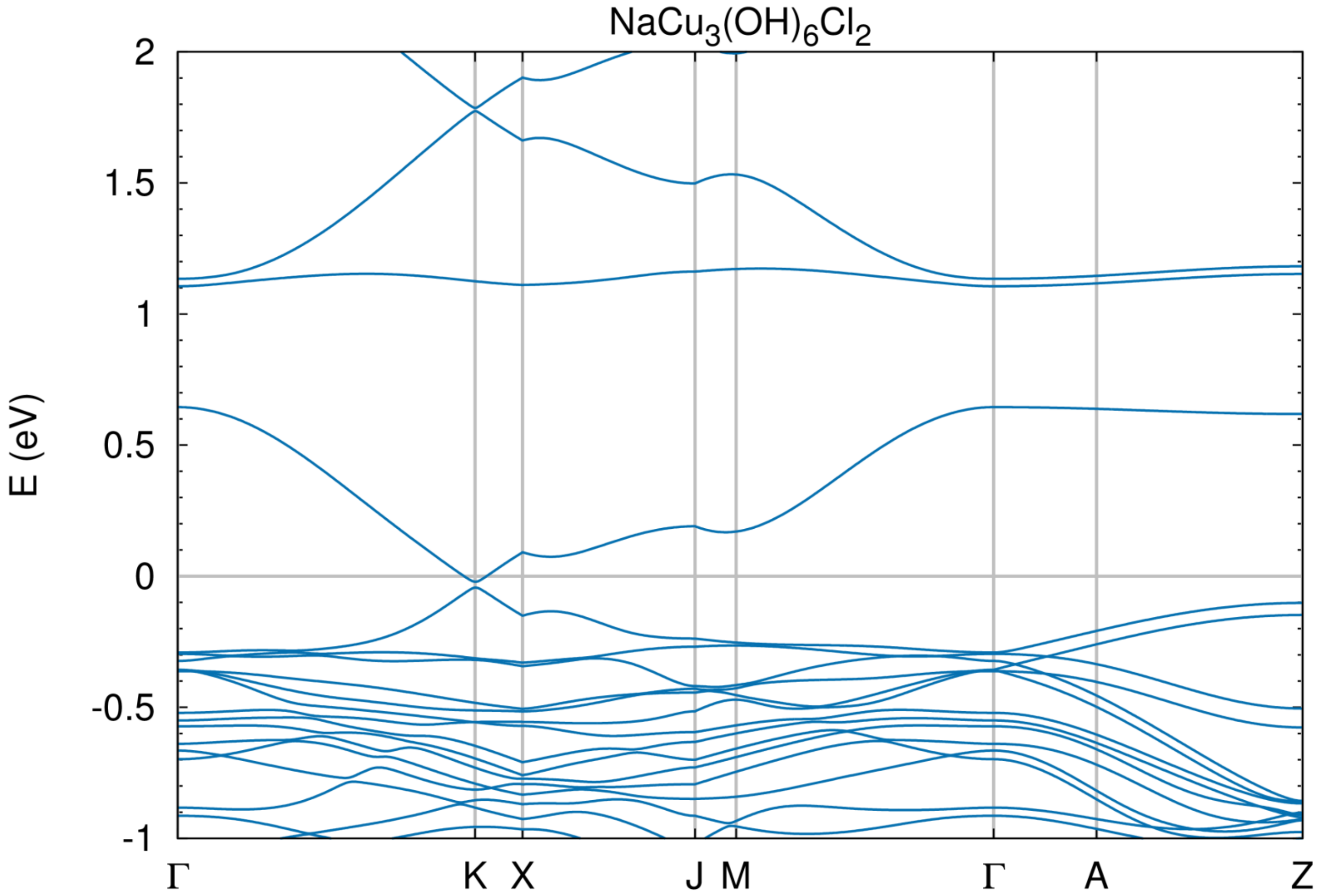
2 electrons/ 3 sites



Ferromagnetic ground state

2 electrons/ 3 sites

Spin-orbit effects?

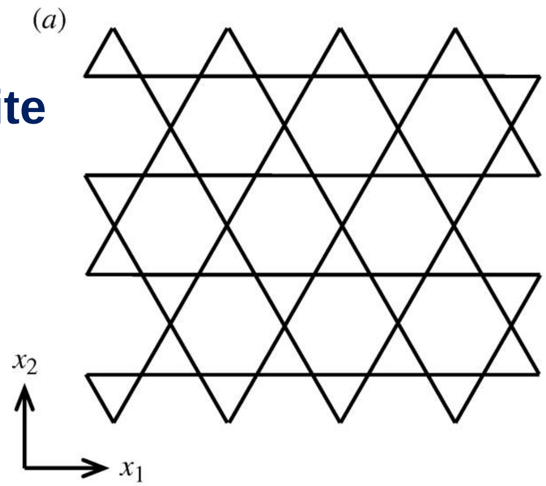


Ferromagnetic ground state

Opening of a gap at
the Dirac point ~ 6-10 meV

Extension to other systems and lattices

Herbertsmithite
Kapellasite
Haydeeite
Barlowite

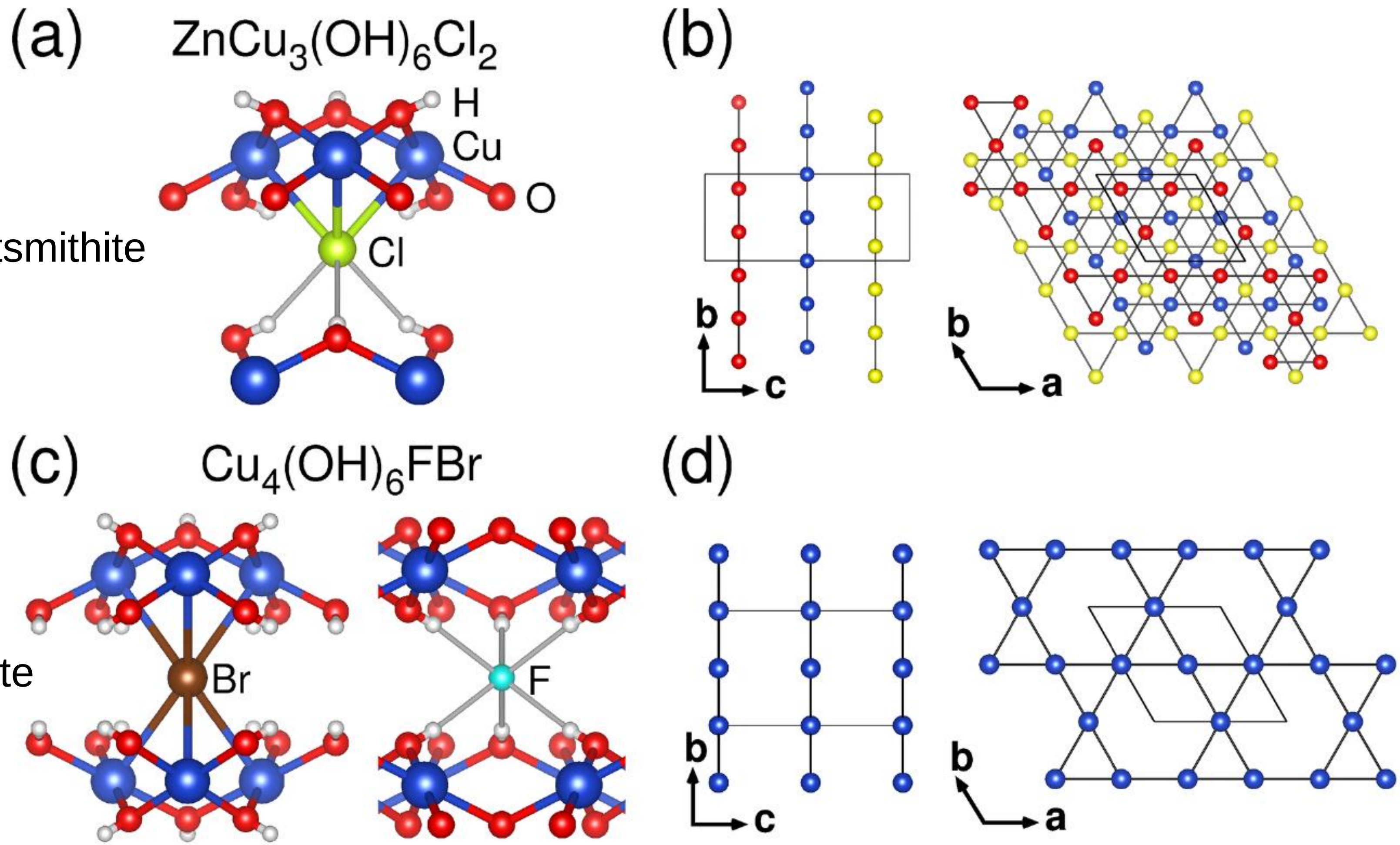


kagome

Kagome Barlowite

Herbertsmithite

Barlowite



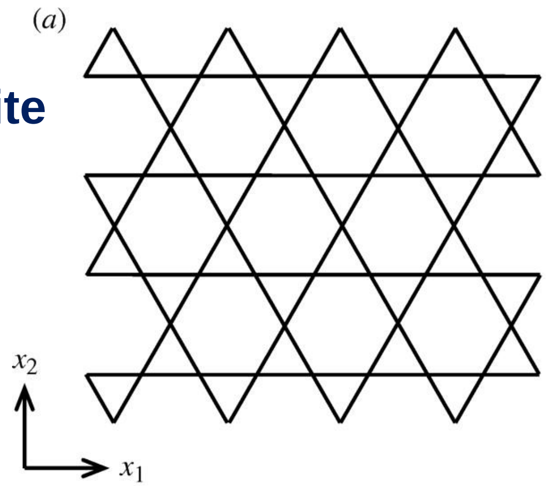
John Schlueter

Han,Singleton,Schlueter, PRL 113, 227203 (2014)

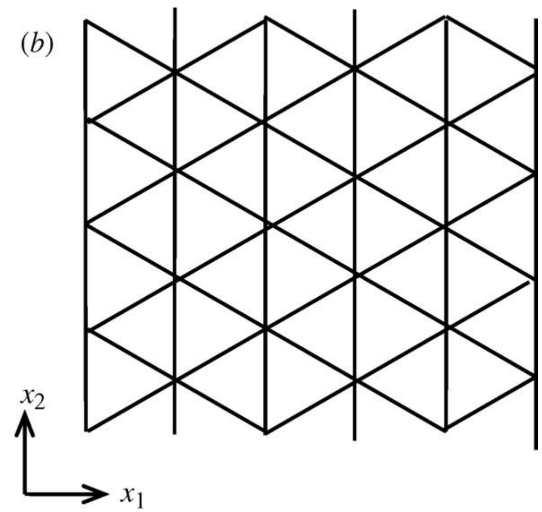
Jeschke, Salvat-Pujol,Gati,Hoang,Wolf,Lang,Schlueter, RV arXiv:1412.4688

Extension to other systems and lattices

Herbertsmithite
Kapellasite
Haydeeite
Barlowite

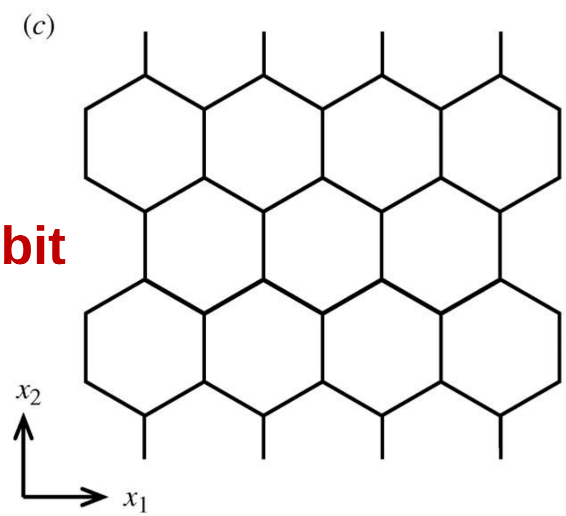


kagome



organic
charge
transfer salts

triangular



honeycomb

Correlations + spin-orbit

4d Ru, Rh
5d Ir

Summary

density functional theory + many-body methods (DMFT,DCA)
powerful method to describe correlated materials from first principles

- ***Correlated materials:***
  - **Fe-based superconductors**
    - * orbital selective renormalization of bands in agreement with (ARPES, de Haas van Alphen, optical conductivity, specific heat)
    - * spectral properties (Hund ←→ Mott physics)
- ***Predict new correlated materials with unconventional superconducting properties***
  - ***Ga-doped Herbertsmithite:*** **Correlated Dirac metal**
    f-wave superconductor?
  - **Effects of doping, magnetism, spin-orbit coupling, lattice geometry**

THANK YOU FOR YOUR ATTENTION!