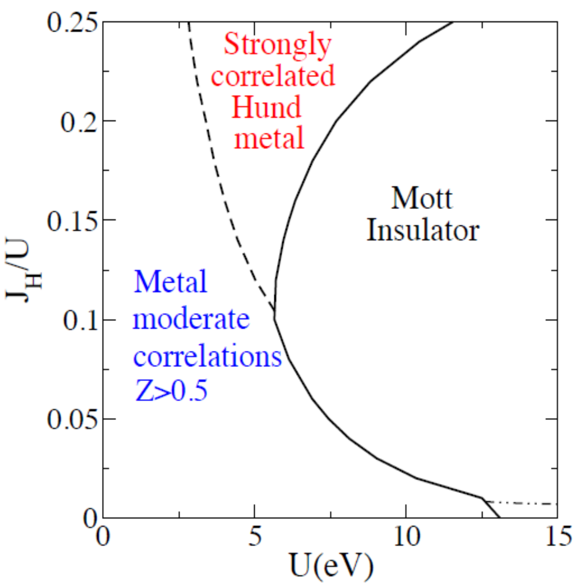
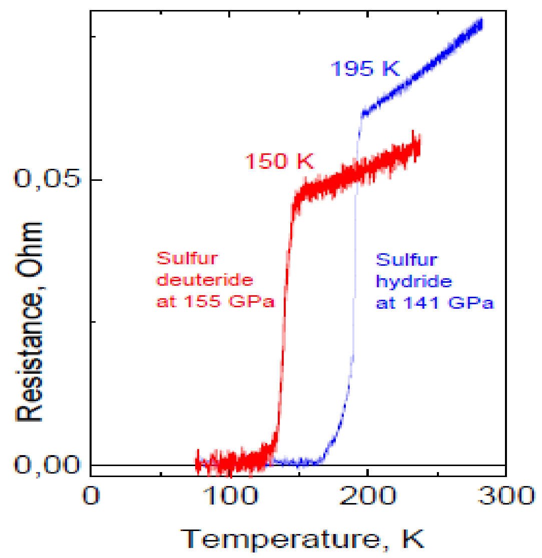
New perspectives in superconductors

E. Bascones
Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)





ICMM
CSIC
Consejo Superior de Investigaciones Científicas
Gobierno de España
Ministerio de Economía y Competitividad

Outline

- Talk I: Correlations in iron superconductors
  - Introduction to iron superconductors
  - Correlations in single-orbital. Cuprates
  - Correlations in multiorbital systems.
    - Equivalent orbitals. The Hund metal
    - Unequivalent orbitals. Iron superconductors
  - The magnetic state phase diagram
  - Comparison with experiments. Iron superconductors in a (U,J_H) phase diagram
- Talk II: A few new superconducting materials
  - Superconductivity and competing phases
    - CrAs and MnP
    - Ti-oxypnictides. Superconductivity emerging from a nematic state?
  - New quasi-1D superconductors
  - Hydrides. A new record for high-Tc?

A few superconducting compounds

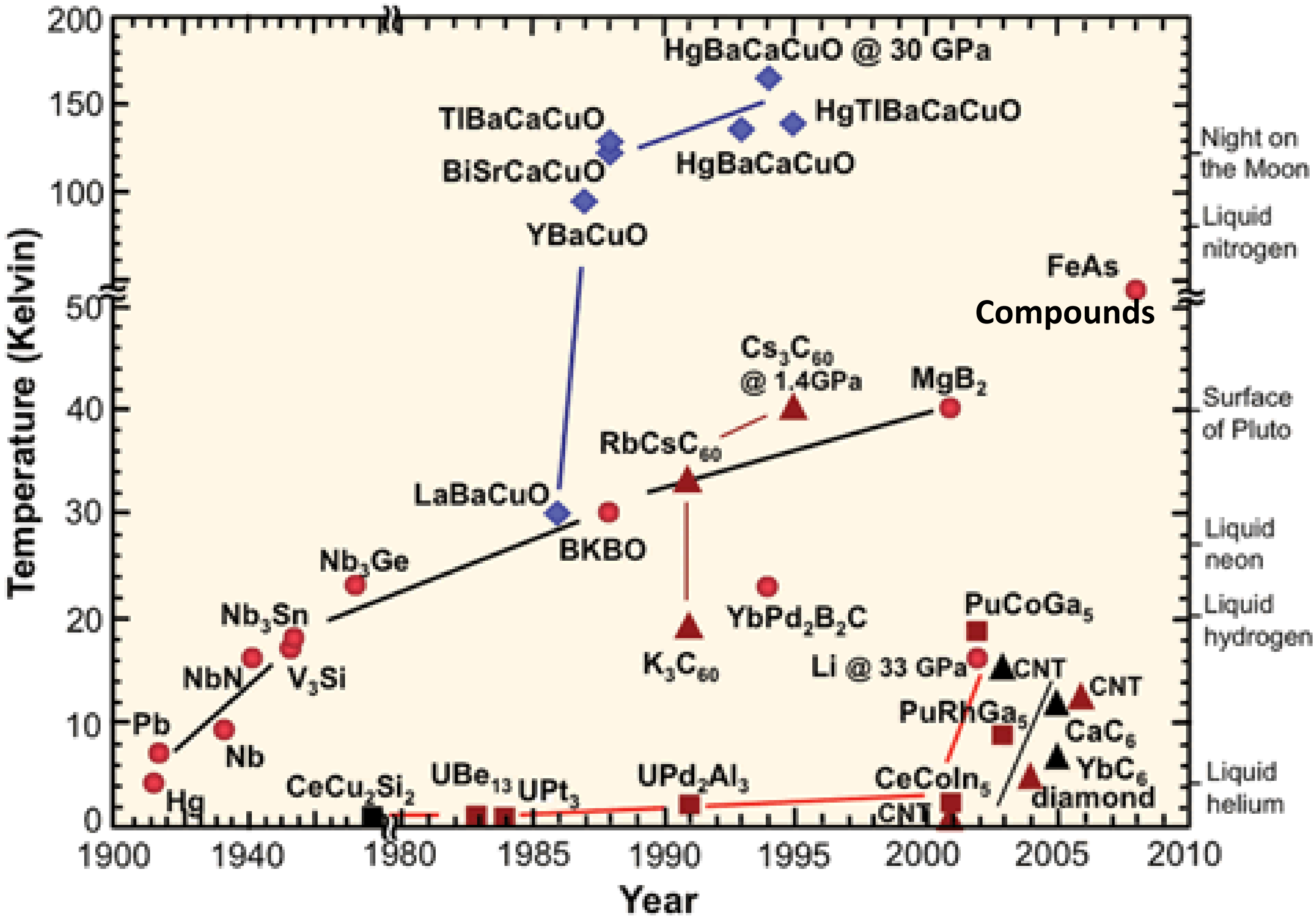


Fig: http://www.ccas-web.org/superconductivity

Superconducting families

Elements and simple compounds Nb, NbN	A15's Nb_3Ge	Doped semiconductors CB_x	Intercalated graphite C_6Ca
Hydrides (PdH)	Dichalcogenides $NbSe_2$	Chevrel phases $PbMo_6S_8$	Magnesium diborides MgB_2
Bismuthates $Ba_{1-x}K_xBiO_3$	Fullerenes $RbCs_2C_{60}$	Borocarbides $YPd_5B_3C_{0.3}$	Bismuth sulfides $YbO_{0.5}F_{0.5}BiS_2$
Heavy fermions and Pu superconductors UPd_2Al_3, $PuCoGa_5$	Cuprates $YBa_2Cu_3O_7$	Iron superconductors FeSe, LiFeAs	Organic spcs (charge transfer salts) $(BEDT\text{-}TTF)_2X$
Strontium ruthenate Sr_2RuO_4	Layered nitrides Ca(THF)HfNCl	Ferrromagnetic superconductors UGe_2	Non centrosymmetric superconductors $SrPtSi_3$
Interface superconductivity $LaAlO_3/SrTiO_3$	Hidrated cobaltites $Na_x(H_3O)_zCoO_2.yH_2O$	Topological superconductors $Cu_x(PbSe)_5(Bi_2Se_3)_6$	Aromatic hidrocarbides K_x-Picene

Hirsch et al, Physica C 514, 1 (2015)

3d based superconductors

Group→ ↓Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
		*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
		**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

E. Bascones leni@icmm.csic.es

Superconductivity in CrAs and MnP

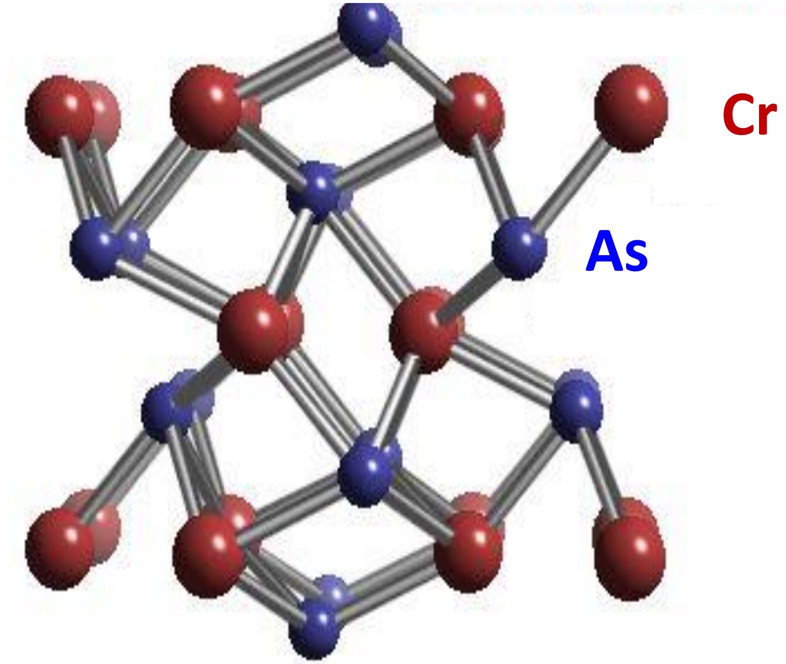
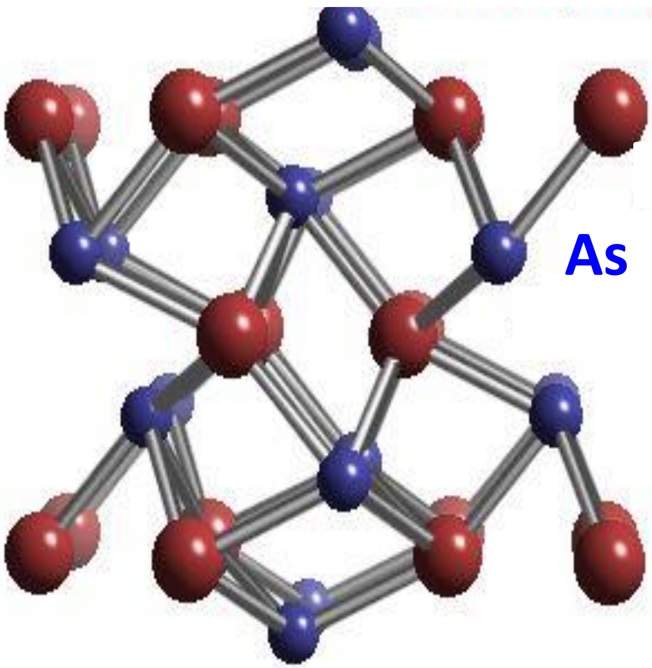
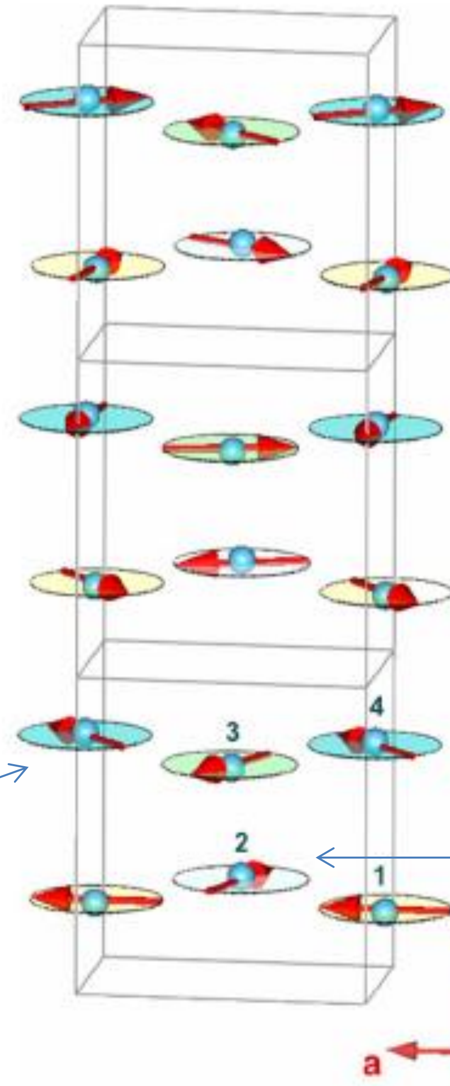


Fig:webelements.com

Superconductivity in CrAs and MnP





Double helical
Structure m~1.7 μ_B

Cr atoms

Ordering momentum along c

$\phi = -110(4)^\circ.$

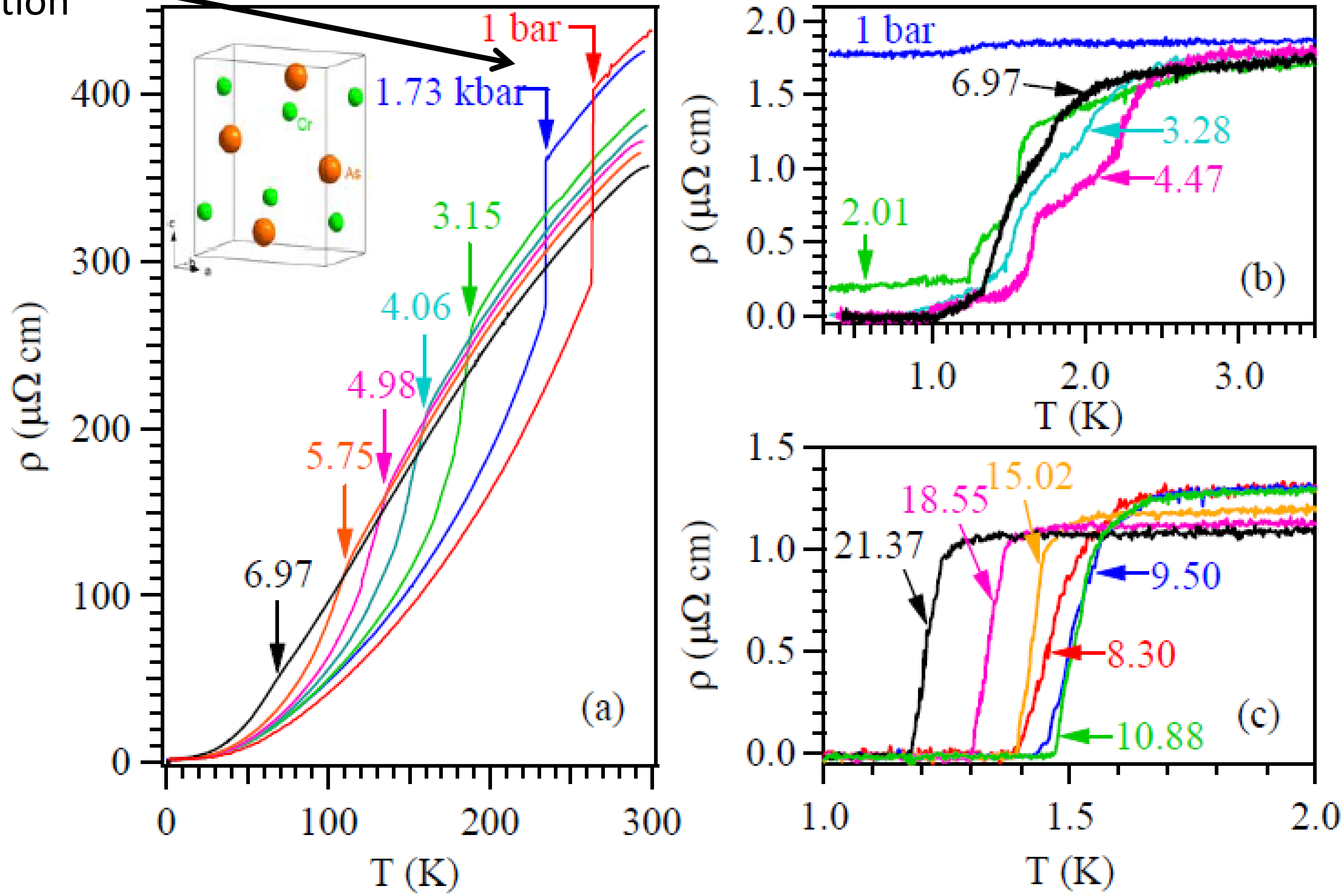
Magnetic moments in ab plane

Fig:webelements.com

Fig:Keller et al, PRB 91, 020409 (2015)

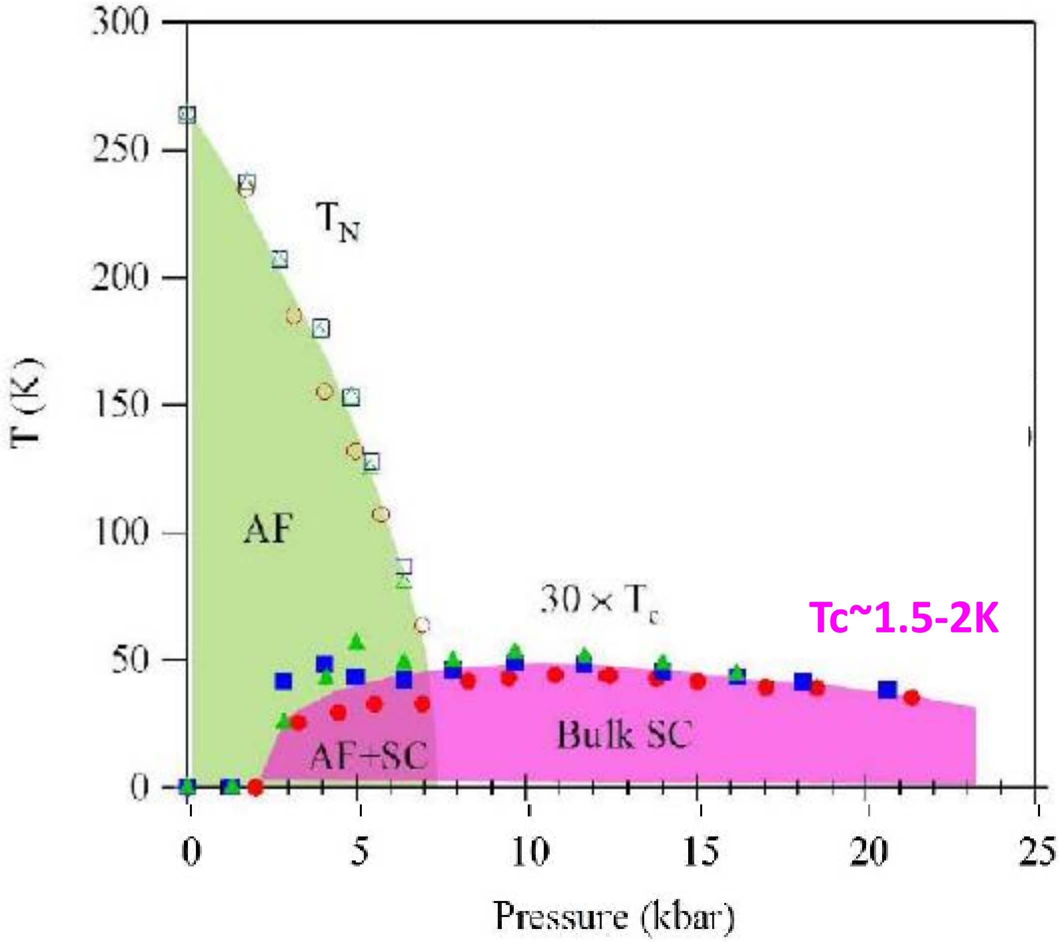
Superconductivity in CrAs and MnP

First order transition



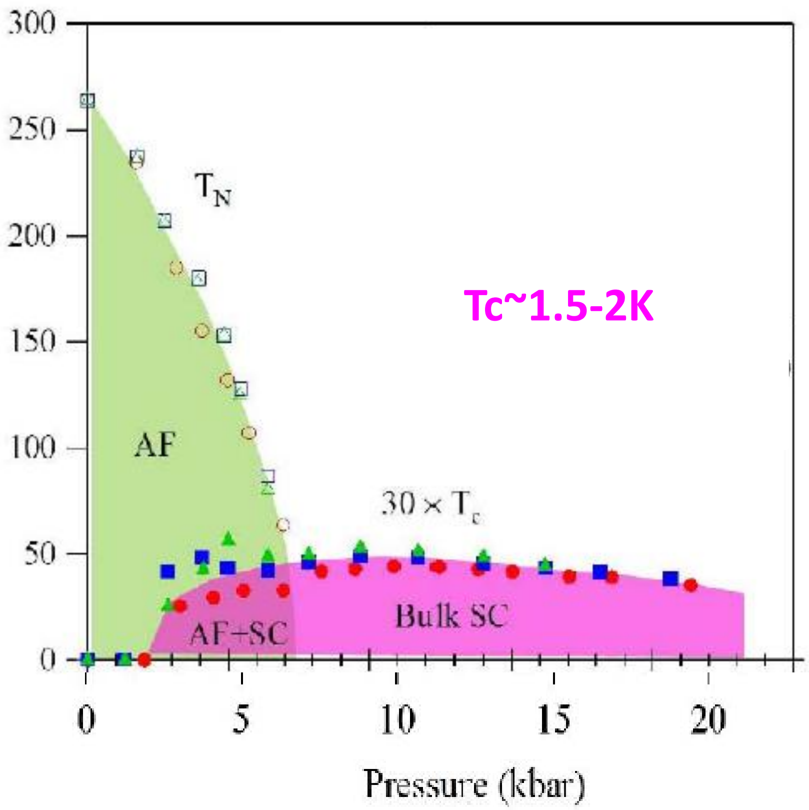
Wu et al, Nat. Comm. 5, 5508 (2014) Kotegawa et al, J. Phys. Soc. Jpn. 83, 093702 (2014)

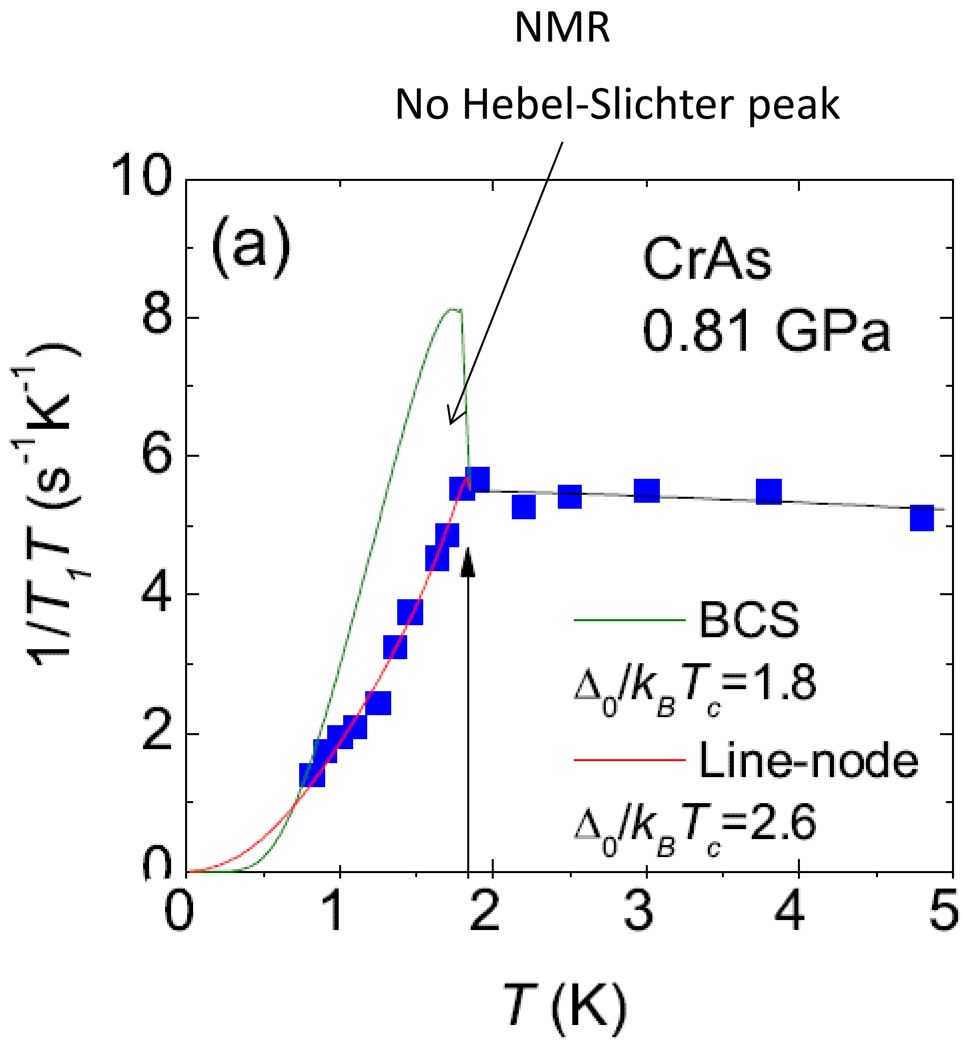
Superconductivity in CrAs and MnP



Wu et al, Nat. Comm. 5, 5508 (2014)   Kotegawa et al, J. Phys. Soc. Jpn. 83, 093702 (2014)

Superconductivity in CrAs and MnP

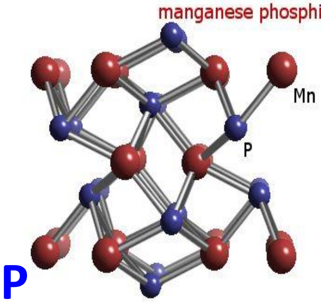




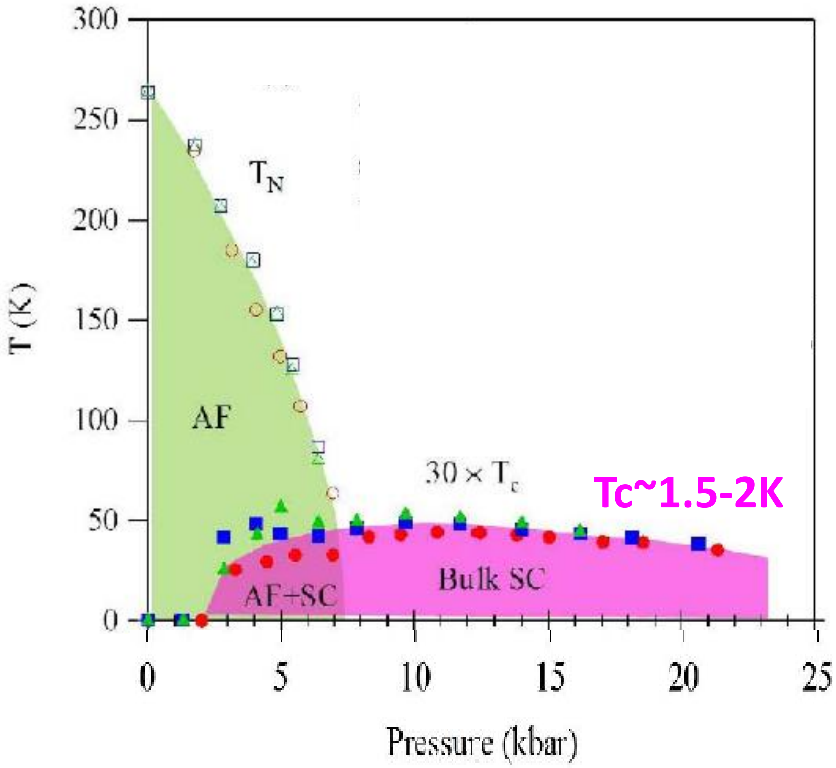
Wu et al, Nat. Comm. 5, 5508 (2014)

Kotegawa et al, Phys. Rev. Lett. 114, 117002 (2015)

Superconductivity in CrAs and MnP

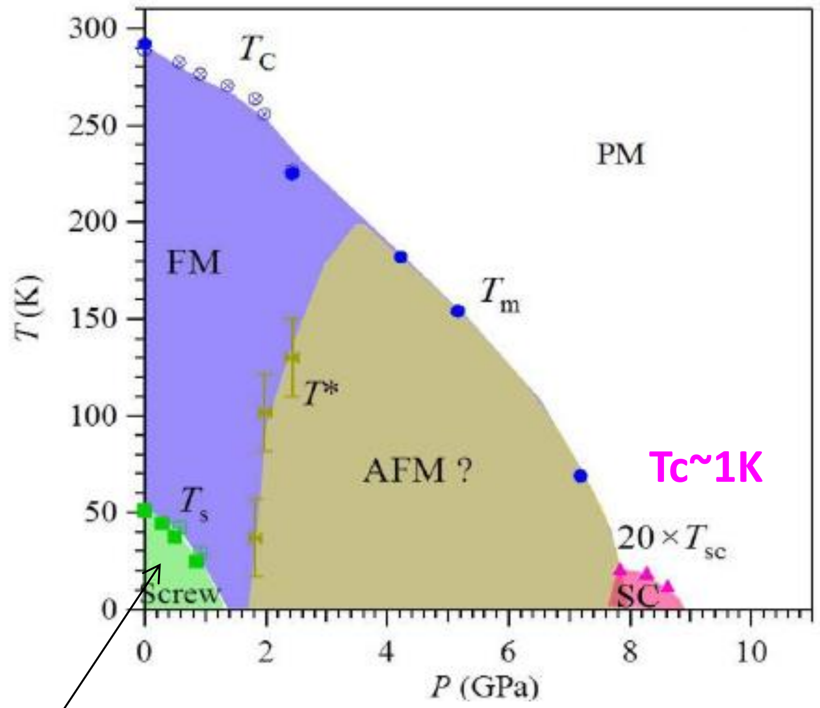


CrAs



Tc~1.5-2K

MnP



Tc~1K

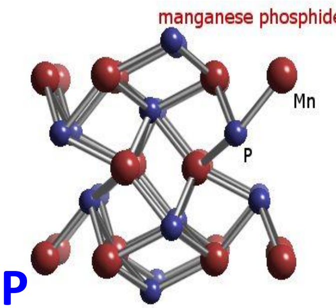
Helimagnet
μ~1.3 μ_B

MnP: First Mn-based superconducting compound

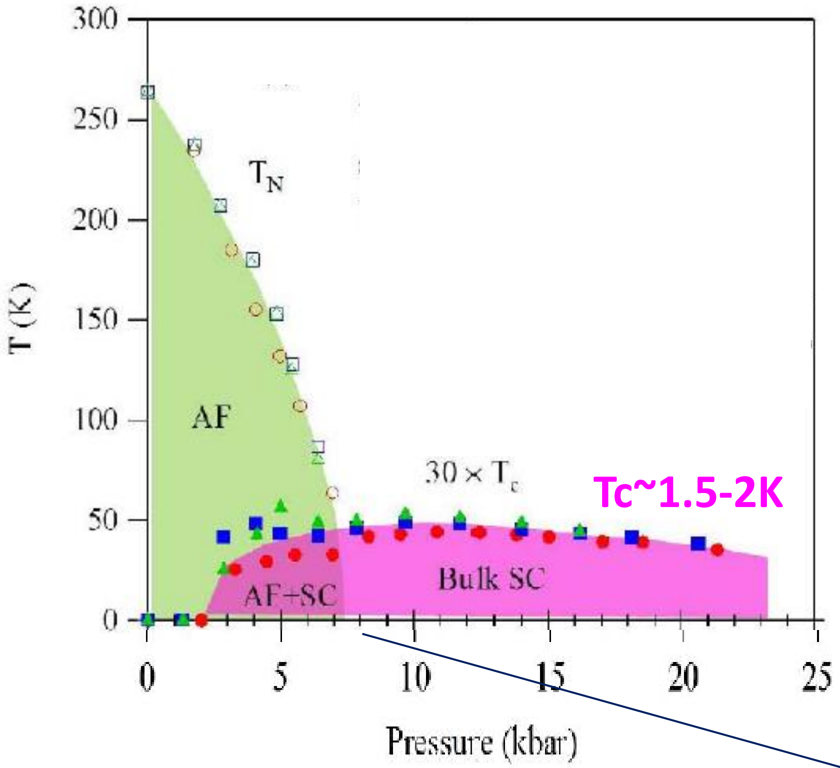
Wu et al, Nat. Comm. 5, 5508 (2014)

Cheng et al, Phys. Rev. Lett. 114, 117001 (2015)

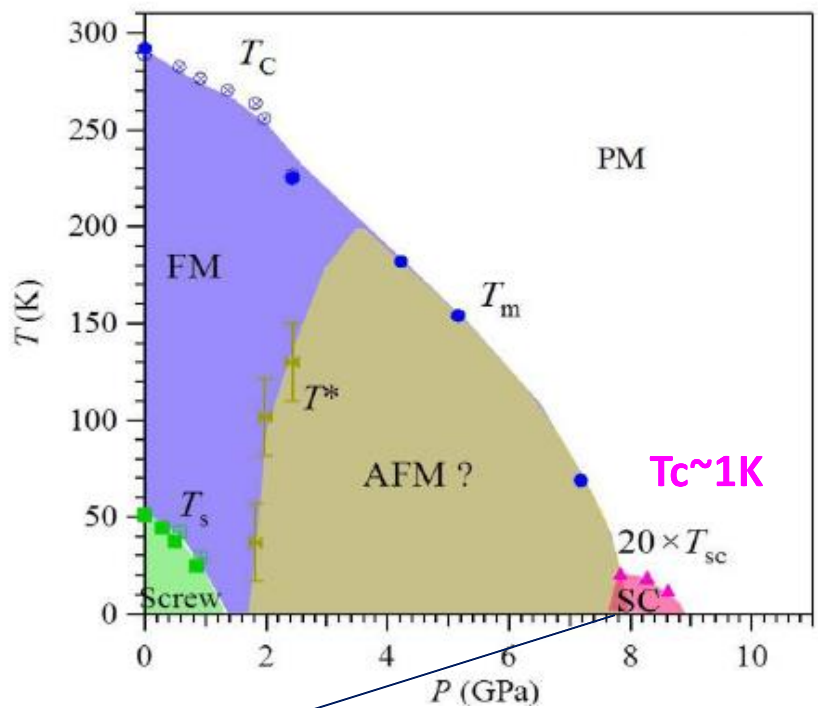
Superconductivity in CrAs and MnP



CrAs



MnP



Quantum Critical Behavior?

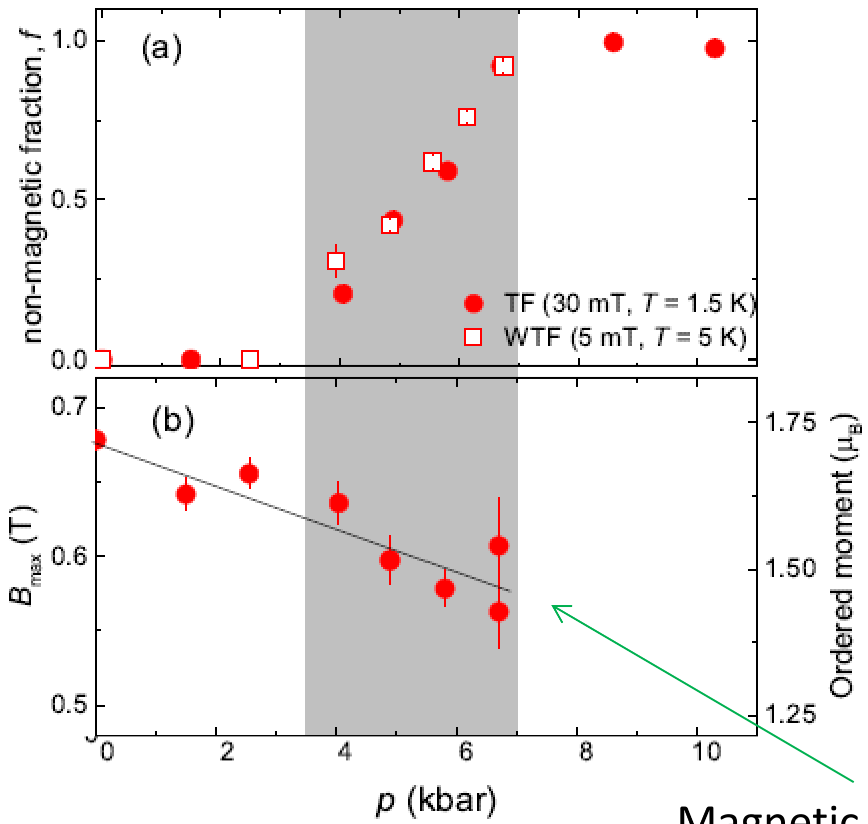
Wu et al, Nat. Comm. 5, 5508 (2014)

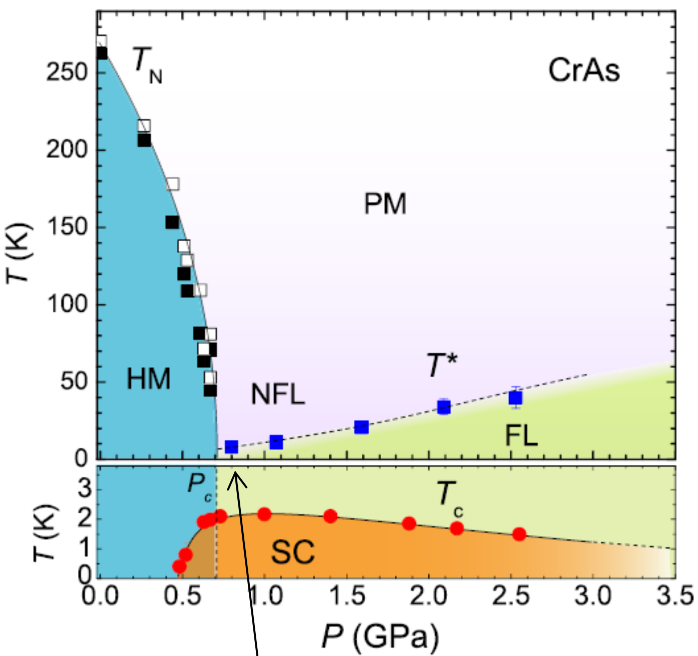
Cheng et al, Phys. Rev. Lett. 114, 117001 (2015)

Superconductivity in CrAs and MnP

- Initial claims in favour of QCP from CrAs and MnP from resistivity measurements

- In CrAS: First order transition and phase separation at P_c from NMR, neutron diffraction and muon spectroscopy





Finite T* @Pc

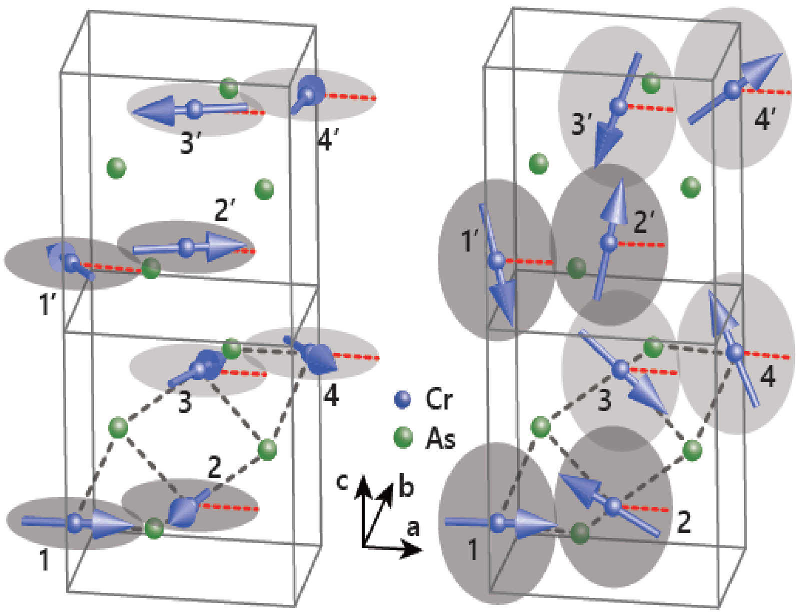
Magnetic moment jumps @ Pc

Keller et al, PRB 91, 020409 (2015), Khasanov et al: arXiv: 1502.07573

Kotegawa et al, PRL 114, 117002 (2015)

Superconductivity in CrAs and MnP

P=0 Gpa T=4 K P=0.6 Gpa T=50 K



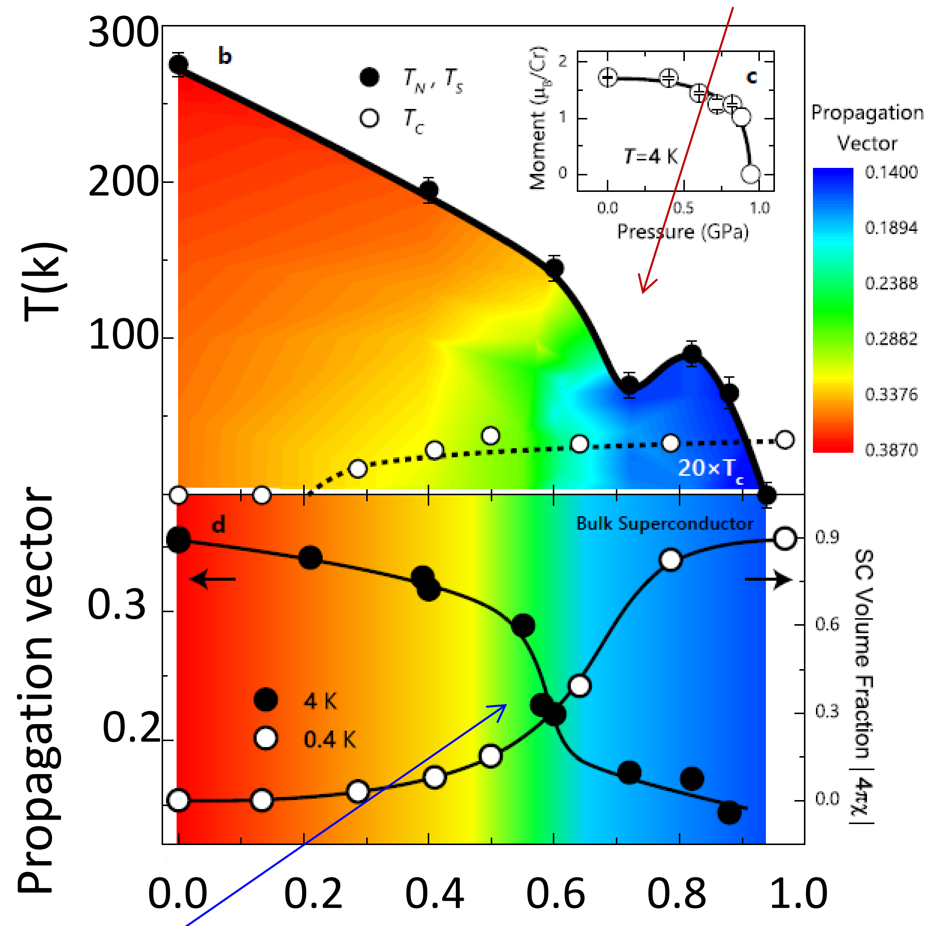
Spins in ab plane

$\phi = -108º$

Spins in ac plane

$\phi = 172º$

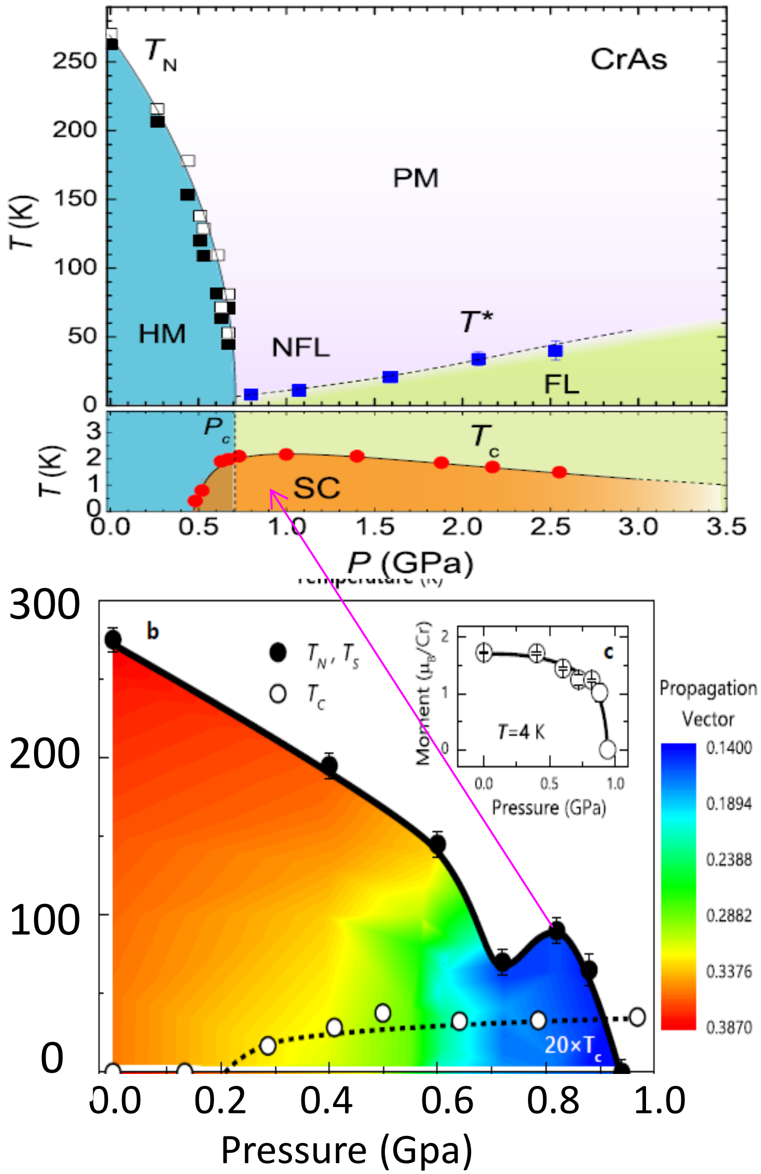
Magnetic reorganization

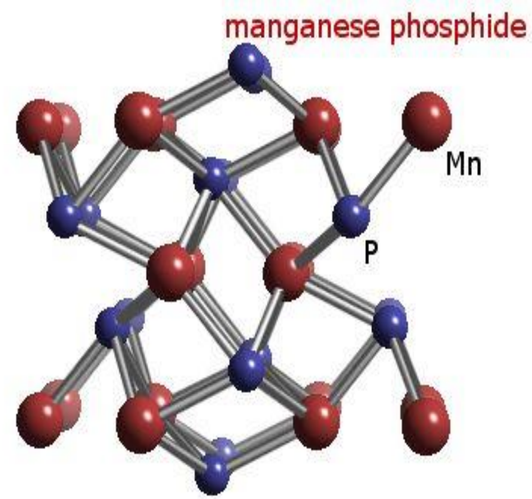


Change in ordering vector k_c

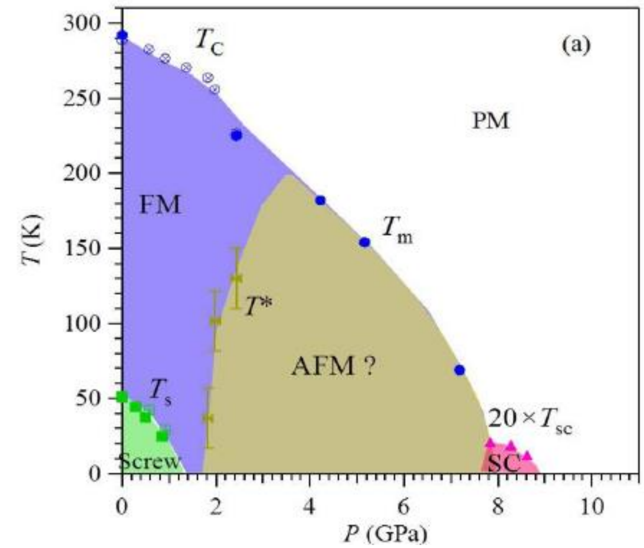
Sheng et al: arXiv: 1409.6615

Superconductivity in CrAs and MnP: Summary





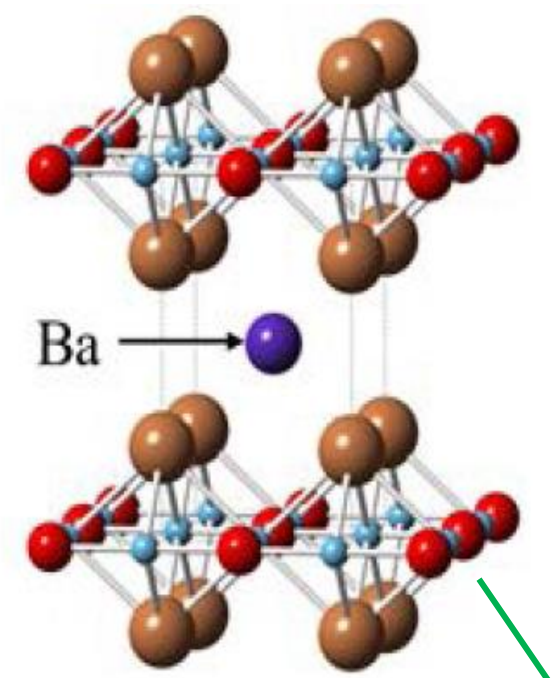
Talk by J. Cheng next week

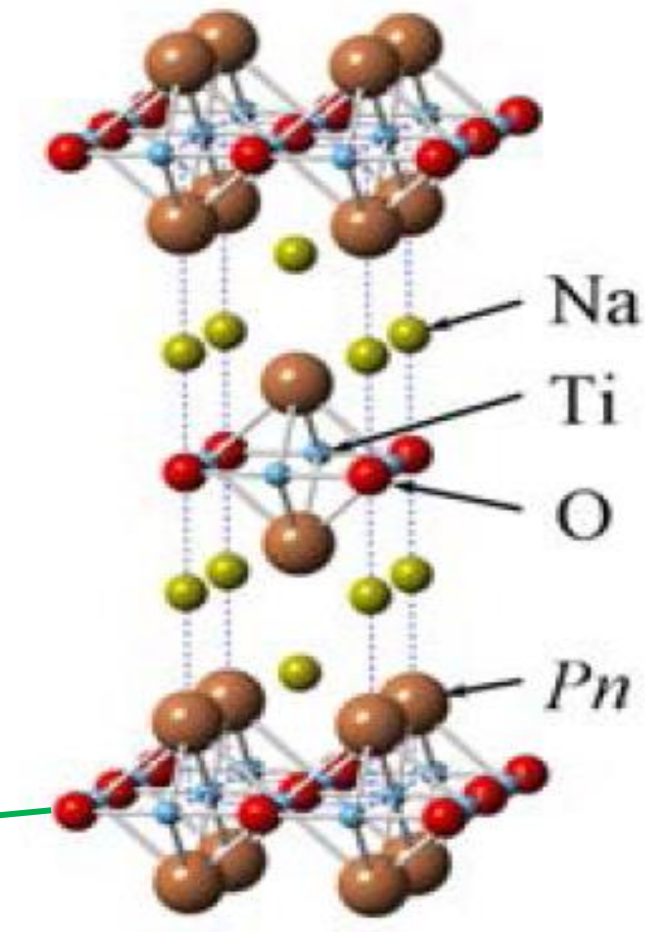


Titanium oxypnictides ATi_2Pn_2O

$A=Na_2$, Ba, $(SrF)_2$ …

Nominal charge +2





TiO_2Pn_4 octahedron layers

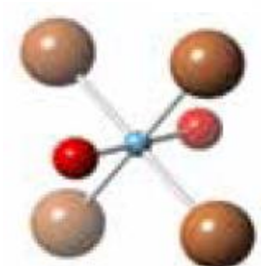


Fig: Hosono et al, Sci. Tech. Adv. Mater. 16, 033503 (2015)

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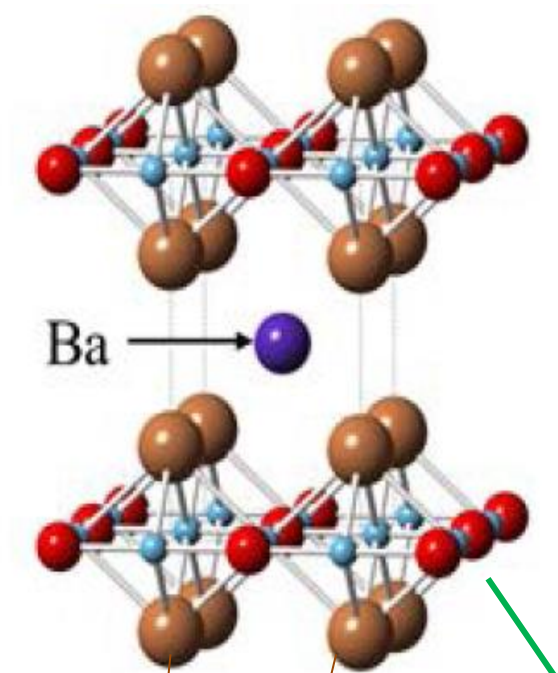
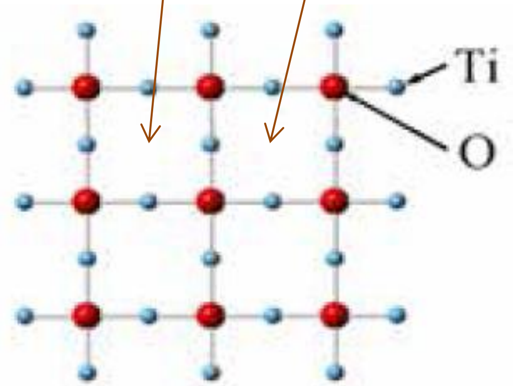
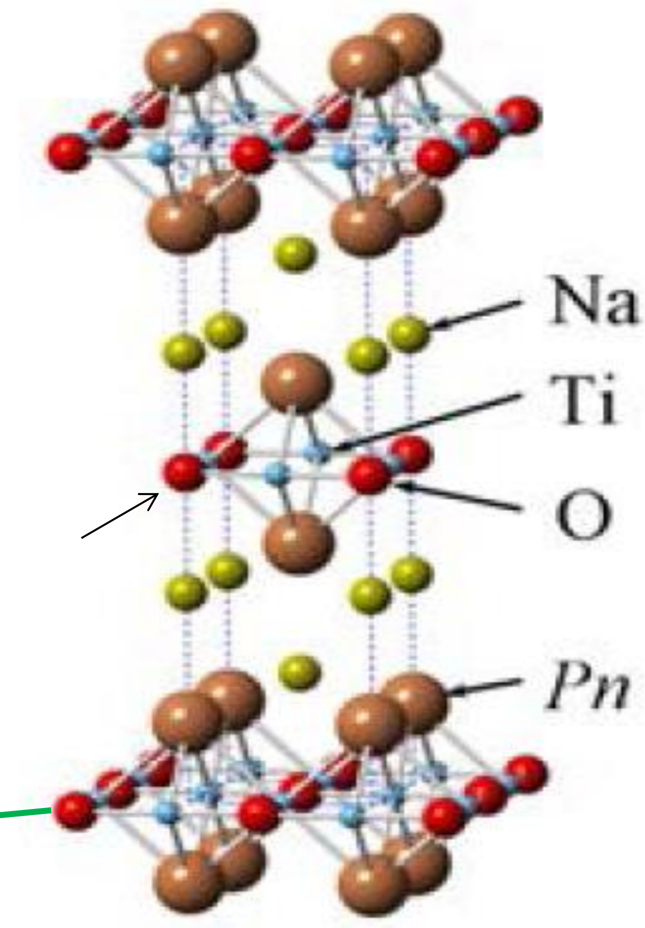






TiO_2Pn_4 octahedron layers

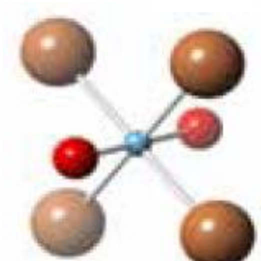
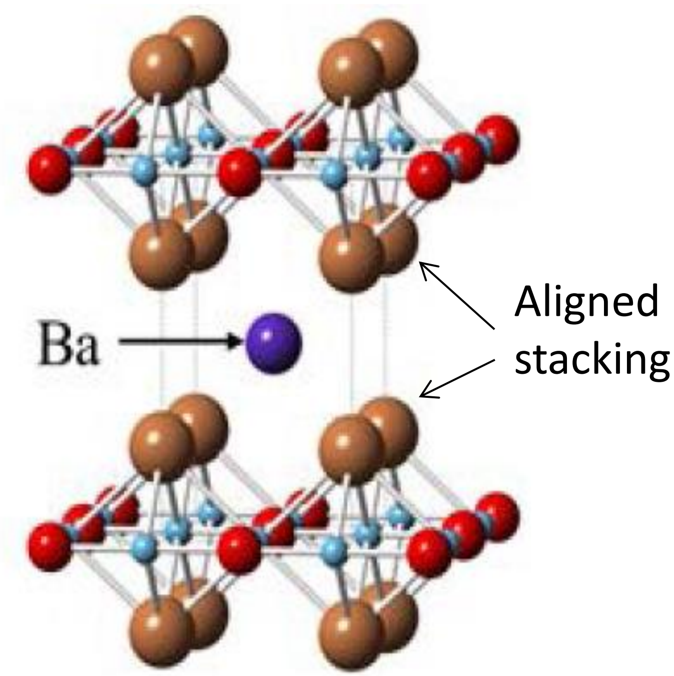


Fig: Hosono et al, Sci. Tech. Adv. Mater. 16, 033503 (2015)

Titanium oxypnictides ATi_2Pn_2O

$A=Na_2$, Ba, $(SrF)_2$ …

Nominal charge +2



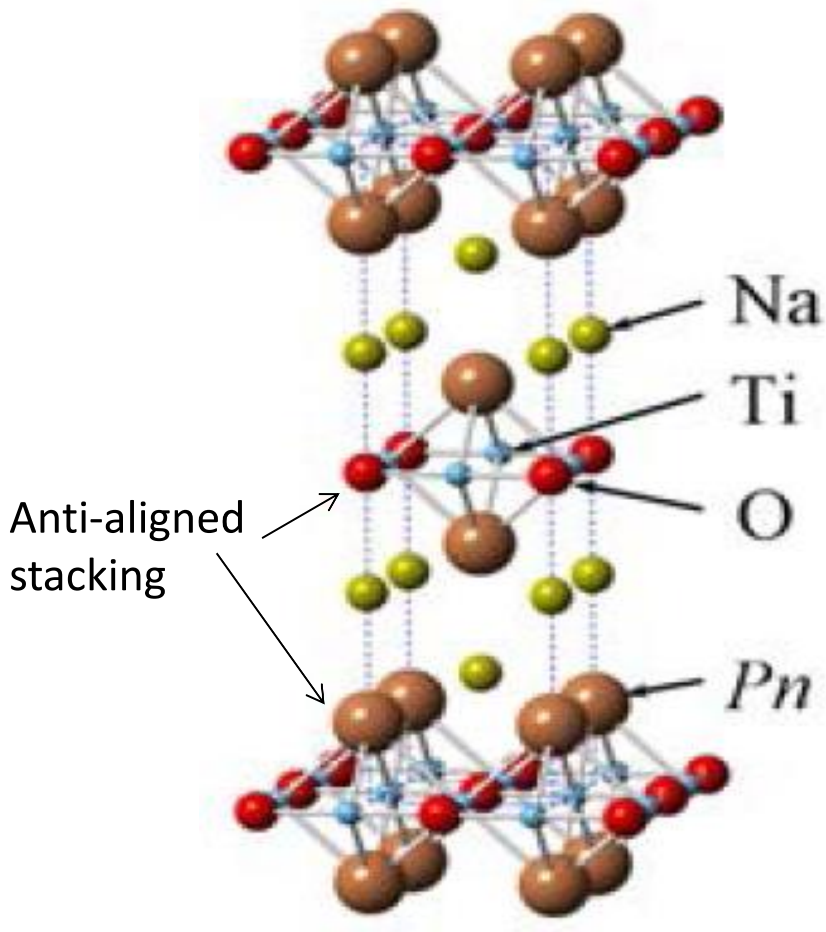
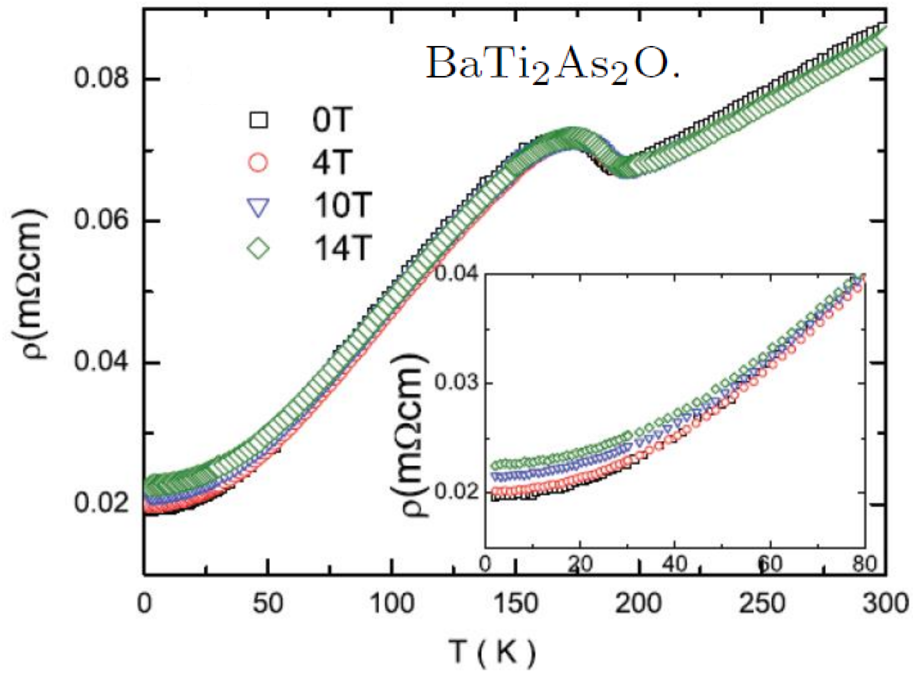
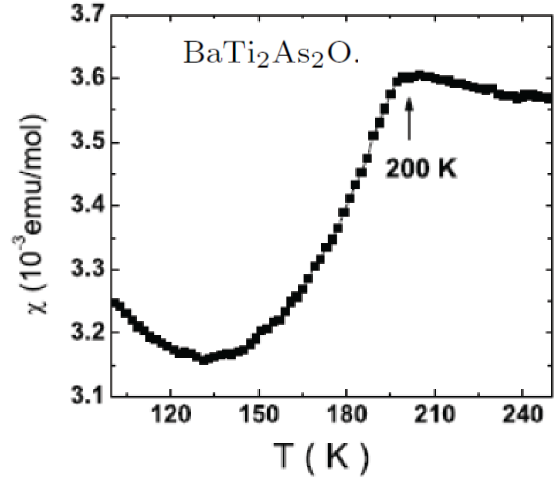


Fig: Hosono et al, Sci. Tech. Adv. Mater. 16, 033503 (2015)

Titanium oxypnictides ATi_2Pn_2O: ordered state

- $Na_2Ti_2As_2O$: T_s~320 K
- $Na_2Ti_2Sb_2O$: T_s ~120 K
- $BaTi_2As_2O$: T_s ~200 K



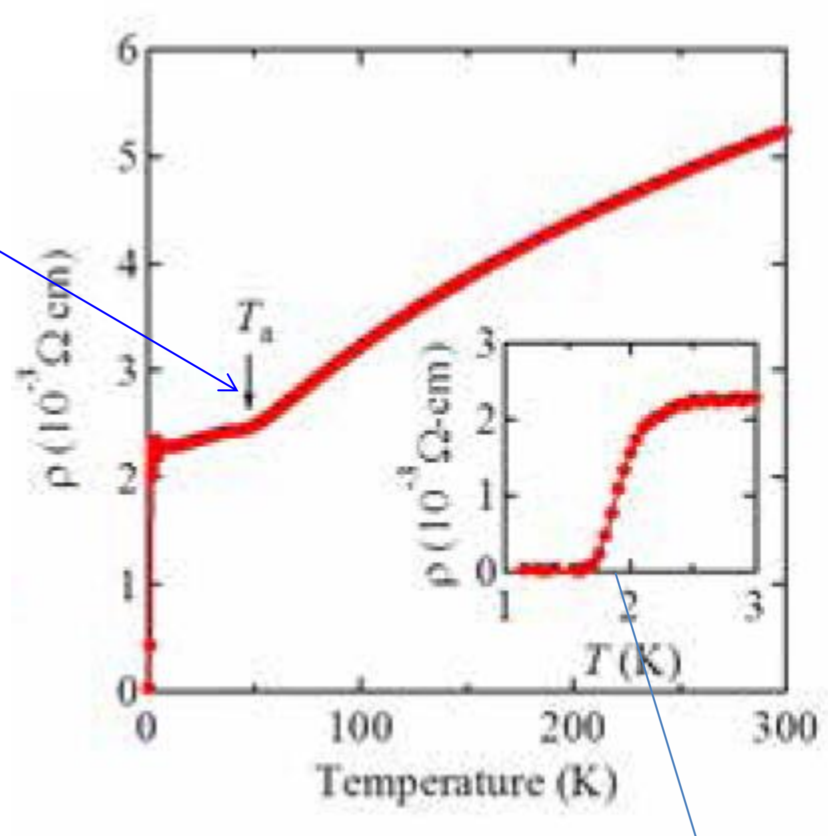


Wang et al, J. Phys. Cond. Mat. 22, 075702 (2010)

Lorenz et al, Int. J. Mod. Phys. B 28, 1430011 (2014)

Superconductivity in $BaTi_2Sb_2O$

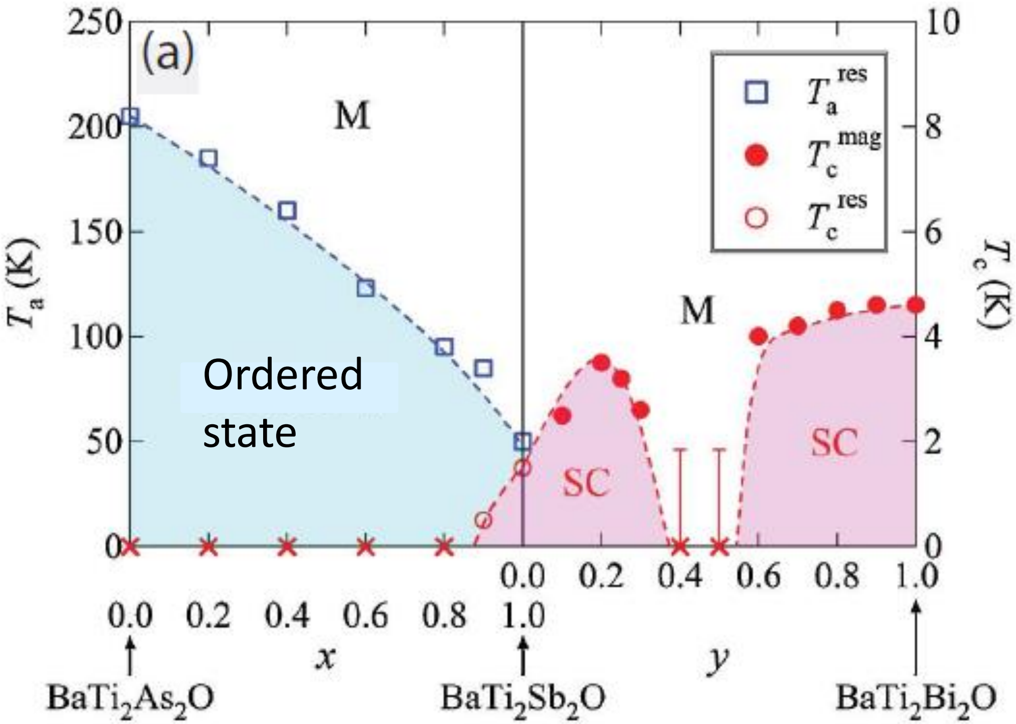
Transition T_s~54 K



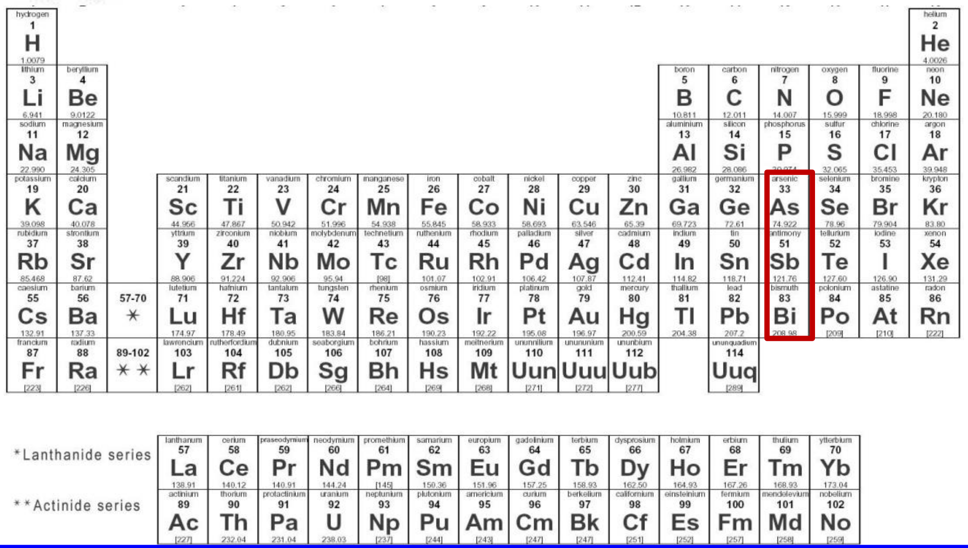
Superconductivity T_c ~ 1.2 K

Tajima et al, J. Phys. Soc. Jpn. 81, 103706 (2012)

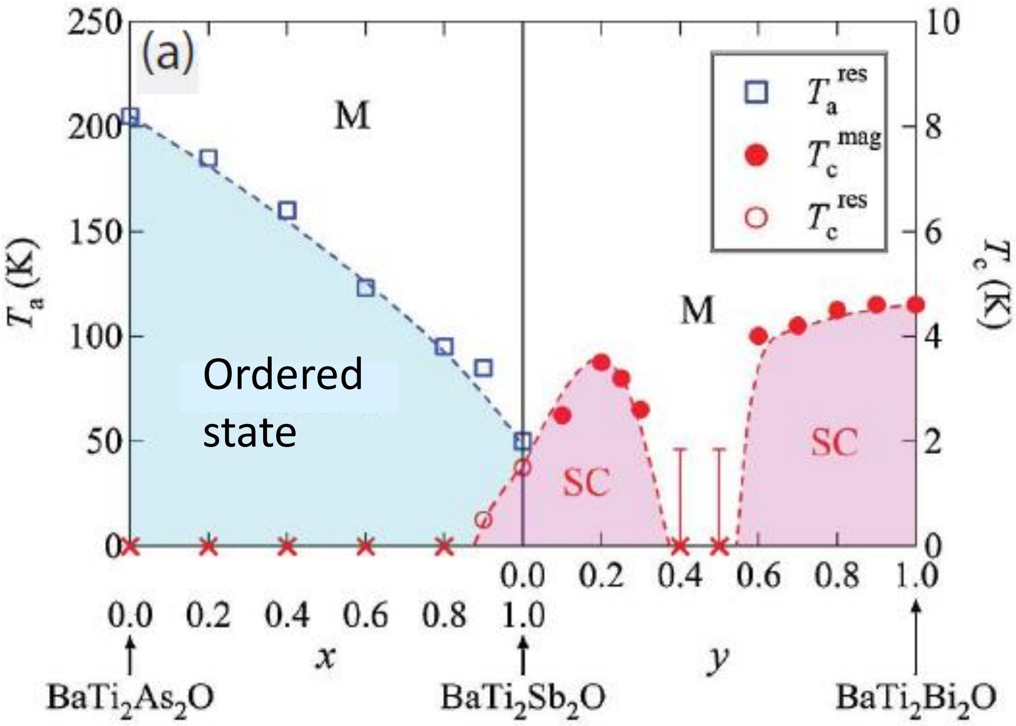
Superconductivity in substituted $BaTi_2Pn_2O$



Tajima et al, J. Phys. Soc. Jpn. 82, 033705 (2013)

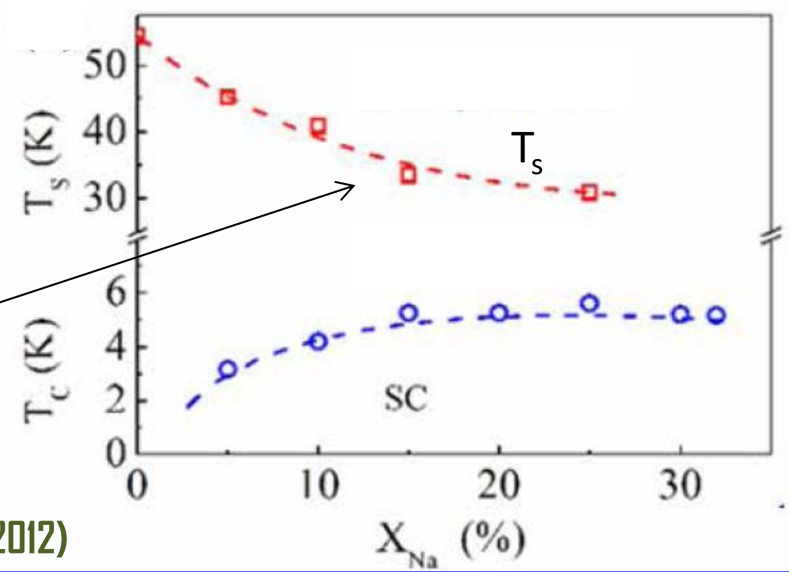


Superconductivity in substituted $BaTi_2Pn_2O$



Tajima et al, J. Phys. Soc. Jpn. 82, 033705 (2013)

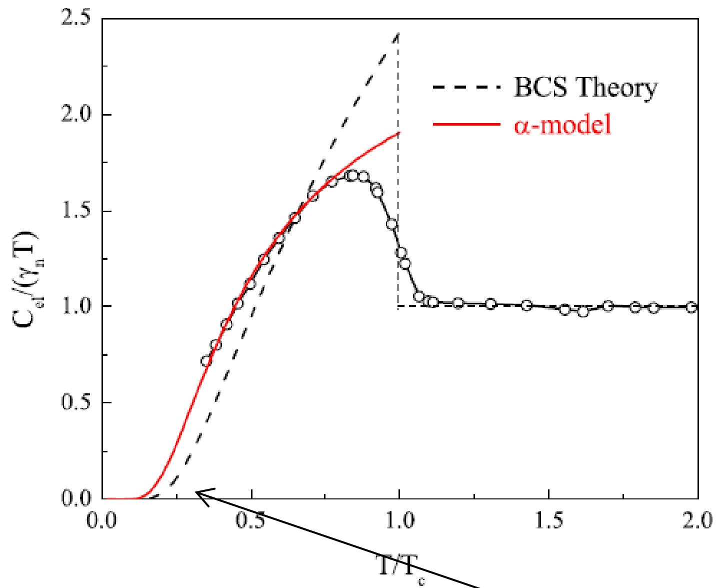
Hole-doping $Ba_{1-x}Na_xTi_2Pn_2O$



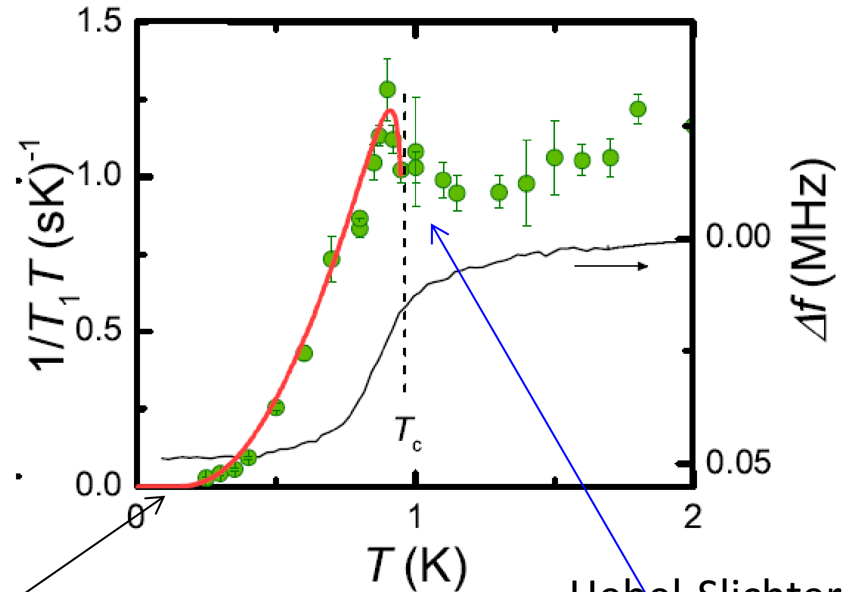
Doan et al, JACS. 134, 16520 (2012)

Superconductivity in $BaTi_2Sb_2O$

Specific heat



NQR



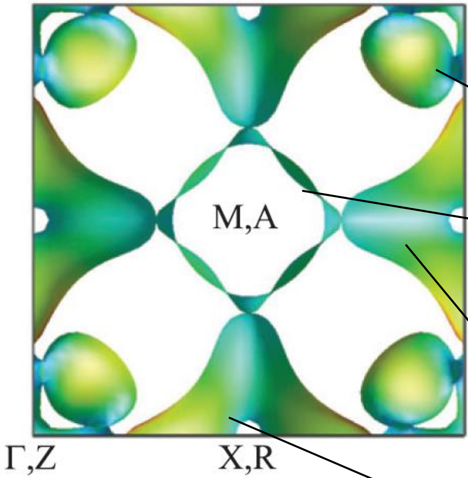
Hebel-Slichter peak

Fully gapped

Gooch et al, PRB 88, 064510 (2013)   Kitagawa et al, PRB 87, 060510 (2013)

Nested Fermi surfaces in titanium oxypnictides

Small mass enhancement ~1-1.5



FS $BaSb_2Ti_2O$

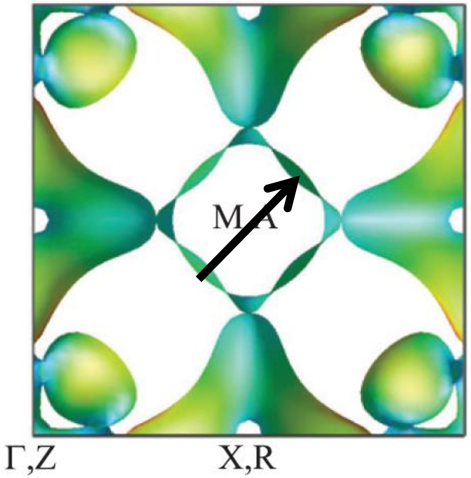
Singh , NJP 14, 123003 (2013)

Electron pockets

Hole pockets

Nested Fermi surfaces in titanium oxypnictides

Small mass enhancement ~1-2



FS **$BaSb_2Ti_2O$**

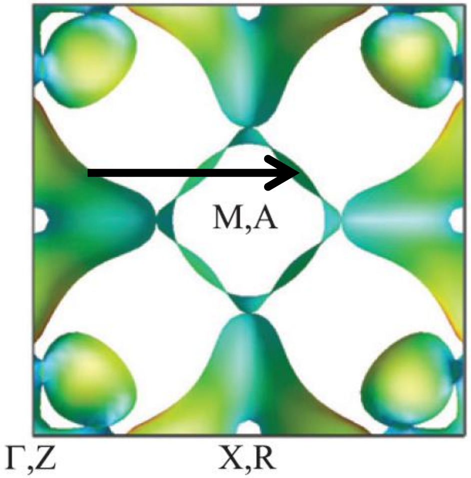
Singh , NJP 14, 123003 (2013)

$Na_2Sb_2Ti_2O$ (Ts~120K, no SC)

- Inconmensurate CDW/SDW Q_M=(0.22,0.22,0)π/a
  Pickett, PRB 58, 4335 (1998)
- Inconmensurate CDW Q_X=(0.27,0,0)π/a or (0,0.27,0)π/a
  Possible second transition with Q_M
  Biani et al, Inorg. Chem. 7, 5810 (1998)

Nested Fermi surfaces in titanium oxypnictides

Small mass enhancement ~1-2



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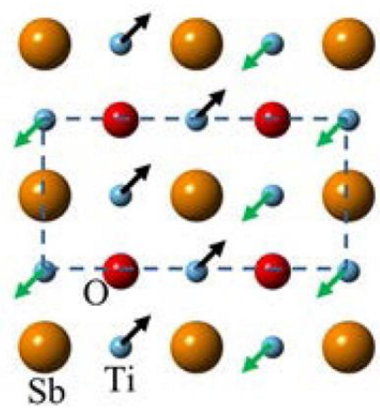
Singh , NJP 14, 123003 (2013)

$Na_2Sb_2Ti_2O$ (Ts~120 K, no SC)

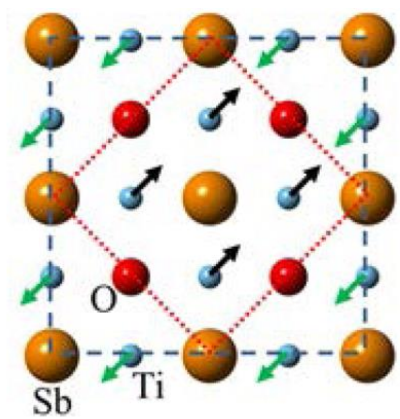
- Inconmensurate CDW/SDW $Q_M=(0.22\pi,0.22\pi,0)$
  Pickett, PRB 58, 4335 (1998)
- Inconmensurate CDW $Q_X=(0.27\pi,0,0)$ or $(0,0.27\pi,0)$
  Possible second transition with Q_M
  Biani et al, Inorg. Chem. 7, 5810 (1998)

Commensurate SDW

$Na_2Sb_2Ti_2O$ (Ts~120 K, no SC)



$Na_2As_2Ti_2O$ (Ts~200 K, no SC)



μ ~0.5 μ_B

Wang & Lu, JPCM 25, 365501 (2013)

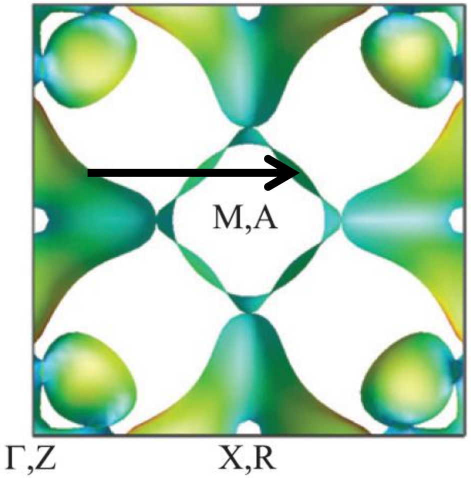
Double stripe SDW $Q_{XM}=(\pi,0)$ or $(0,\pi)$

Blocked checkerboard SDW

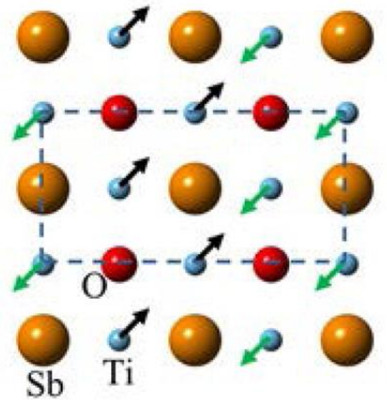
Fig: Hosono et al, Sci. Tech. Adv. Mater. 16, 033503 (2015)

Nested Fermi surfaces in titanium oxypnictides

Small mass enhancement ~1-2



$BaSb_2Ti_2O$ (Ts~54 K, SC~1.2 K)

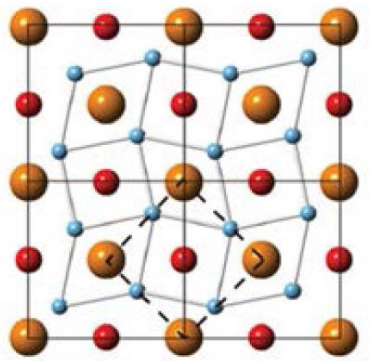


Double stripe SDW

$Q_{XM}=(\pi,0)$ or $(0,\pi)$

μ ~0.2 μ_B

Singh , NJP 14, 123003 (2013)



CDW $Q=(\pi,\pi)$

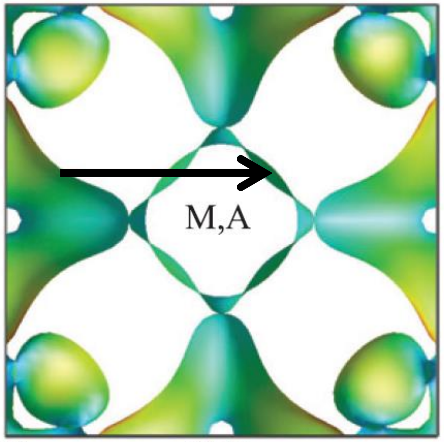
Phonon anomaly

Subedi, PRB 87, 054506 (2013)

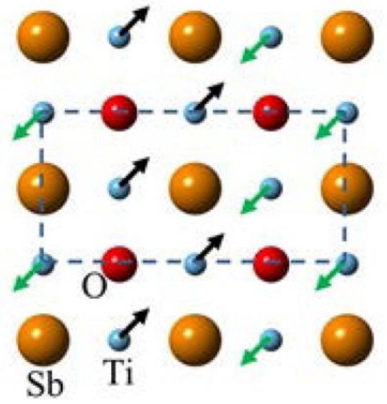
Fig: Hosono et al, Sci. Tech. Adv. Mater. 16, 033503 (2015)

Nested Fermi surfaces in titanium oxypnictides

Small mass enhancement ~1-2



$BaSb_2Ti_2O$ (Ts~54 K, SC~1.2 K)



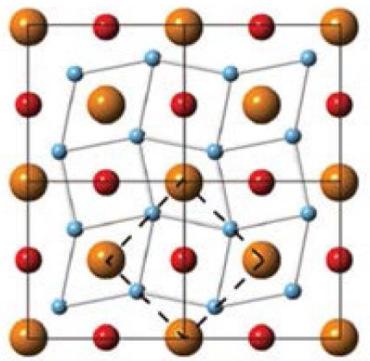
Double stripe SDW

$Q_{XM}=(\pi,o)$ or $(0,\pi)$

μ ~0.2 μ_B

Magnetically mediated SC **$s^{\pm}$**

Singh , NJP 14, 123003 (2013)



CDW $Q=(\pi,\pi)$

Phonon anomaly

Phonon mediated SC **s-wave,** Tc ~5 K

Subedi, PRB 87, 054506 (2013)

Fig: Hosono et al, Sci. Tech. Adv. Mater. 16, 033503 (2015)

A nematic state below T_s in titanium oxypnictides?

- NMR/NQR in **$BaTi_2Sb_2O$** at Sb site
  - Excludes Inconmensurate CDW/SDW correlations.
  - Breaking of Tetragonal symmetry at Sb site

Kitagawa et al,
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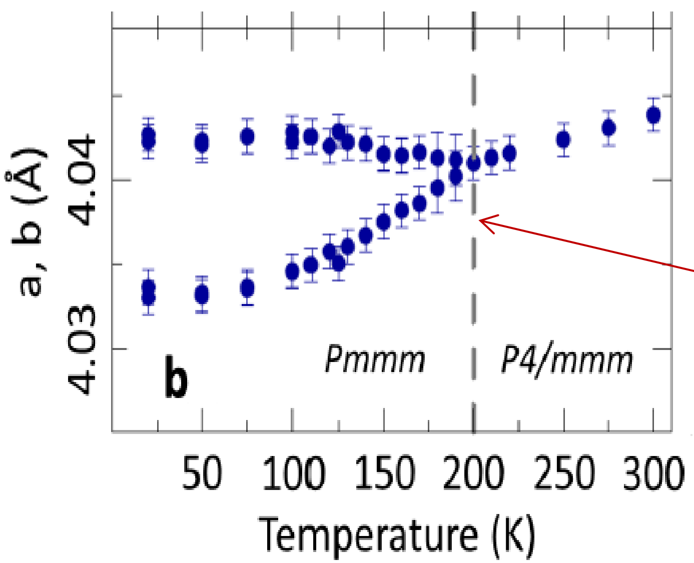
Kitagawa et al, PRB 87, 060510 (2013)

- No superlattice peaks in high sensitivity electron diffraction

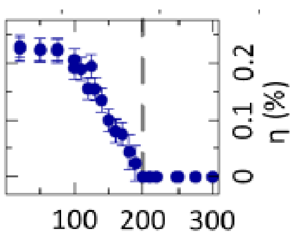
$BaTi_2As_2O$ (Ts ~200 K, no Sc)

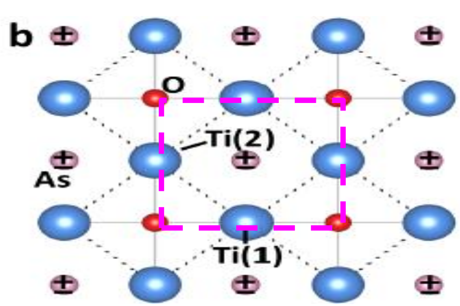


Neutron diffraction

Frandsen et al, Nat. Comm. 5, 5761 (2014)

Tetragonal-Orthorhombic Structural transition





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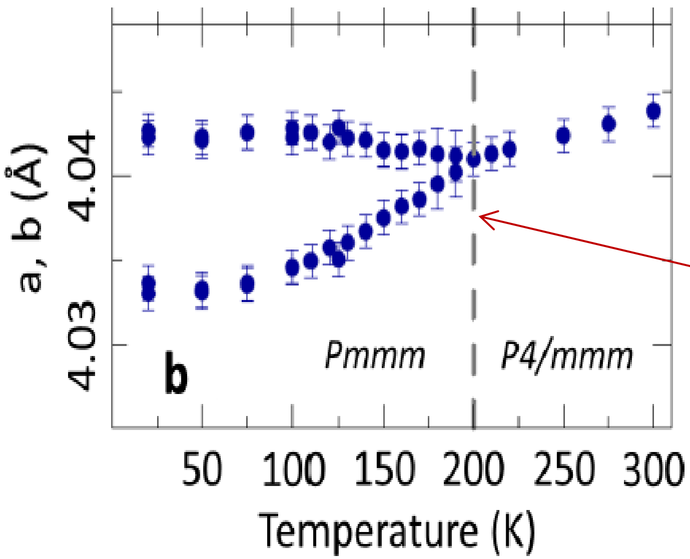

Frandsen et al,
Nat. Comm. 5,
5761 (2014)

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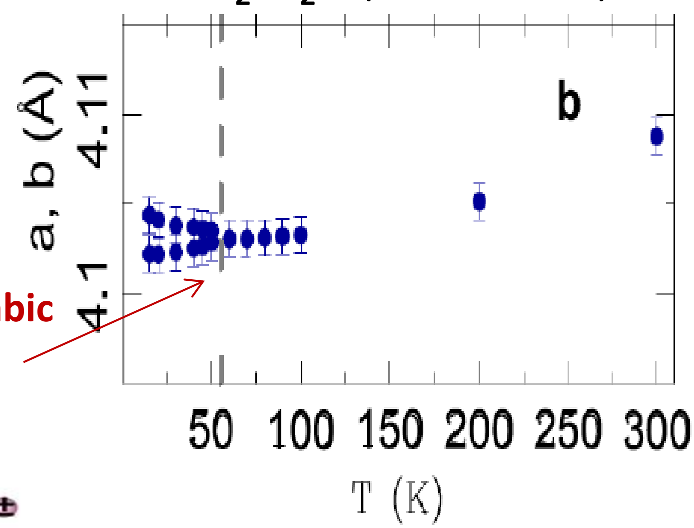

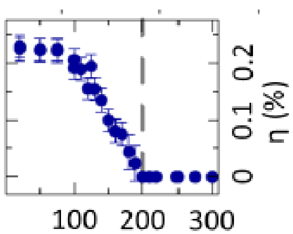

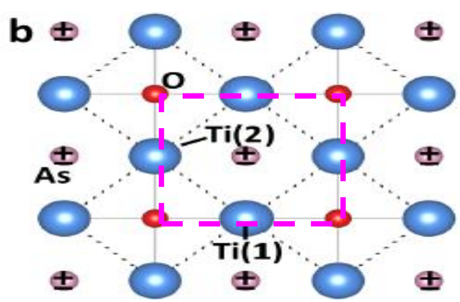

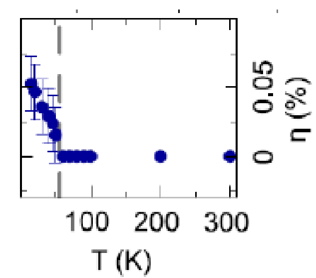

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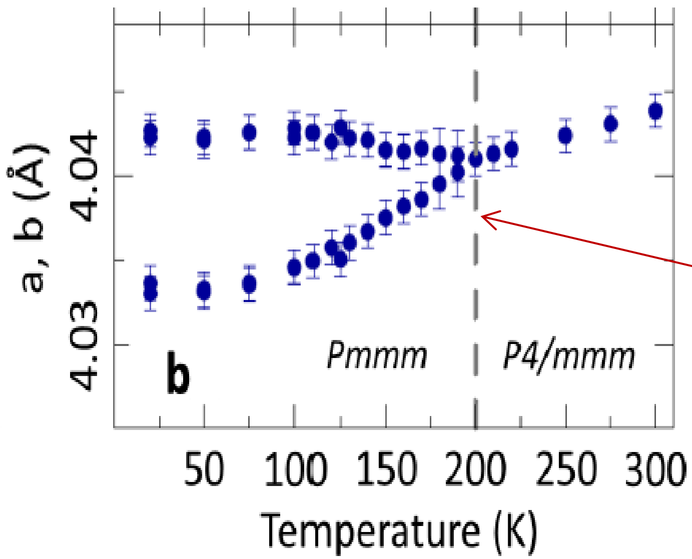
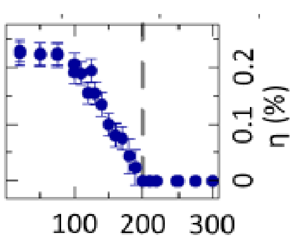
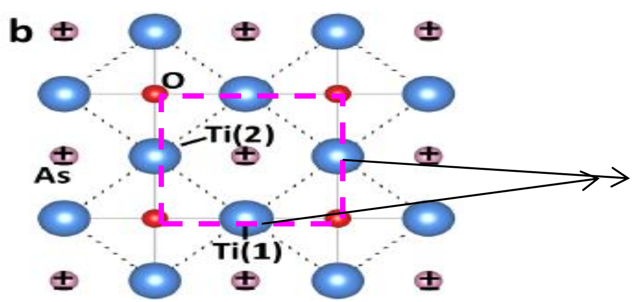


Frandsen et al, Nat. Comm. 5, 5761 (2014)

Intra unit cell nematic state with d-wave charge ordering

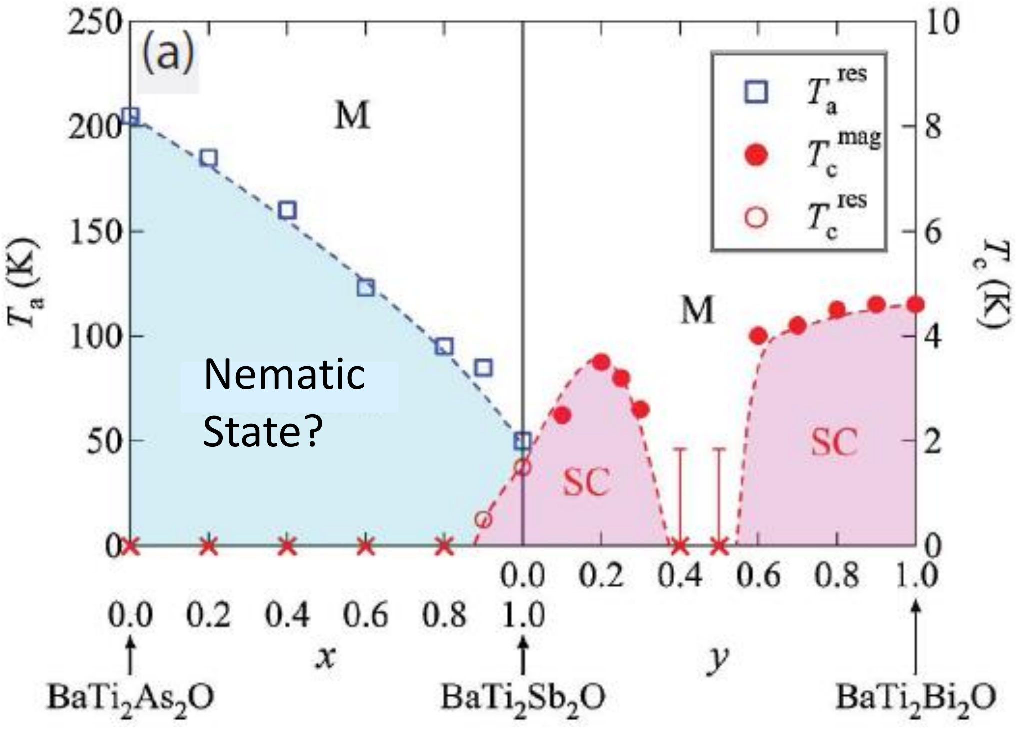
Tetragonal-Orthorhombic Structural transition





Different charge filling

Superconductivity emerging from a nematic state?



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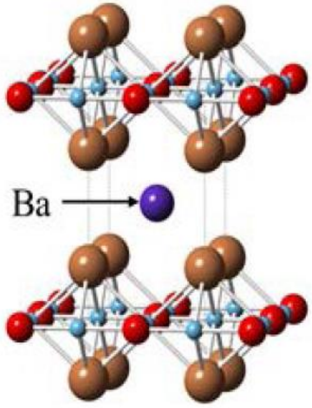
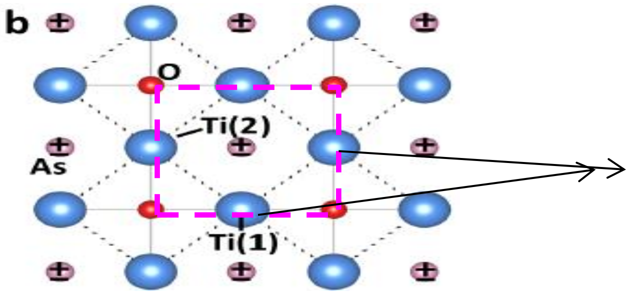




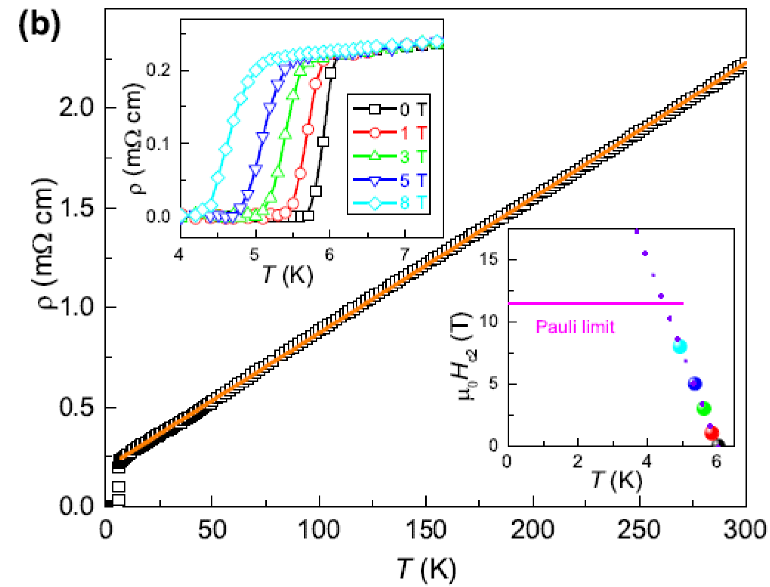
Different charge ordering

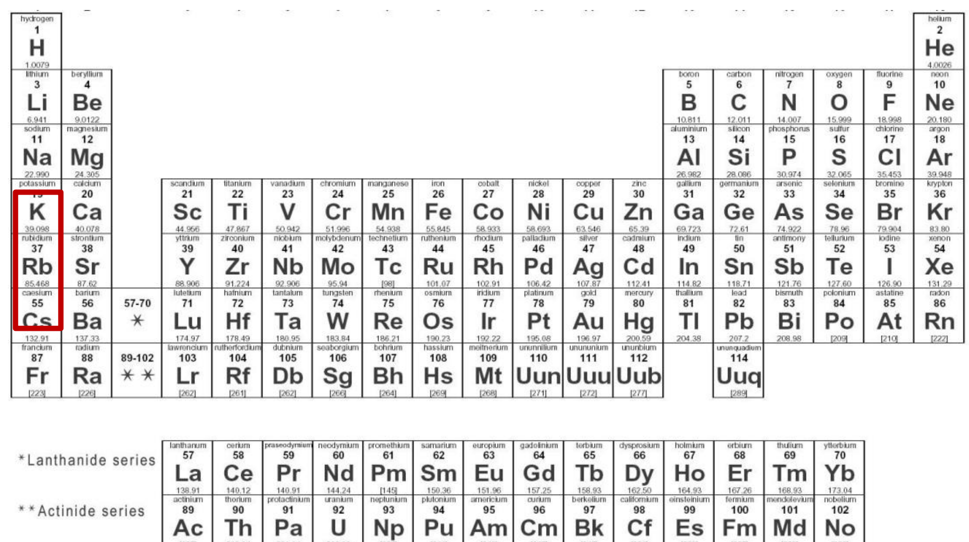
Superconductivity in Quasi-1d $A_2Cr_3As_3$ compounds

$K_2Cr_3As_3$ T_c ~6.1 K

$Rb_2Cr_3As_3$ T_c ~4.8 K

$Cs_2Cr_3As_3$ T_c ~2.2 K





Bao et al, arXiv:1412.0067,
Tang et al, arXiv:1412.2596
Tang et al, arXiv: 1501.02065

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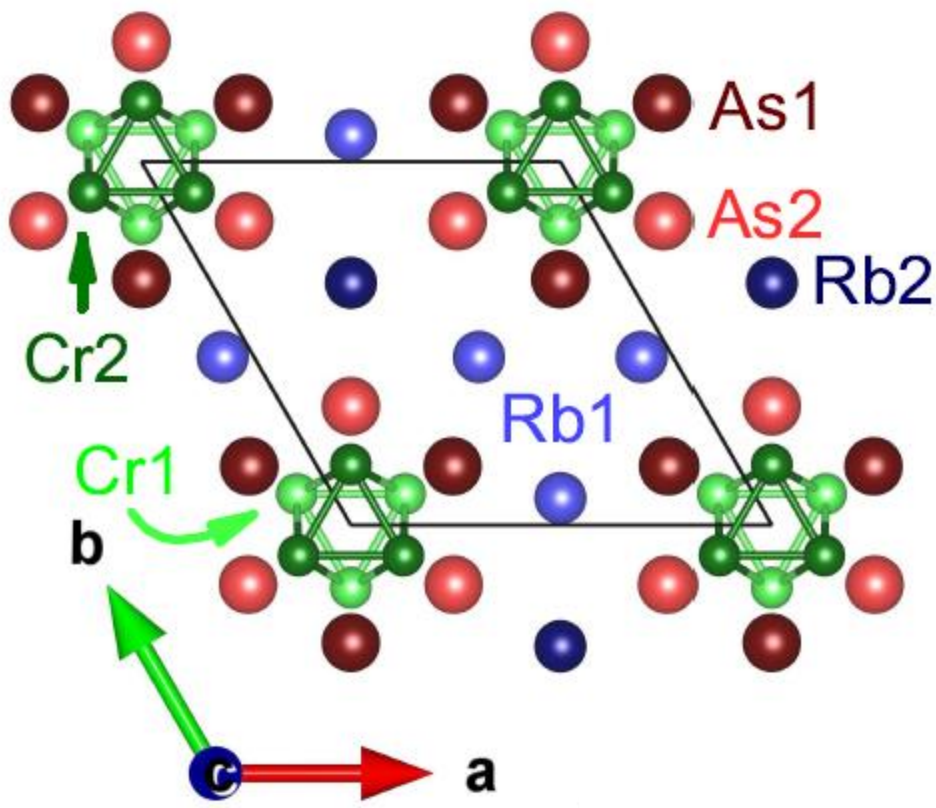
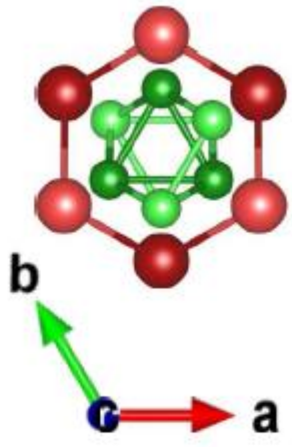
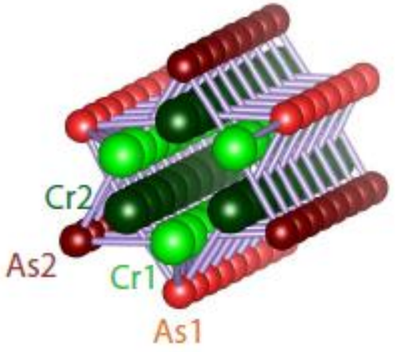




Double wall nanotubes

As (outer shell) Cr (inner shell)

Quasi-1d lattice structure



Bao et al, arXiv:1412.0067

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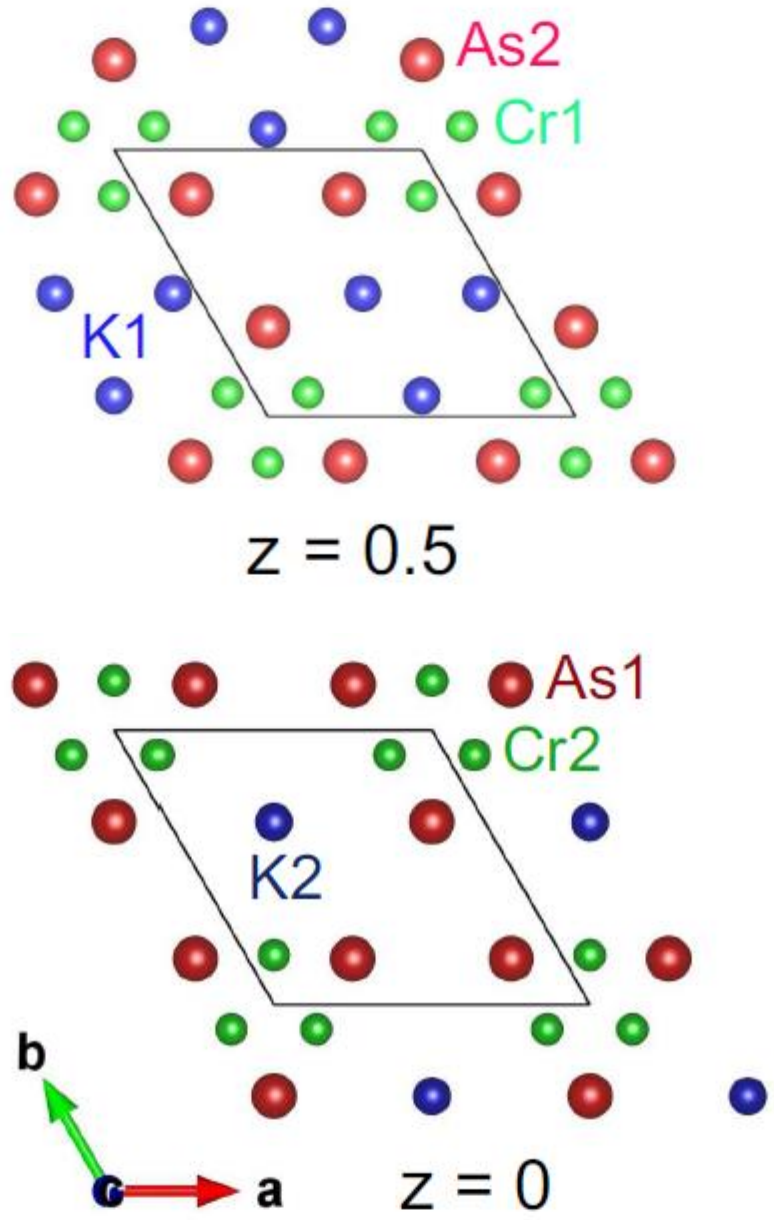

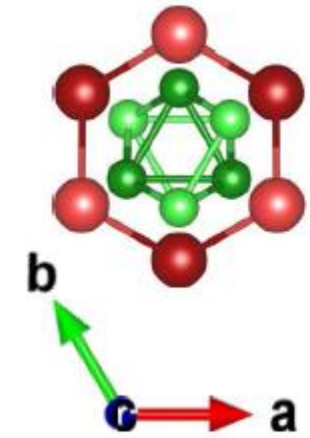

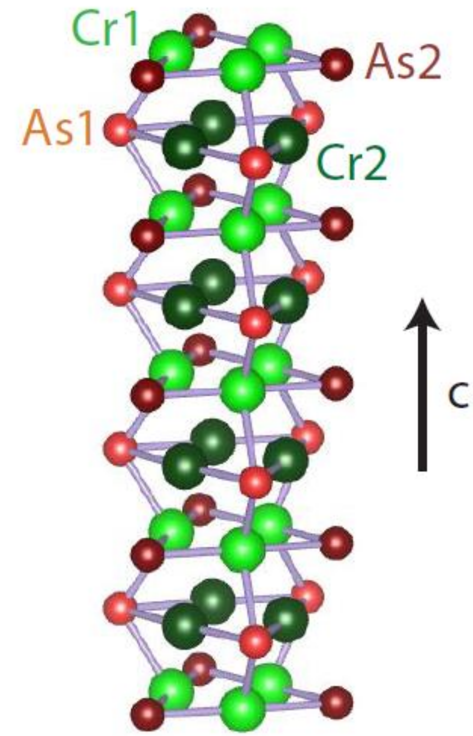

Superconductivity in Quasi-1d $A_2Cr_3As_3$ compounds

- Only very few quasi-1d superconducting materials
- Interacting 1d electronic systems : Luttinger liquids

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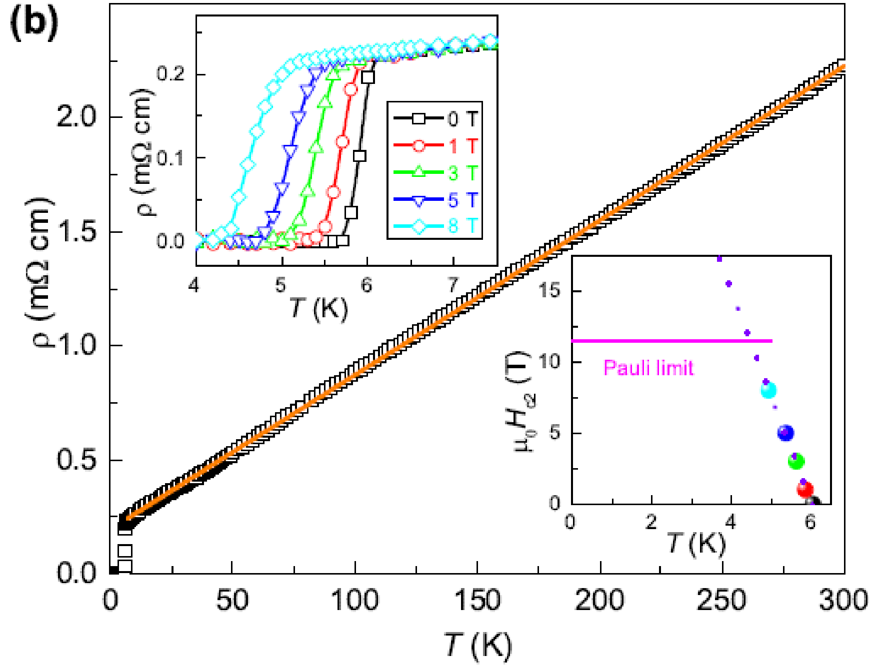
- Very large Sommerfeld constant γ ($C_e = \gamma T$) ⟹ Correlated system

$\gamma \propto m^* \sim 3\text{-}4\ m$ in $K_2Cr_3As_3$



Bao et al, arXiv:1412.0067

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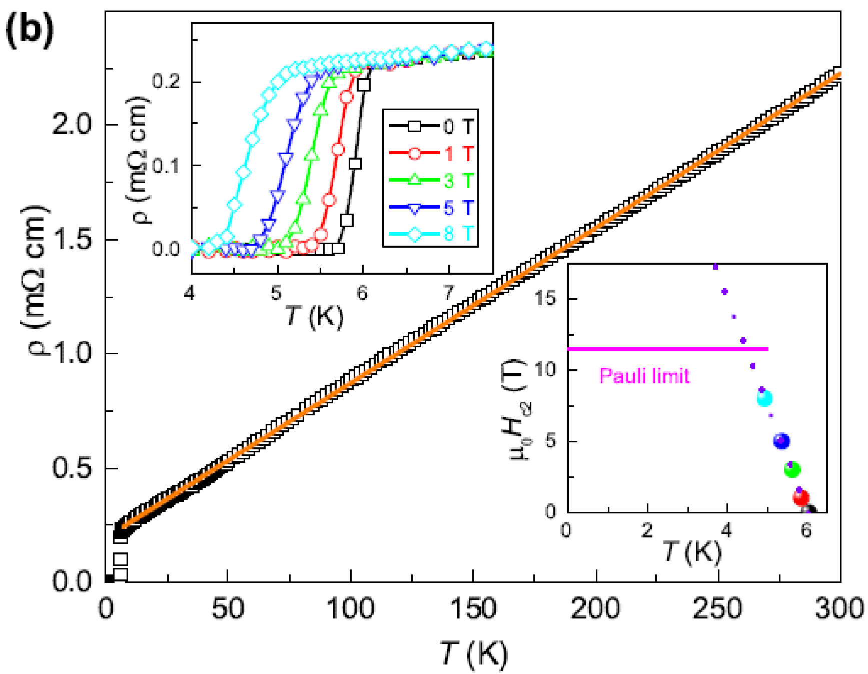
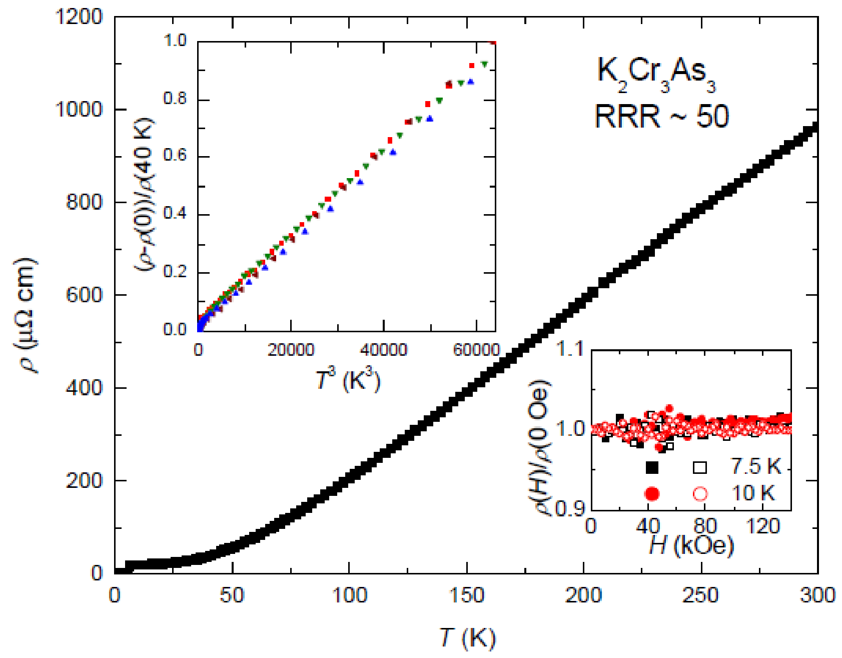




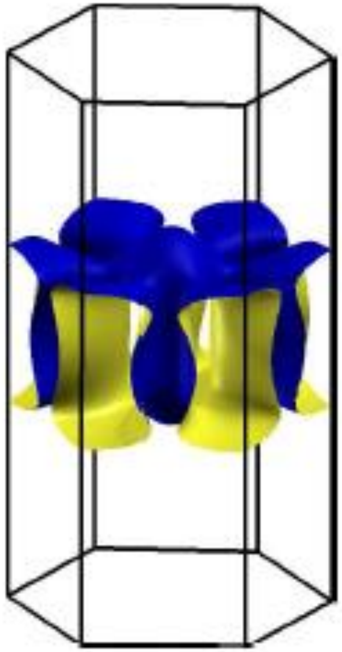
Bao et al, arXiv:1412.0067

Kong et al, arXiv:1501.01554

E. Bascones leni@icmm.csic.es

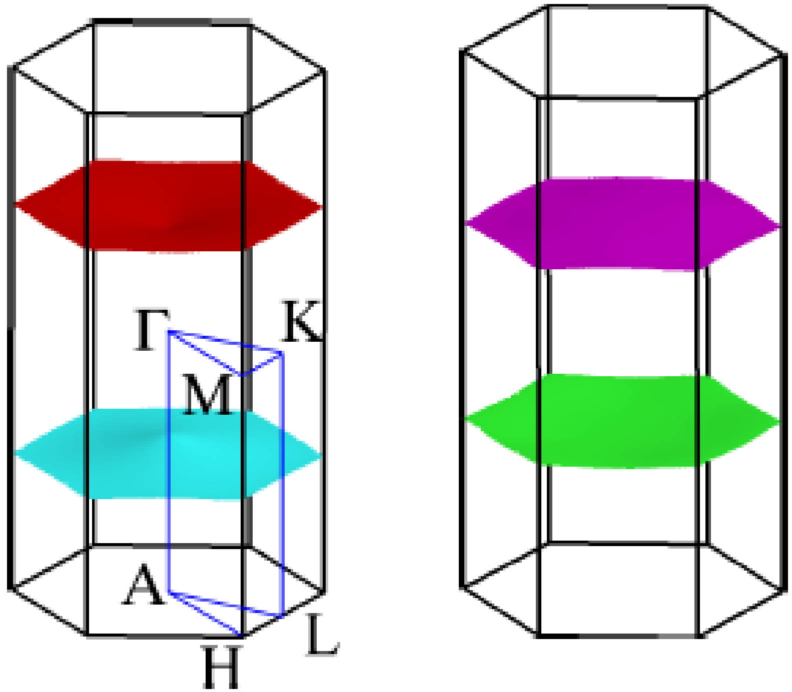
Quasi-1d $A_2Cr_3As_3$ compounds: Fermi surface

3d Fermi pocket



Large density of states

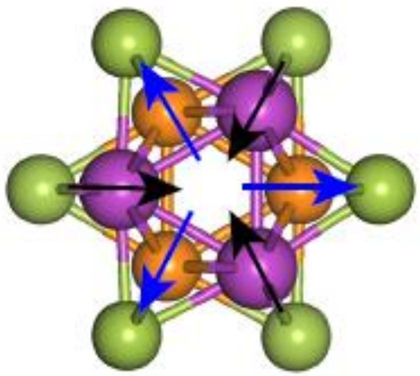
Quasi-1d Fermi pockets



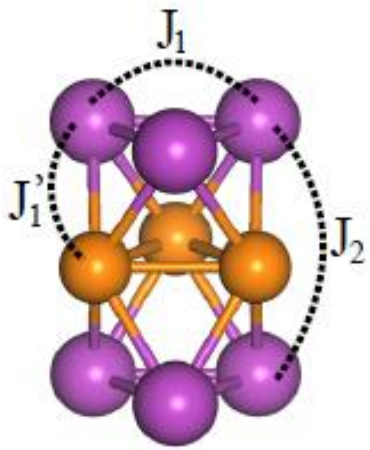
Jiang et al, arXiv:1412.1309

E. Bascones leni@icmm.csic.es

Magnetic tendencies



In-Out Coplanar
Antiferromagnetic Ordering
(ferromagnetic ordering along the chain)



Wu et al, arXiv:1412.1309

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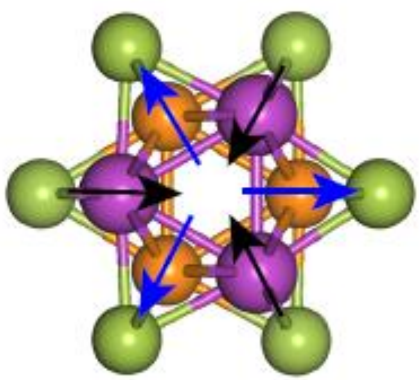

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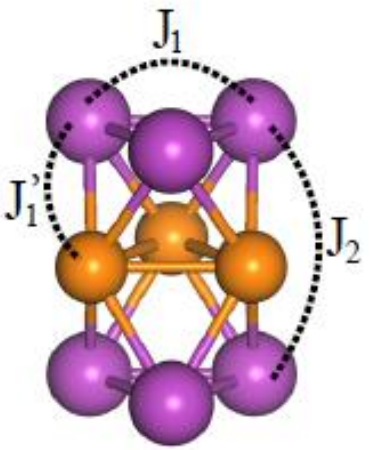
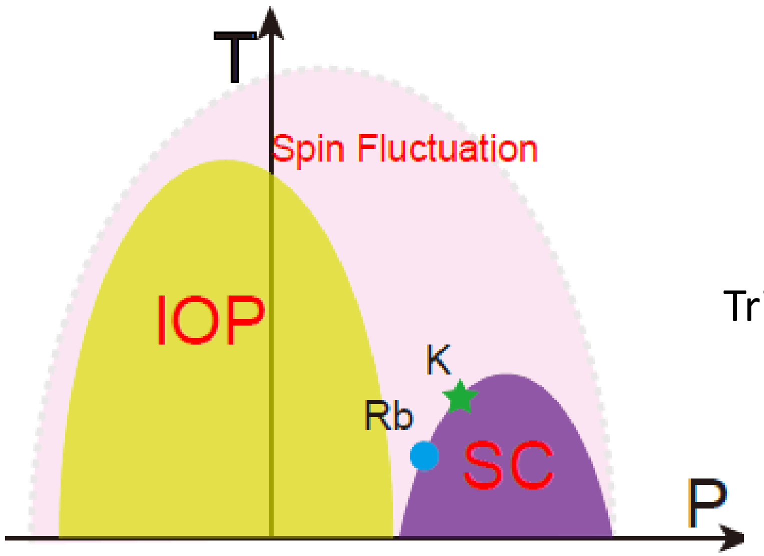


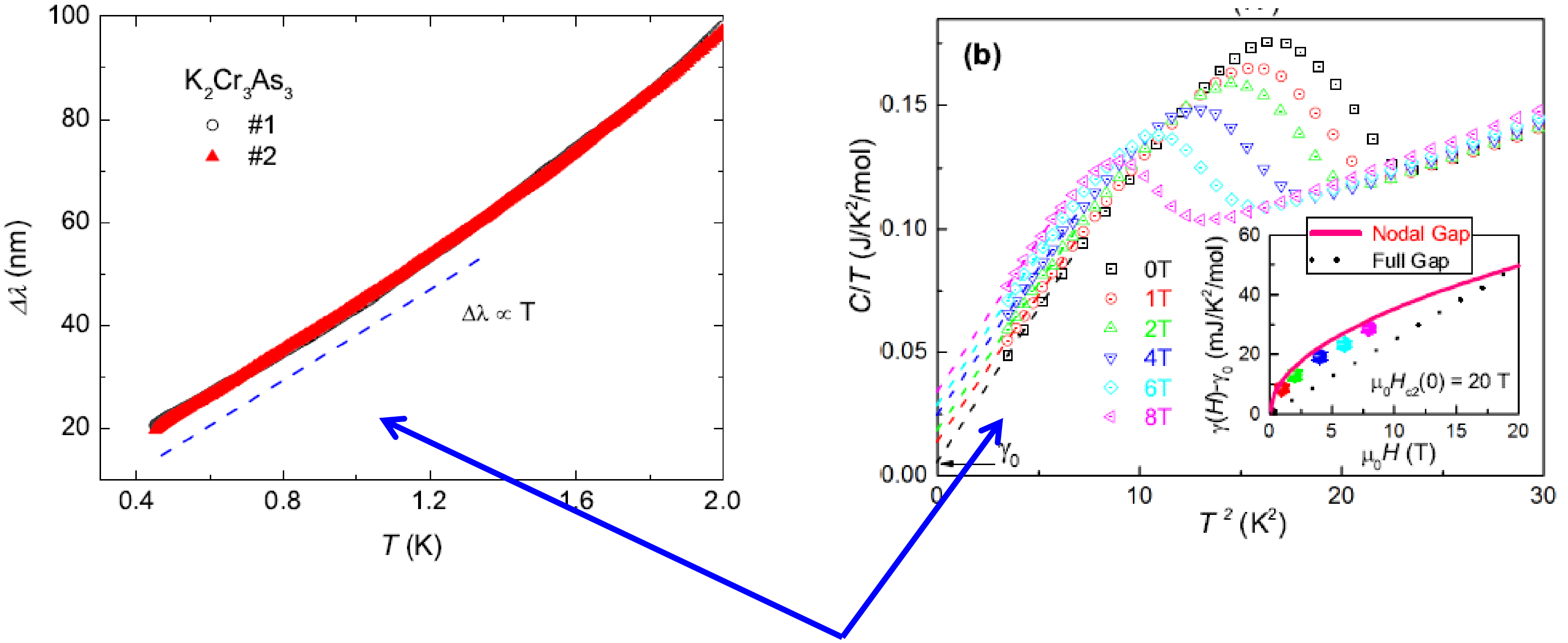


Triplet pz

Wu et al, arXiv:1501.00412, 1503.06707

Idea later supported by explicit calculations,; electron-phonon superconductivity also claimed

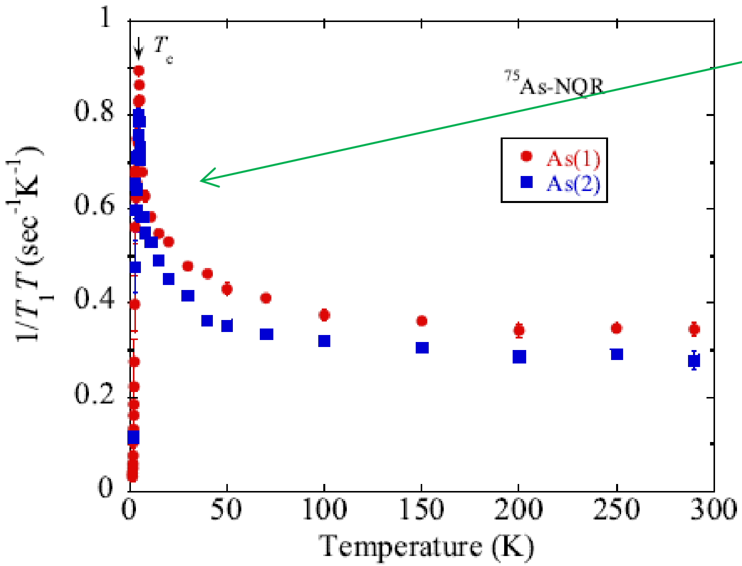
In favour of triplet superconductivity



It seems consistent with the presence of line nodes.

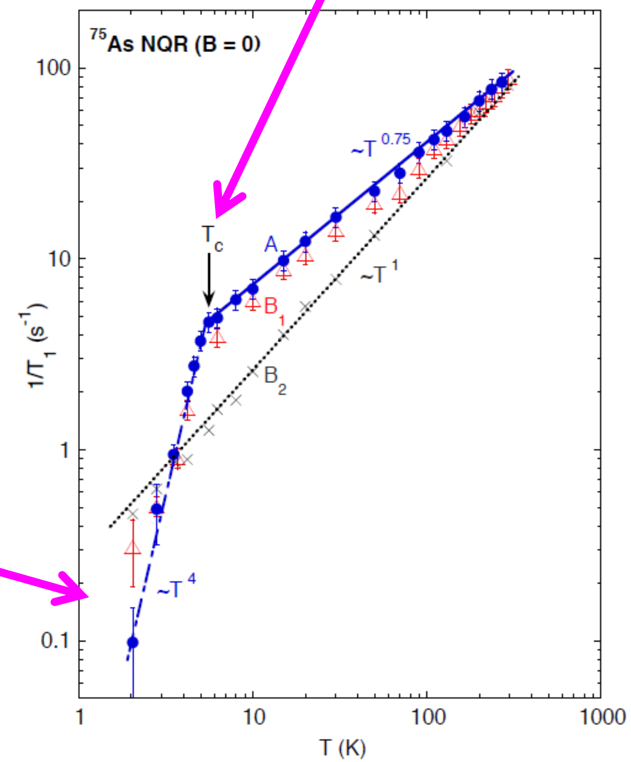
Pang et al, arXiv:1501.01880

In favour of triplet superconductivity



Enhancement of magnetic fluctuations
Towards Tc

No Hebel-Slichter peak



Very small internal magnetic
Field detected by muon spectroscopy
0.003 G

No
exponential
suppression
at low T

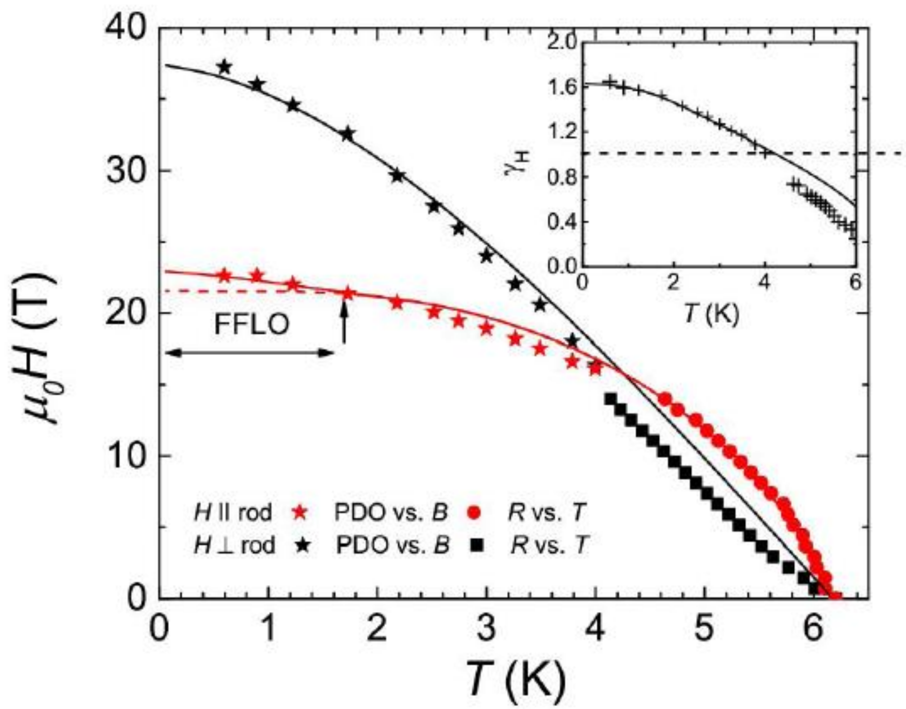
Zhi et al, arXiv:1505.05743

Zhi et al, arXiv:1501.00713

Against triplet superconductivity

- Tc insensitive to impurities
- Hc parallel to the chains Pauli limited.
  Hc perpendicular to the chains not Pauli limited.

Singlet pairing with spins blocked along the chain direction?



Talk G.Cao
Next week

Balakirev et al, arXiv:1505.05547

Lack of inversion center: spin-triplet mixing?

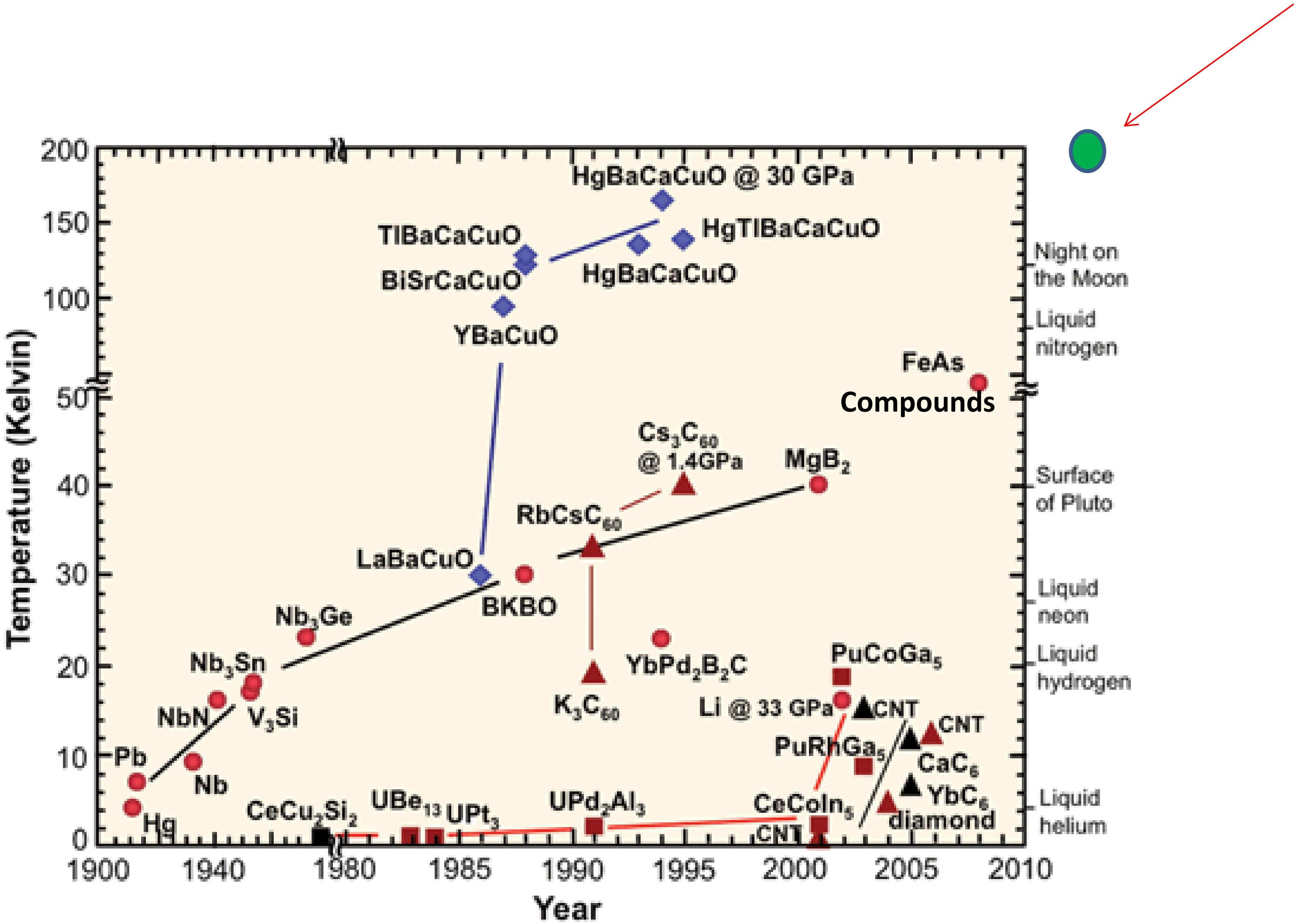


Fig: http://www.ccas-web.org/superconductivity

Metallic Hydrogen: a high-Tc superconductor?

$$T_c = \frac{\omega_{ln}}{1.2} exp\left(\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$

Characteristic phonon frequency

Electron-phonon coupling constant

Coulomb pseudopotential

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Large λ + high ω_{ln} ⟹ High T_c

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⇓

Metallic Hydrogen

Aschroft, PRL 21, 1748 (1968)

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Coulomb pseudopotential

- ❑ Large ω_{ln}: small mass
- ❑ Large λ: as H^+ ion lacks inner structure.
  strong bare electron ion interaction
- ❑ High Density of States. Small μ^* due to screening

T_c ~10^2 K
(at present ~240 K)

Aschroft, PRL 21, 1748 (1968)

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T_c ~10^2 K

but

$P_{H\text{-metal}}$ ~ 400 GPa

Aschroft, PRL 21, 1748 (1968)

Städele & Martin, PRL 84, 6070 (2000)

Hydrogen-rich alloys: high-Tc superconductors?

Hidrogen-rich covalent hydrides MH_4 M: C, Si, Ge, Sn

group IV

- High frequency phonons (H-ions)
- Compensated semimetal with high density of states
- Wideband (μ^* favourable)
- Large electron-ion interactions (H-M)
- Low and large q- electron-phonon coupling

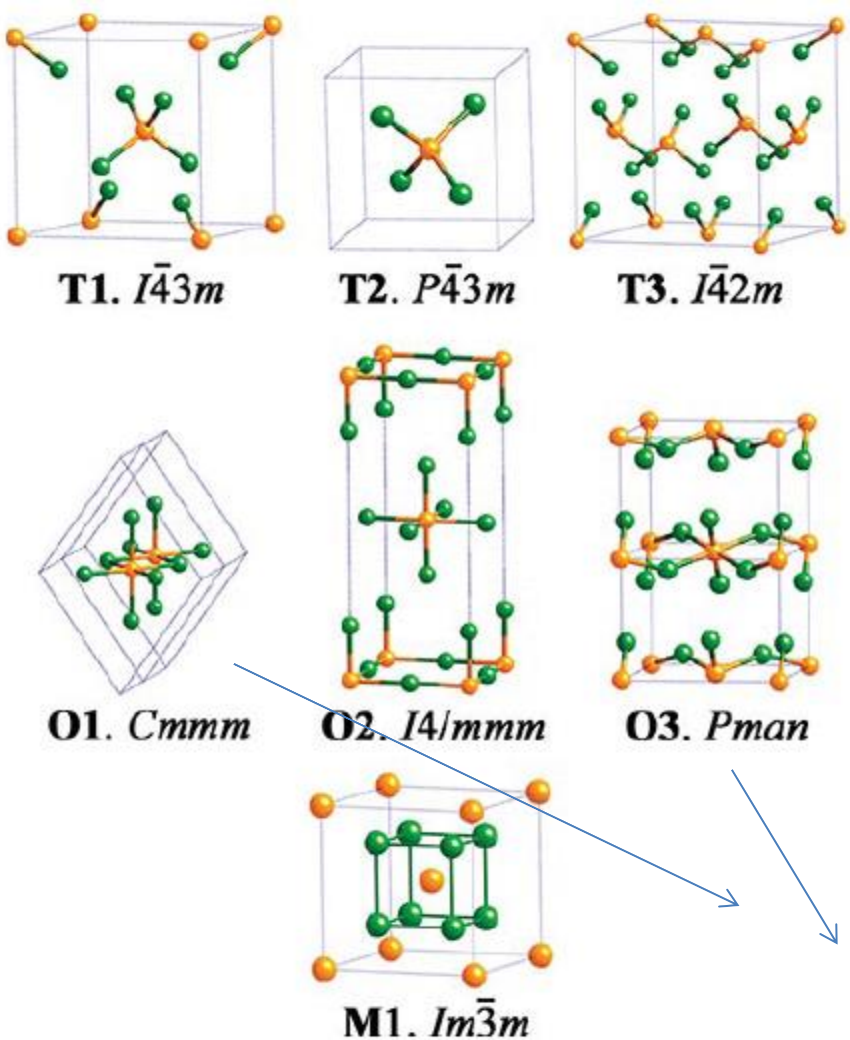
Possibility to tune Tc through M substitutions

smaller P_{metal}

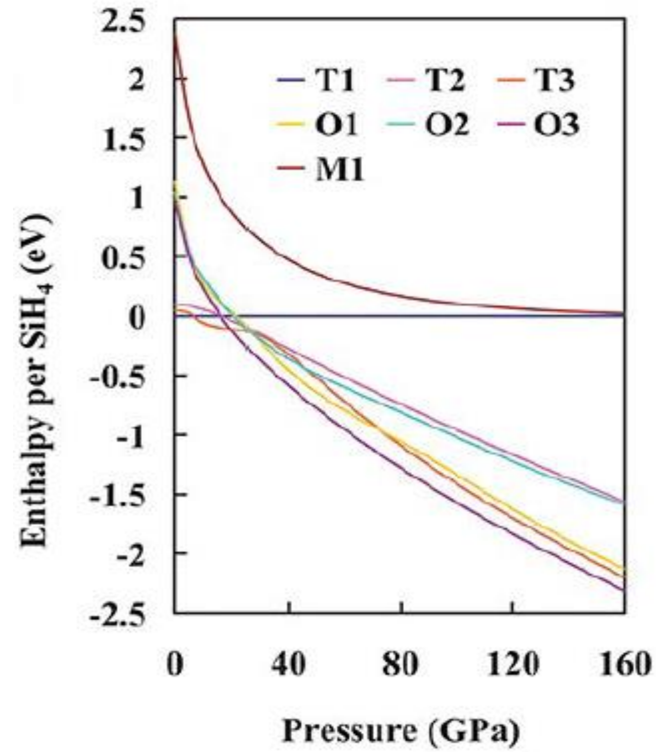
Aschroft, PRL 92, 187002 (2004)

Hydrogen-rich alloys: search for high-Tc superconductors

SiH_4 : stability of different phases



Low pressure phases:
Insulating molecular crystals



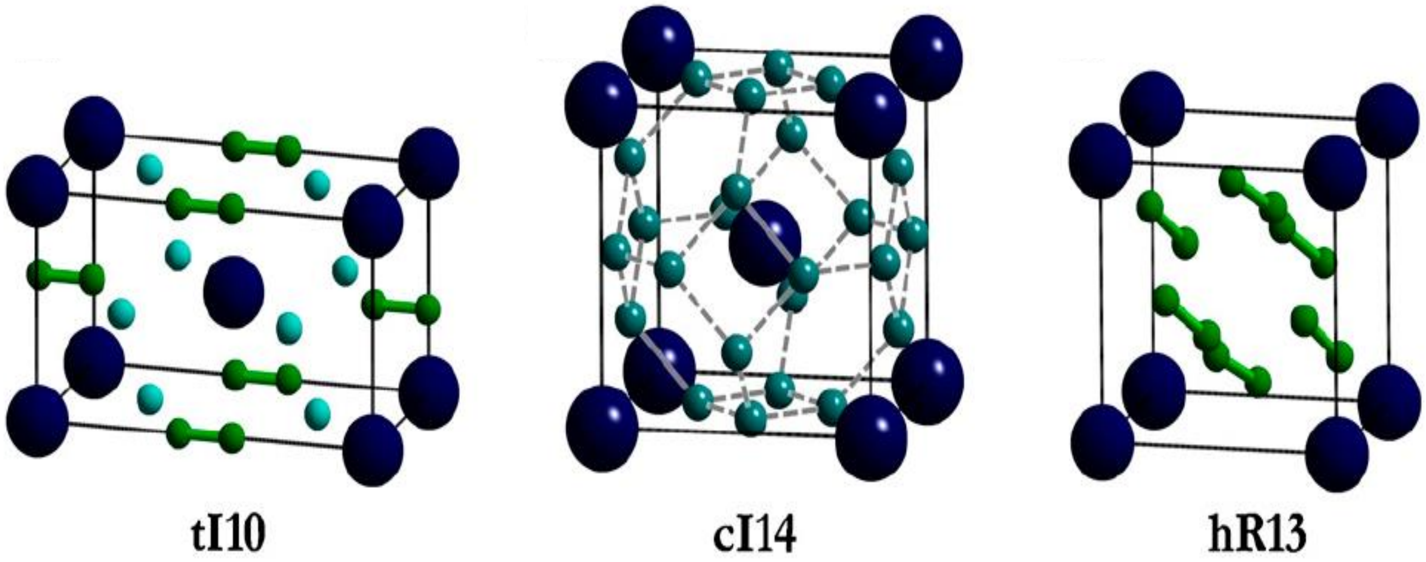
Compact metallic phases
at high pressure

Feng et al, PRL 96, 017006 (2006)

Hydrogen-rich alloys: search for high-Tc superconductors

Ca_mH_n

stability of different compositions & structures as a function of pressure



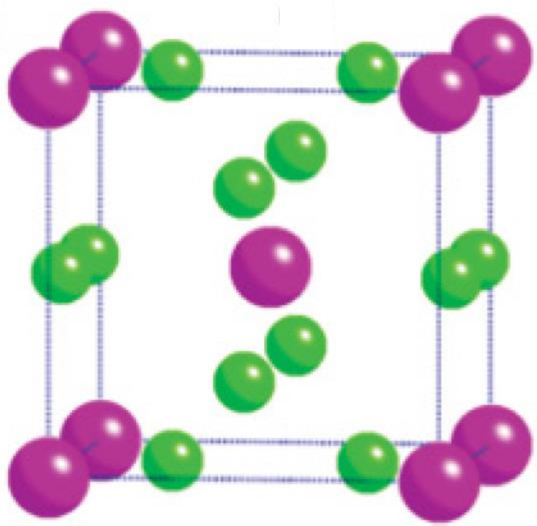
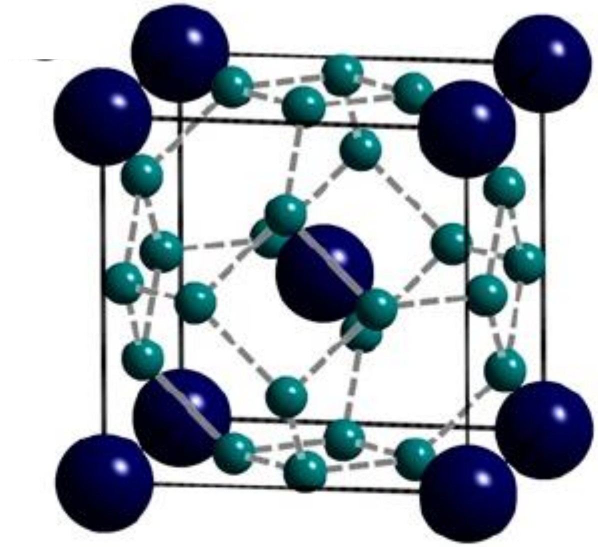
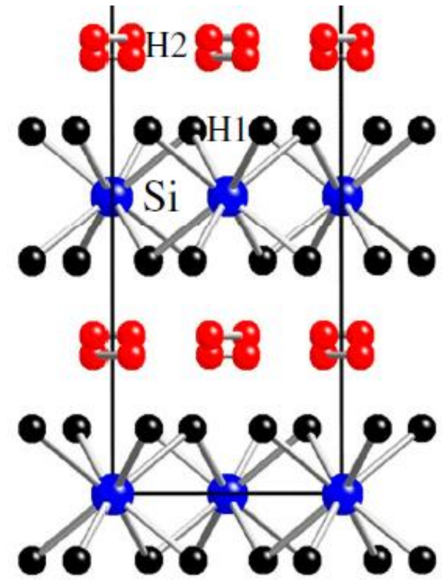
CaH_4
50-200 GPa

CaH_6
150-200 GPa

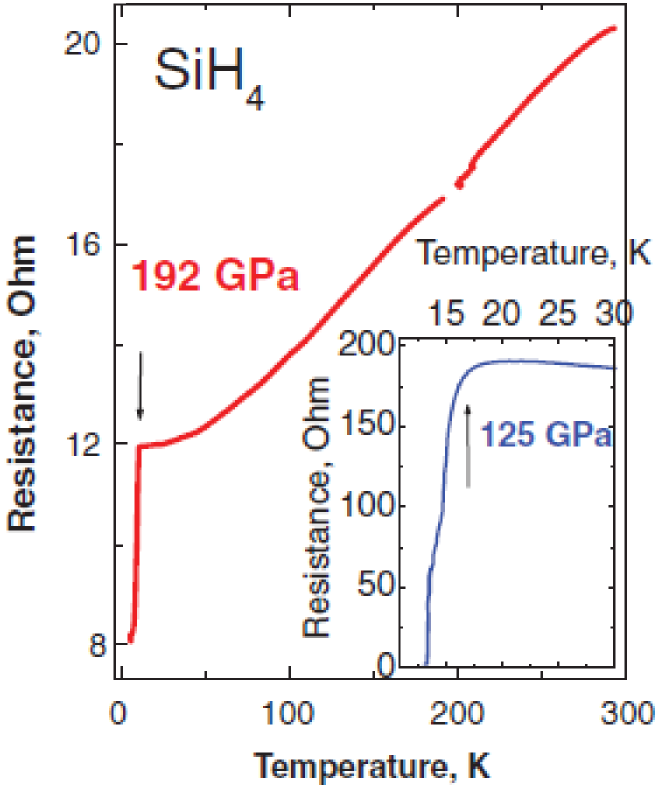
CaH_{12}
100-200 GPa

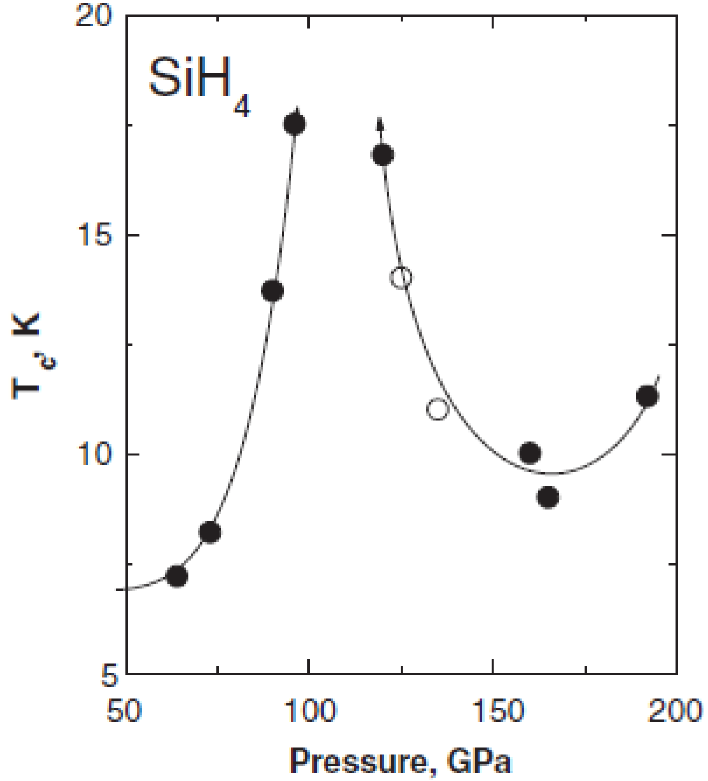
Wang et al, PNAS 109, 6463 (2012)

Hydrogen-rich alloys: search for high-Tc superconductors

GaH_3	CaH_6	$SiH_4(H_2)_2$
		
T_c ~80 K @ 160 GPa	T_c ~220 K @ 150 GPa	T_c ~100 K @ 250 GPa
Gao et al, PRB 84, 06411 (2011)	Wang et al, PNAS 109, 6463 (2012)	Li et al, PNAS 107, 15708 (2010)

Superconductivity in SiH_4 under high-pressure



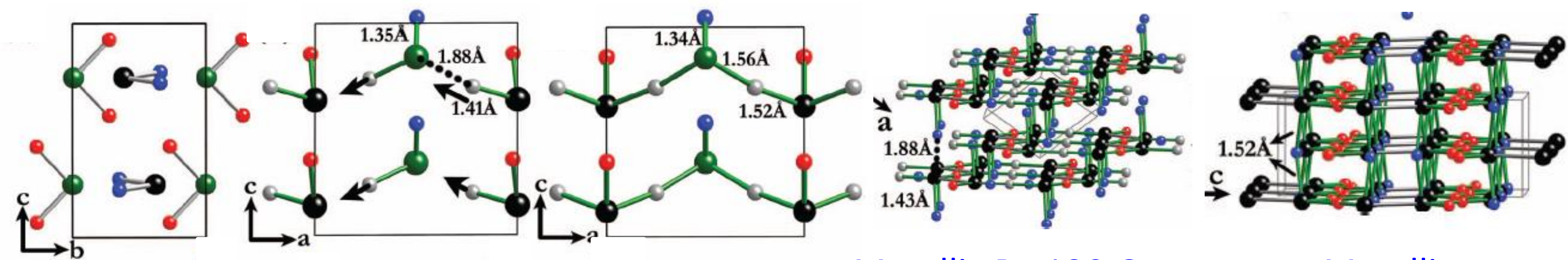


Eremets et al, Science 319, 1506 (2008)

Sulfur hydrides: search for high-Tc superconductors

H_2S under pressure

P2/c (P>8,7 GPa) P2/c (8,7-29 GPa) Pm2c1 (29-65 GPa) P1 (80-158 GPa) Cmca (P>158 GPa)



Li et al, J. Chem. Phys. 140, 174712 (2014)

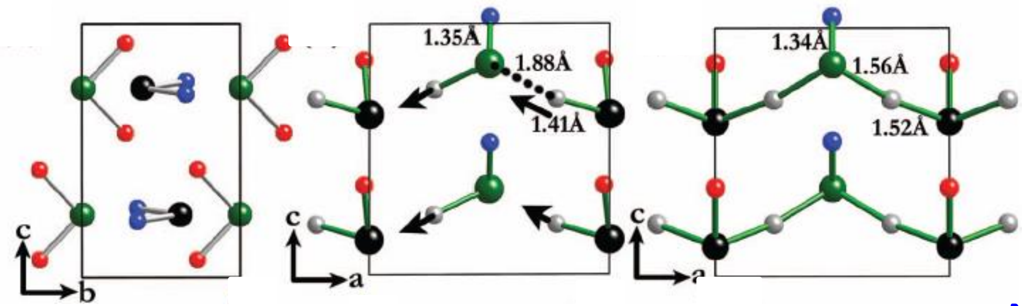
Metallic P> 130 Gpa
Tc~33-60 K

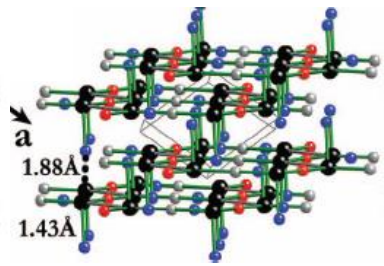
Metallic
Tc~80 K @158 GPa

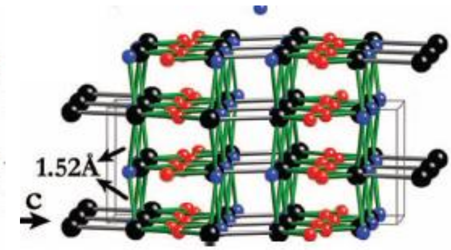
Sulfur hydrides: search for high-Tc superconductors

H_2S under pressure

P2/c (P>8,7 GPa) Pc (8,7-29 GPa) Pm2c1 (29-65 GPa) P1 (80-158 GPa) Cmca (P>158 GPa)







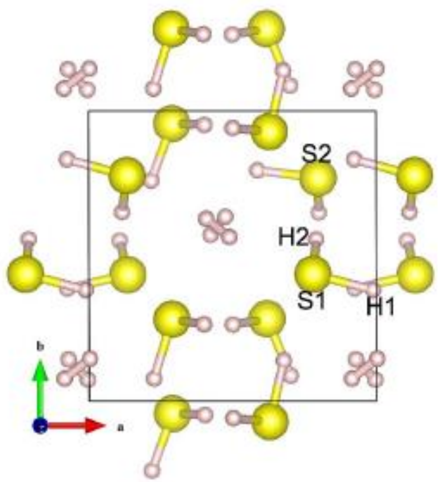
Li et al, J. Chem. Phys. 140, 174712 (2014)

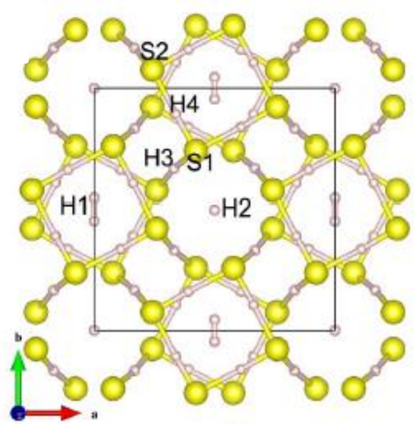
Metallic P> 130 Gpa
Tc~33-60 K

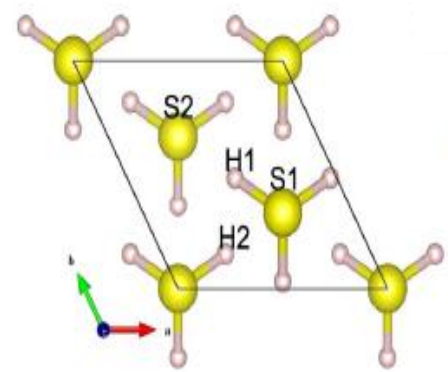
Metallic
Tc~80 K @158 GPa

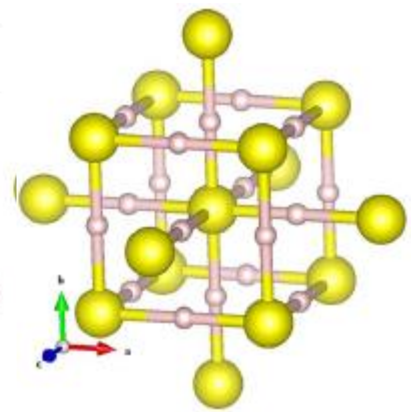
$(H_2S)_2H_2$ under pressure ⟶ H_3S

P1 (P< 37 GPa) Cccm (37-111 GPa) R3m (111-180 GPa) I3-3m (P > 180 GPa)









Metallic
Tc~160 K

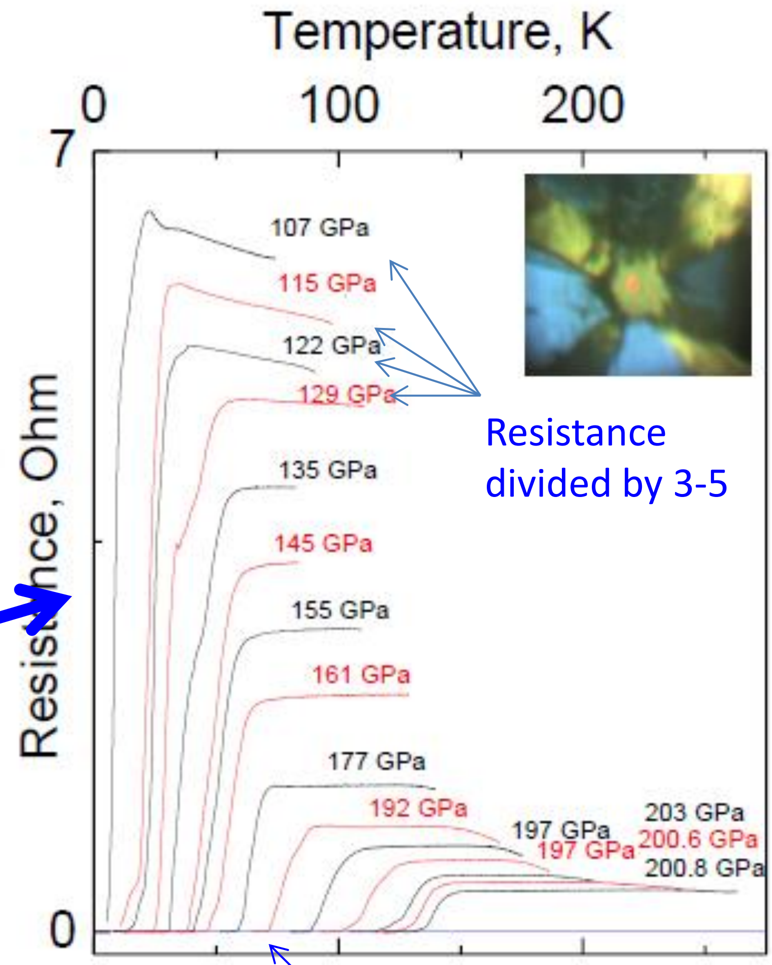
Metallic
Tc~200 K

Duan et al, Sci. Rep. 4, 6968 (2014)

H_2S under high-pressure

- In electrical measurements it starts to conduct at P ~ 50 Gpa
- At 90-100 GPa further drop in resistance.

Sharp drop in resistance with cooling at "Tc" .

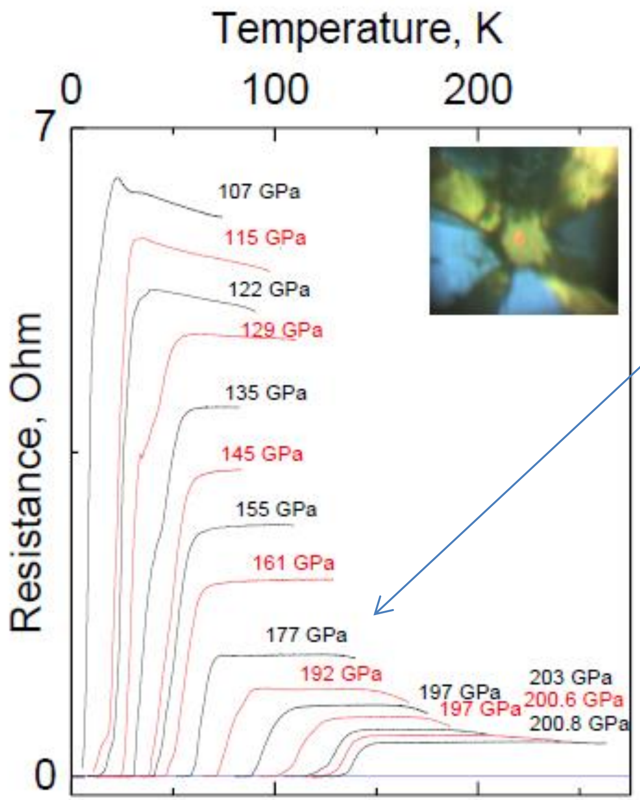


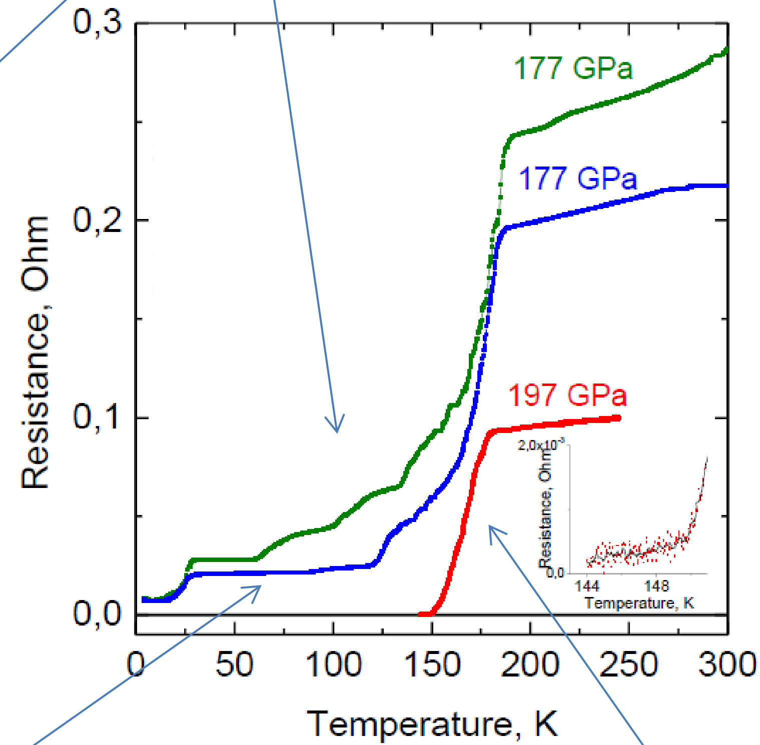
Transition temperature depends on pressure

Drozdov, Eremets,Troyan arXiv:1412.0460 Drozdov et al, arXiv:1506.08190

H_2S under high-pressure

The transition temperature depends on the route followed to reach the Pressure & Temperature conditions



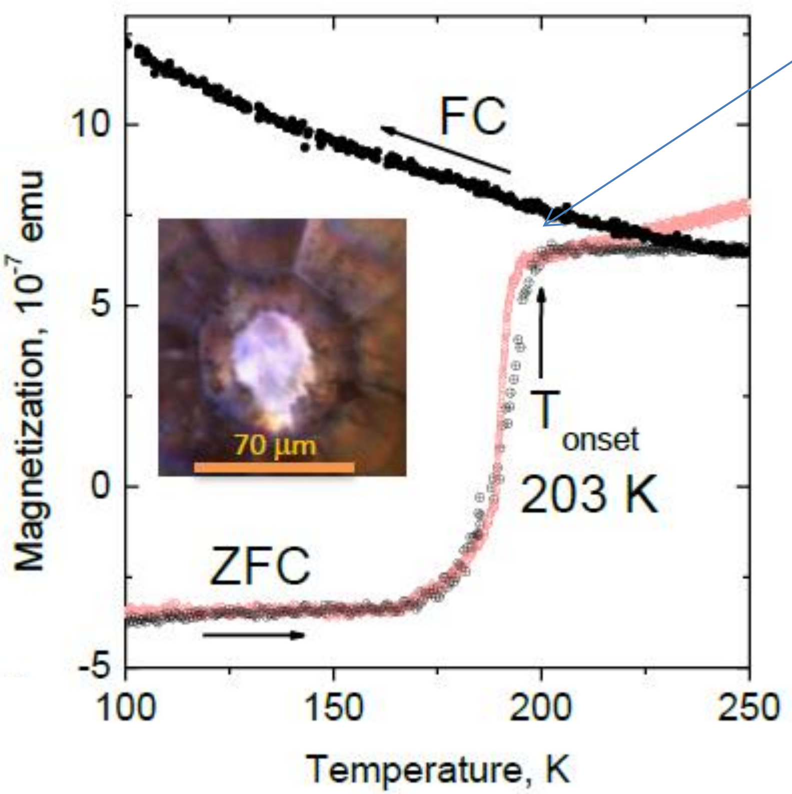


Temporary steps appear in some curves

Broad transitions

Drozdov, Eremets,Troyan arXiv:1412.0460 Drozdov et al, arXiv:1506.08190

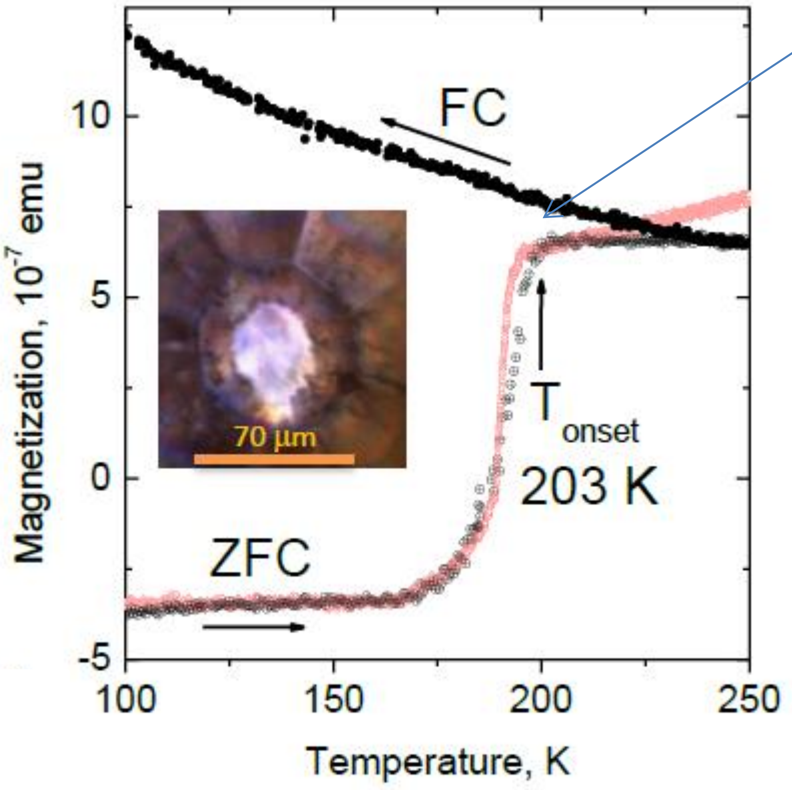
H_2S under high-pressure



Diamagnetic signal

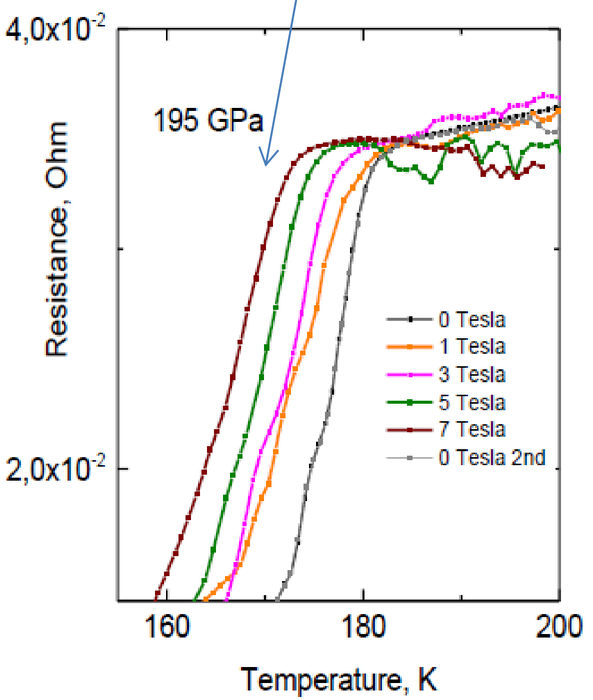
Drozdov et al, arXiv:1506.08190

H_2S under high-pressure



Diamagnetic signal

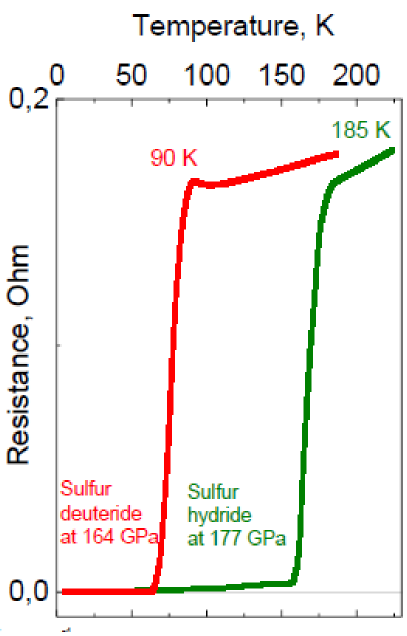
Transition temperature reduced with magnetic field

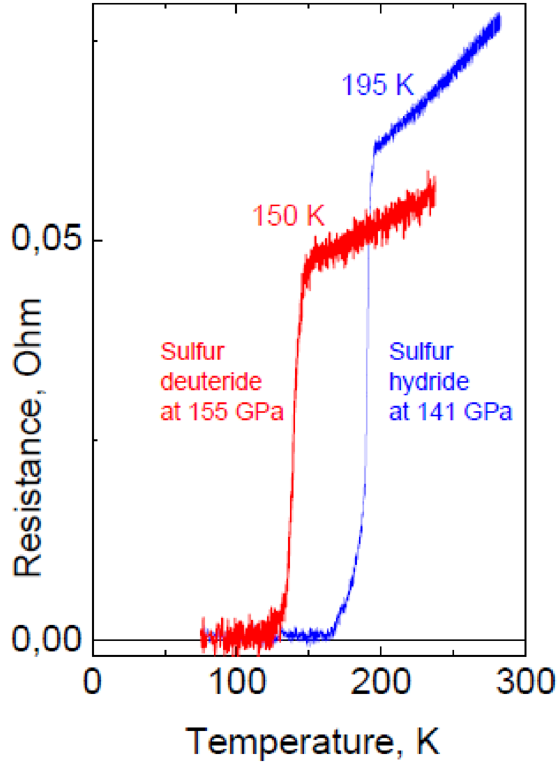


Drozdov, Eremets,Troyan arXiv:1412.0460   Drozdov et al, arXiv:1506.08190

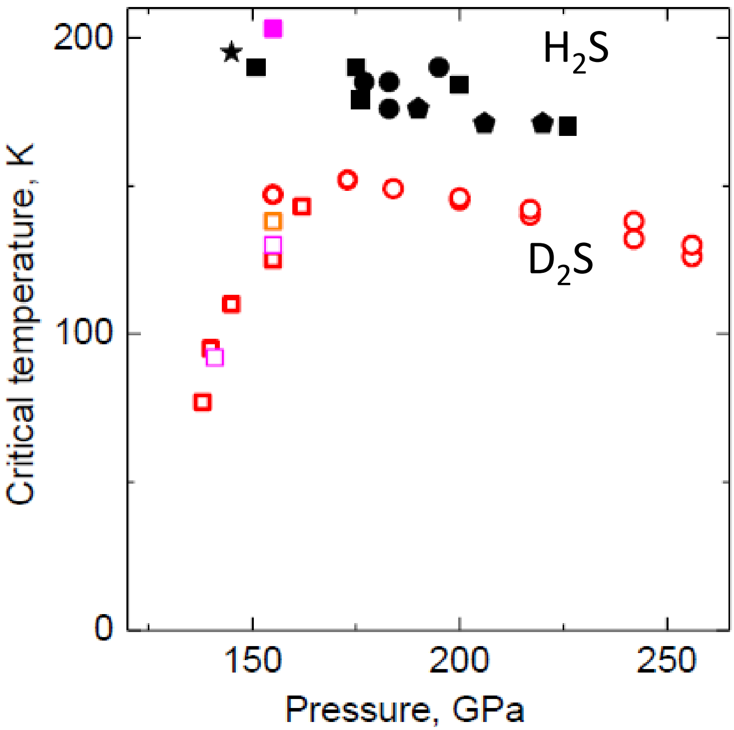
H_2S under high-pressure

Isotope effect





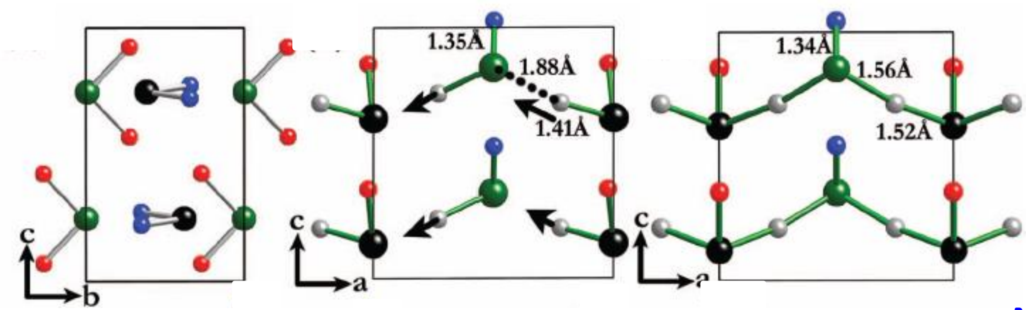
Annealed samples

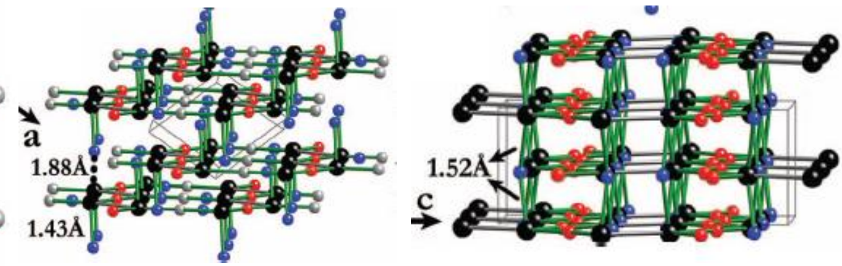


Drozdov, Eremets,Troyan arXiv:1412.0460 Drozdov et al, arXiv:1506.08190

H_2S under high-pressure

P2/c (P>8,7 GPa) Pc (8,7-29 GPa) Pm2c1 (29-65 GPa) P1 (80-158 GPa) Cmca (P>158 GPa)

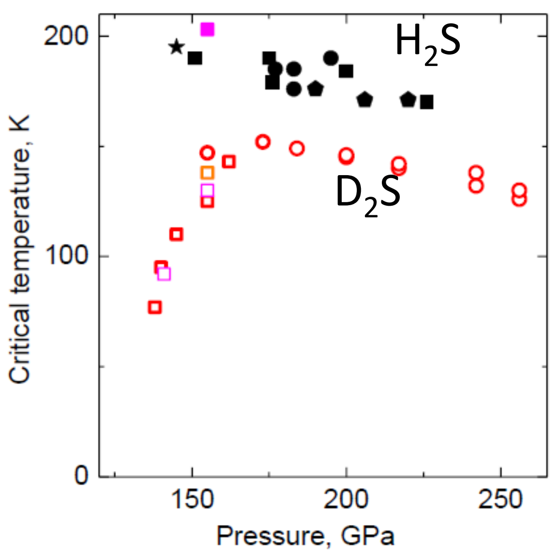




Li et al, J. Chem. Phys. 140, 174712 (2014)

Metallic P> 130 Gpa
Tc~33-60 K

Metallic
Tc~80 K @158 GPa



Drozdov, Eremets,Troyan arXiv:1412.0460 Drozdov et al, arXiv:1506.08190

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H_2S under high-pressure

Stability of H_2S under pressure revisited

P2/c (P>8,7 GPa)   Pc (8,7-29 GPa)   Pm2c1 (29-65 GPa)   P1 (80-158 GPa)   Cmca (P>158 GPa)

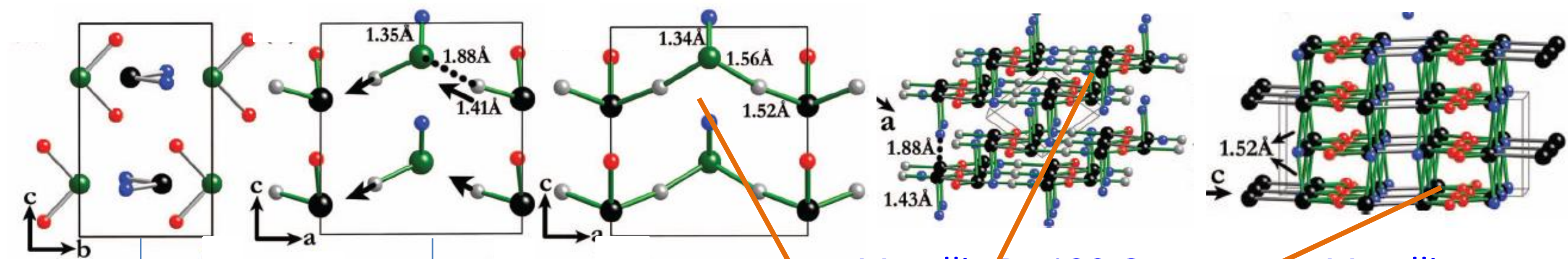


Fig: Li et al, J. Chem. Phys. 140, 174712 (2014)

Metallic P> 130 Gpa
Tc~33-60 K

Metallic
Tc~80 K @158 GPa

P2/c (20-30 GPa)   Pc (30-50 GPa)

Not stable

Decomposition
@ 50 GPa

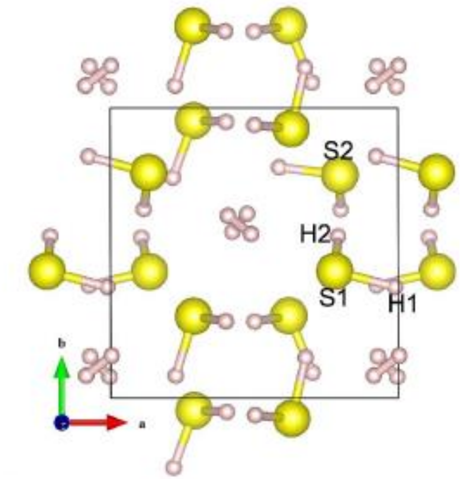
$$3\,H_2S \longrightarrow 2H_3S + S$$

Duan et al, PRB 91, 180502 (2015), Bernstein et al, PRB 91, 060511 (2015), Errea et al, PRL 114, 157004 (2015)

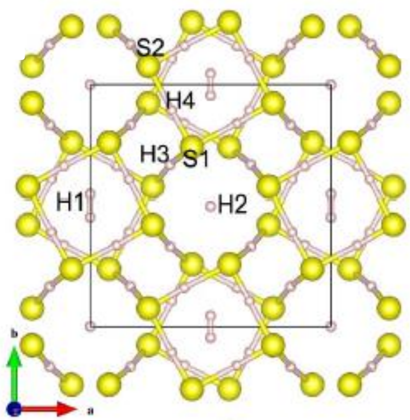
H_3S under high-pressure

$(H_2S)_2H_2$ under pressure → H_3S

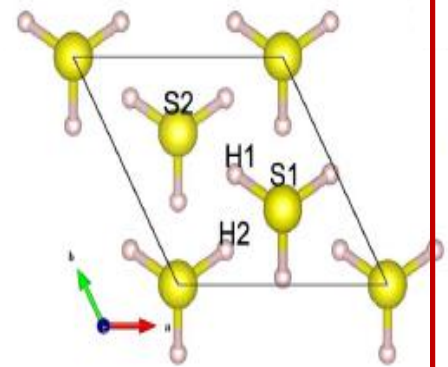
P1 (P< 37 GPa)



Cccm (37-111 GPa)

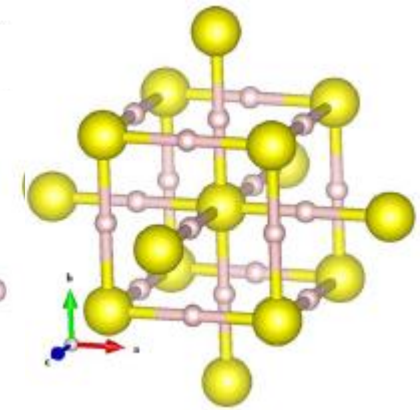


R3m (111-180 GPa)



Metallic
Tc~160 K

I3-3m (P > 180 GPa)



Metallic
Tc~200 K

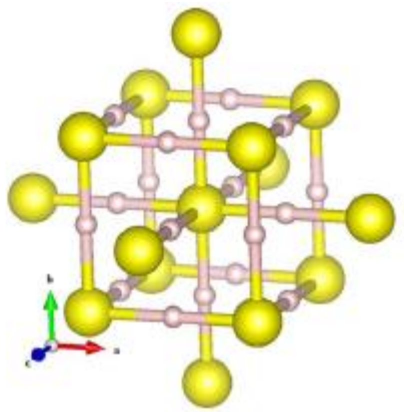
Duan et al, Sci. Rep. 4, 6968 (2014)

H_3S under high-pressure: Calculations revisited

Different approximations/ab-initio codes

- Tc ~ 150-250 K @ 200 Gpa
  λ ~ 1.6- 2.64
  ω_{ln} ~1160-1500 K
  μ^*~0.1-0.16

$$T_c = \frac{\omega_{ln}}{1.2} exp\left(\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$

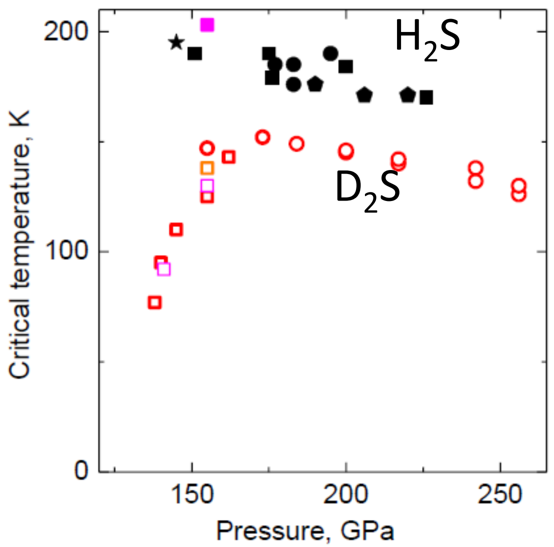


Duan et al, Sci. Rep. 4, 6968 (2014)

- Large e-ph coupling: covalent bonds

- Strongly anharmonic

  (λ: 2.64 $\rightarrow$1.84, Tc: 250K $\rightarrow$194 K)
  Isotope efffect Tc~$M^{-\alpha}$ α: 0.5 $\rightarrow$0.35

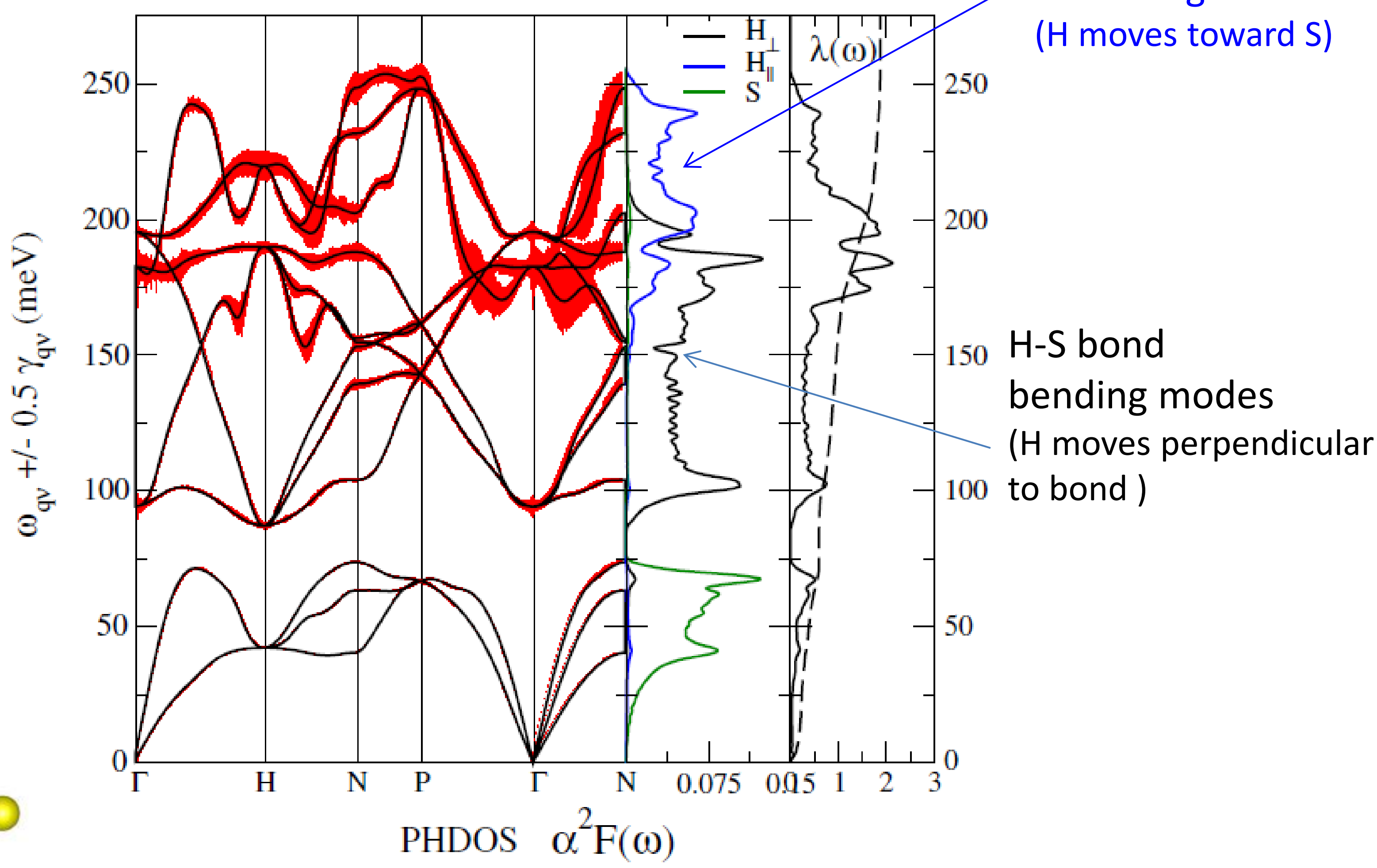


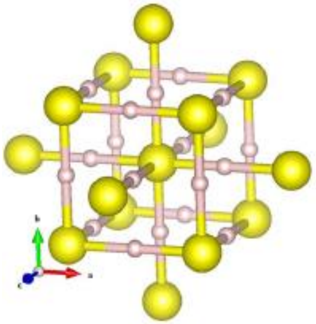
Errea et al PRL 114, 157004(2015), Bernstein et al, PRB 91, 060511(2015), Flores-Livas et al, arXiv:1501.06336, Akashi et al, arXiv: 1502:00936 Zhang et al, arXiv: 1502.02607, Heil-Boeri, arXiv: 1507.02522,

Drozdov et al, arXiv:1506.08190

H_3S under high-pressure

Role played by H vibrations





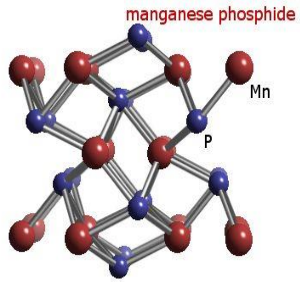
Errea et al, PRL 114, 157004 (2015)

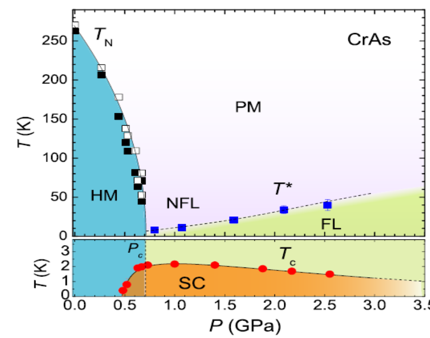
Prospects for new high-Tc superconductors

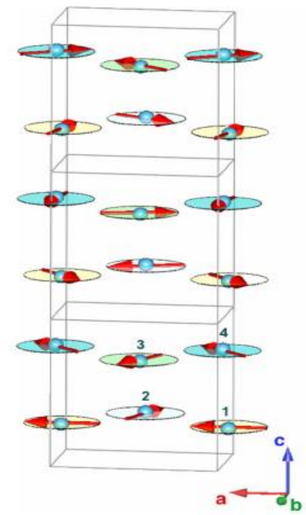
Material	Tc	Ref.
H_2Br	10 K @ 240 GPa	Duan et al, arXiv: 1504.01196
PtH	16 K @ 100 GPa	Szcesniak-Zemla, arXiv 1504.01349
H_4I	13.7 K @ 150 GPa	Shamp & Zurek, arXiv:1507.02616
HSe	39 K @ 250 GPa	Zhang et al, arXiv:1502.02607
PoH_4	41.1 K @ 200 GPa	Liu et al, 1503.08587
$GeH_4(H_2)_2$	80 K @ 250 GPa	J. Phys. Chem. C 116, 5225 (2012).
GaH_3	80 K @ 160 GPa	Gao et al, PRB 84, 06411 (2011)
$SiH_4(H_2)_2$	100 K @ 250 GPa	Li et al, PNAS 107, 15708 (2010)
H_4Te	104 K @ 170 GPa	Zhong et al, 1503.00396
H_3Se	116 K @ 200 GPa	Zhang et al, arXiv:1502.02607
GeH_3	140 K @ 180 GPa	Abe & Aschroft. PRB 88, 174110 (2013).
$H_3O_{0.5}S_{0.5}$	164 K	Heil-Boeri, arXiv:1507.02522
CaH_6	235 K @150 GPa	Wang et al, PNAS 109, 6463 (2012)

New perspectives in superconductors

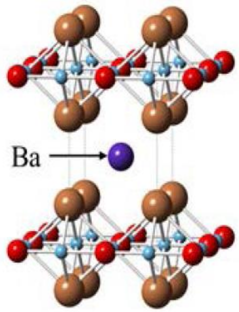
❑ CrAs and MnP, two new superconducting with an helimagnetic parent phase and a possible non trivial relation with magnetism

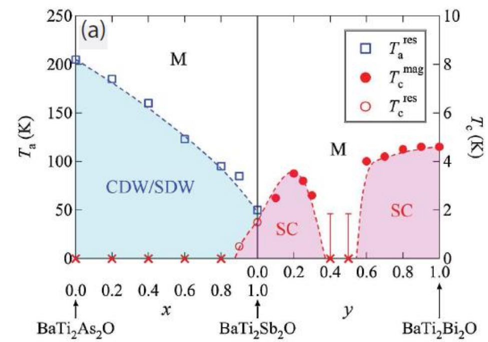


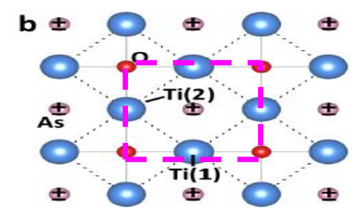




❑ Titanium oxypnictides, superconductivity could emerge from a nematic state

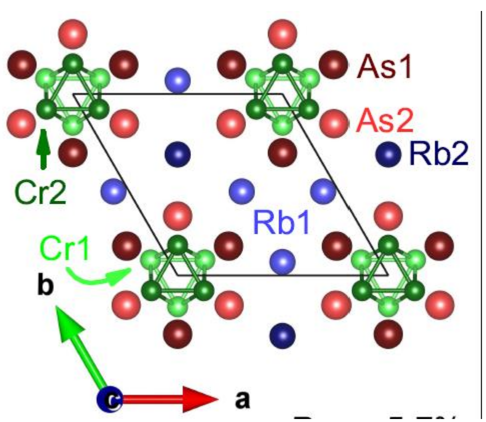




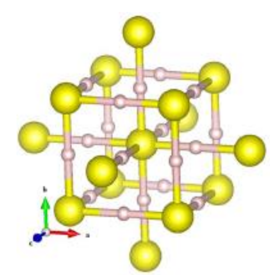


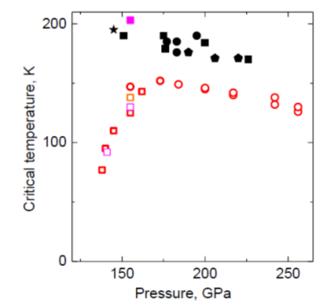
❑ Quasi-1d A2Cr3As3

Triplet SC or Singlet with spin blocking?



❑ H_2S under pressure Possible record of Tc Electron-phonon superconductor





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New perspectives in superconductors

- Many other recently discovered superconductors: $Zr_5Sb_{3-x}Ru_x$, $Ta_4Pd_3Te_{16}$, doped ferromagnetic semiconductor SmN, thermoelectric $CsPb_xBi_{4-x}Te_6$, BiS_2 layered materials,

- Dichalcogenides: metallic $NbSe_2$, … (CDW revisited, single layer),
  semiconducting MoS_2 …(superconductivity in gated single layer or high pressure)
  WTe_2 (SC under pressure suppressing magnetoresistance)

- Strong activity in iron superconductors, cuprates, fullerenes, heavy fermions

M. Capone, N. Hussey, Yakovenko talk

- Superconductivity in heterosctructures

- Topological superconductivity and search for Majorana Fermions

J. Alicea, E.A Kim talk