

Pressure-induced metallization/ superconductivity of
hydrogen-dominant materials

Duck Young, Kim



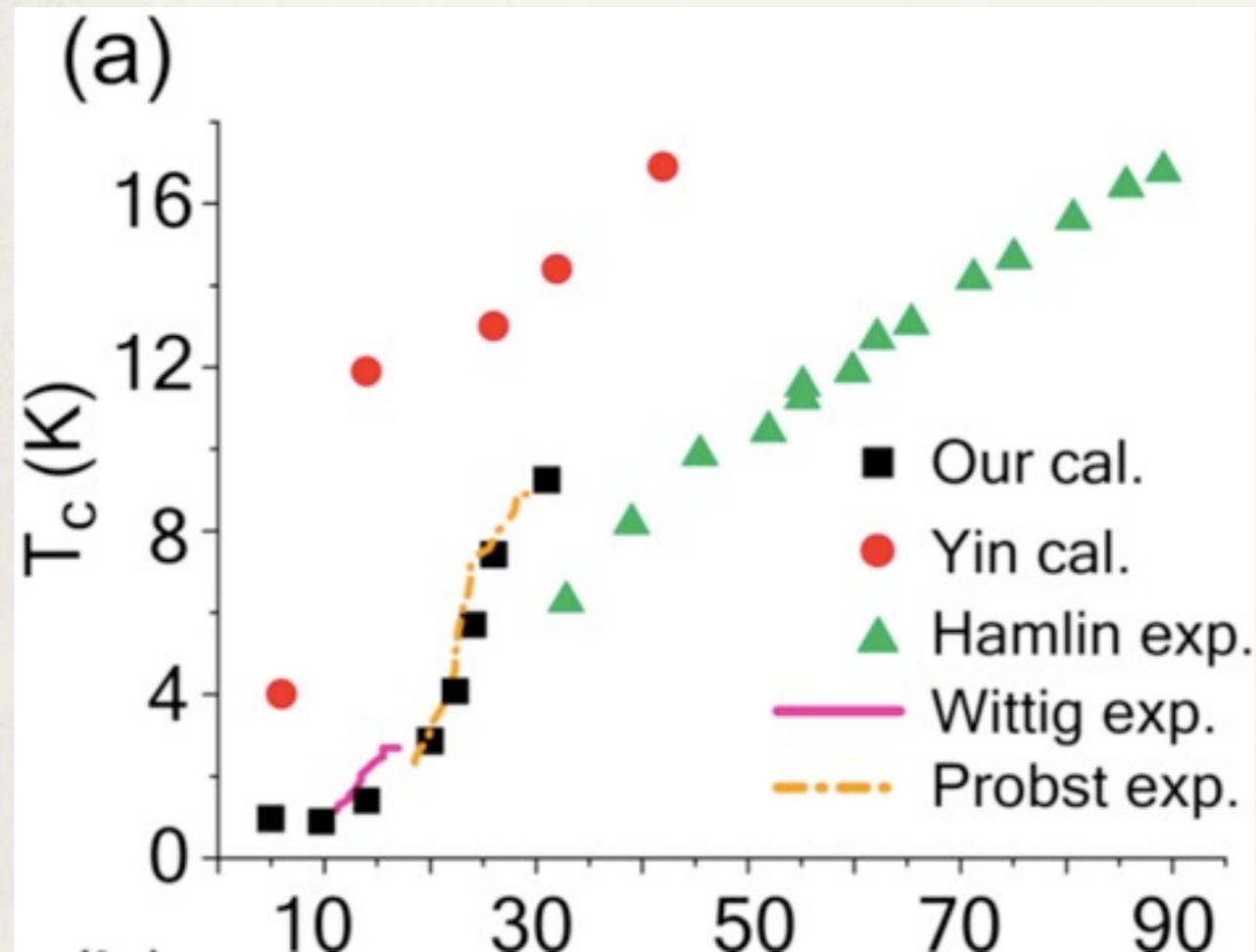
Wenner-Gren Stiftelserna
Wenner-Gren Foundations

2010-04-21 (*ESDG Cavendish*)

Methods

- ❖ DFT calculations
- ❖ Quasiparticle calculations (G_0W_0)
- ❖ Energetic + dynamical stability (phonon)
- ❖ Electron-phonon coupling
- ❖ Superconducting T_c is estimated with Allen-Dynes equation (Modified McMillan equation)

Superconductor: Yttrium



Quantitatively reliable !

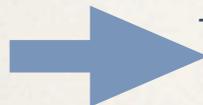
Pressure (GPa)

For T_c estimation at higher pressure, we need crystal structures which are dynamically stabilized.

D. Y. Kim *APL* 96 022510 (2010)

PRESSURE vs H

- ❖ Hydrogen is a strong insulator
- ❖ Pressure induces metallization of materials

 Hydrogen-dominant materials under pressure allow a proxy-study of metallic / superconducting hydrogen via pre-compression (chemical pressure)

N. W. Ashcroft *PRL* 92 187002 (2004)

In 1990s, in the middle of the euphoric times of high-temperature superconductivity, we decided to search for other **superconductors with a potentially high T_c** As starting material we chose yttrium, which is able to absorb 300% hydrogen up to the composition **YH_3** .

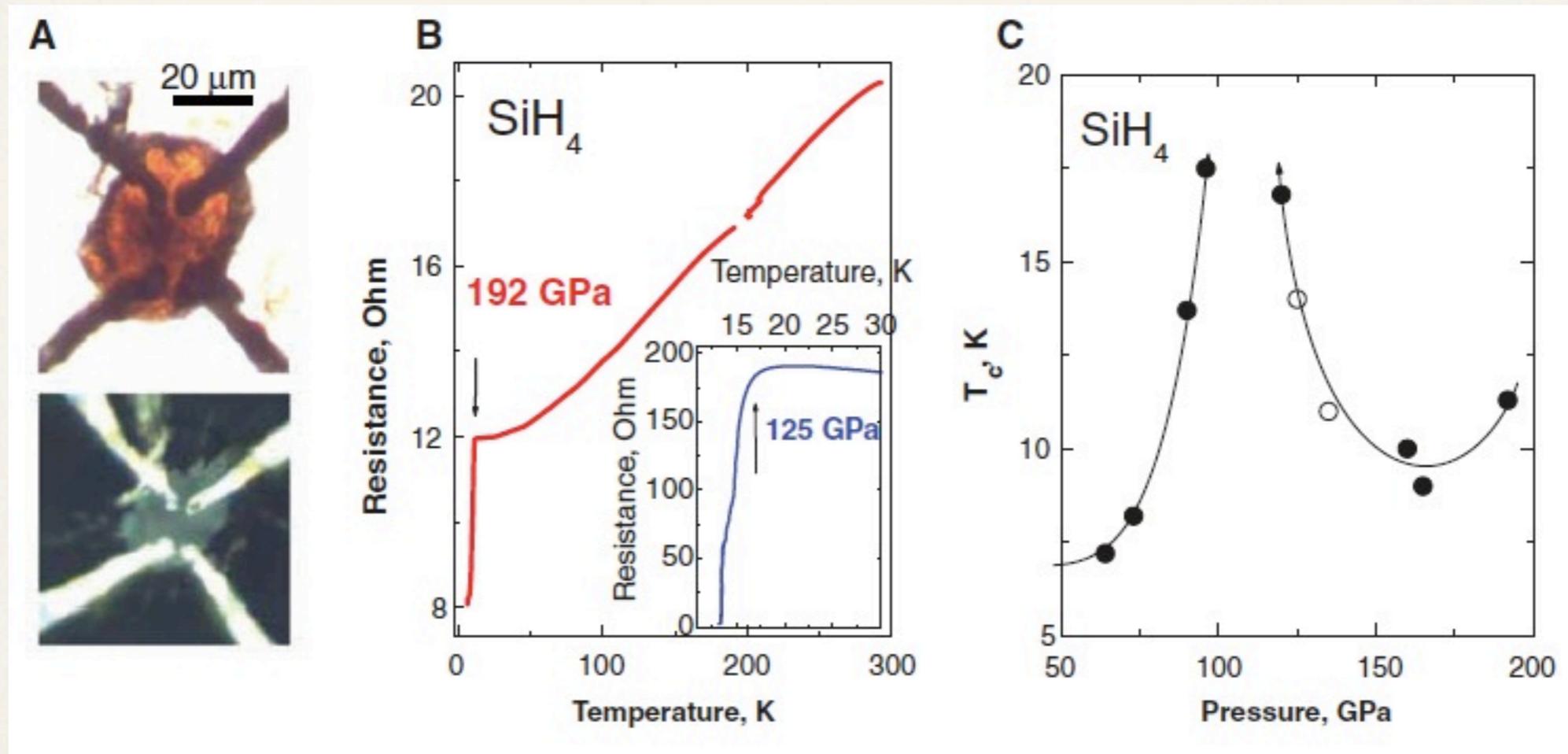
R. Grissen, switchable mirror, *europhysicsnews*, march (2001)

Superconductivity in Hydrogen Dominant Materials: Silane

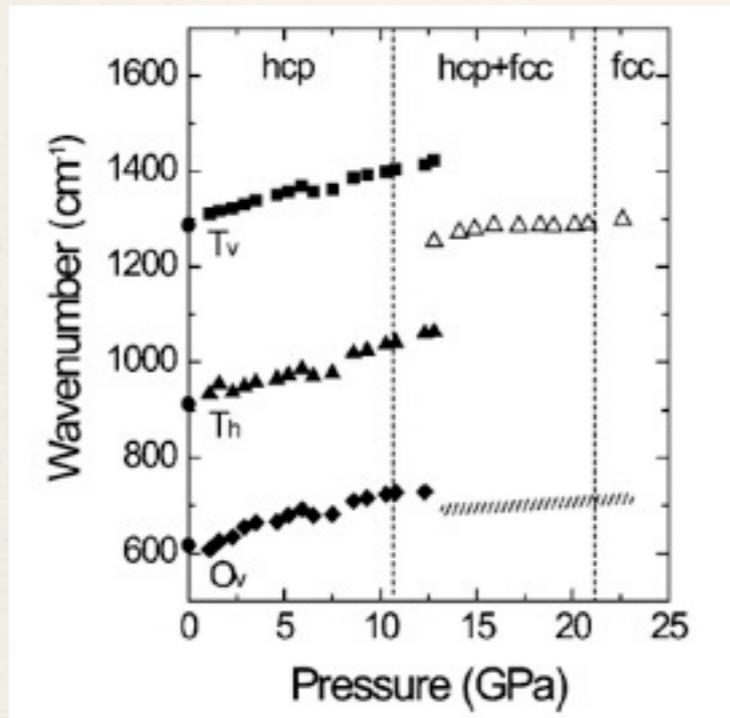
M. I. Erements, *et al.*

Science **319**, 1506 (2008);

DOI: 10.1126/science.1153282

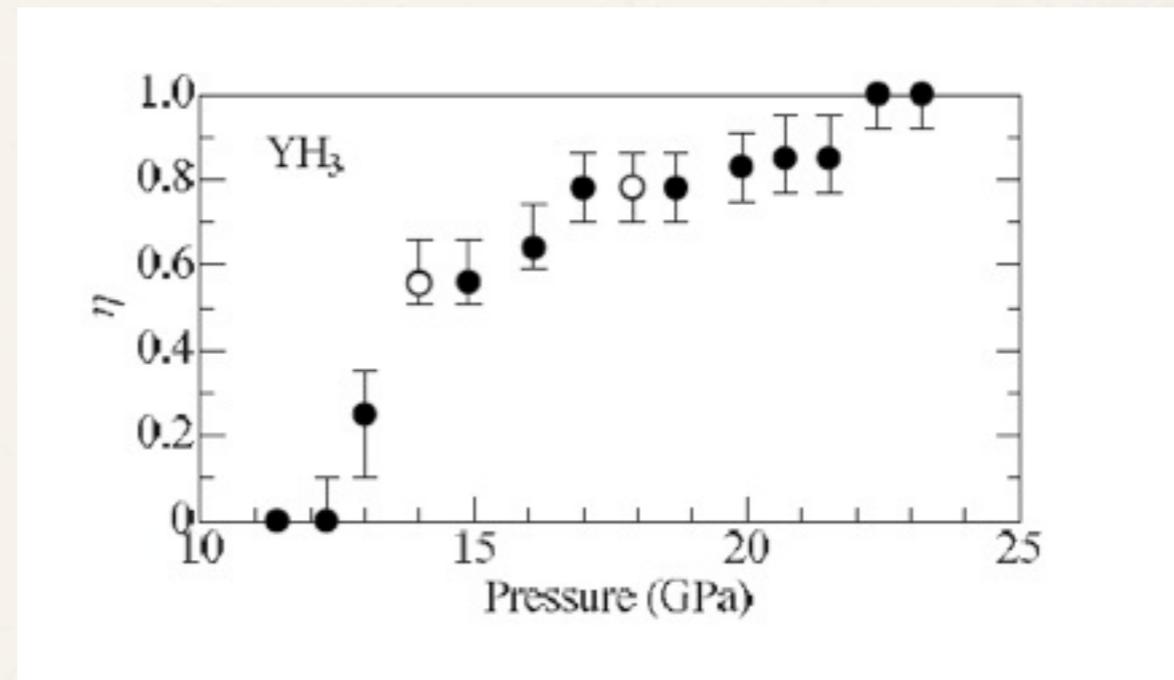


High pressure experiments (YH_3)



fcc(I) - fcc(M) transition

A. Ohmura et al *PRB* 73 104105 (2006)

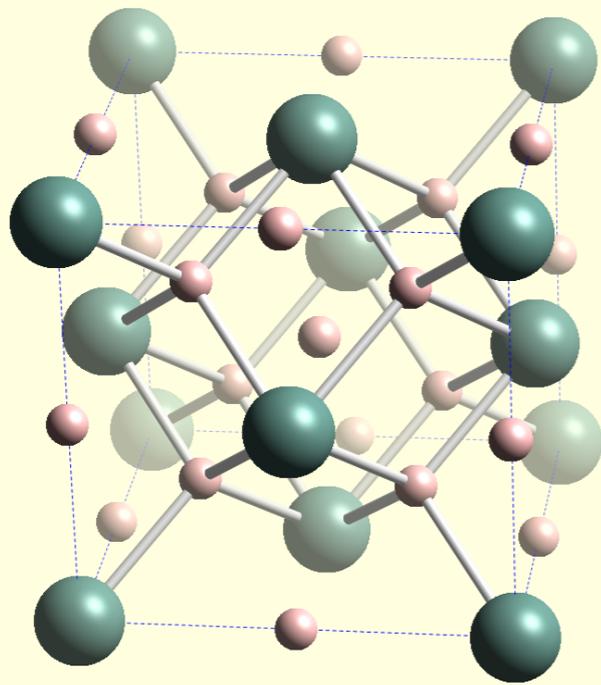


Another intermediate state

A. Machida et al *PRB* 76 052101 (2007)

fcc YH_3 was reported above 20 ~ 23 GPa

fcc YH_3



Space group: No 225 (fcc)

Y at fcc site

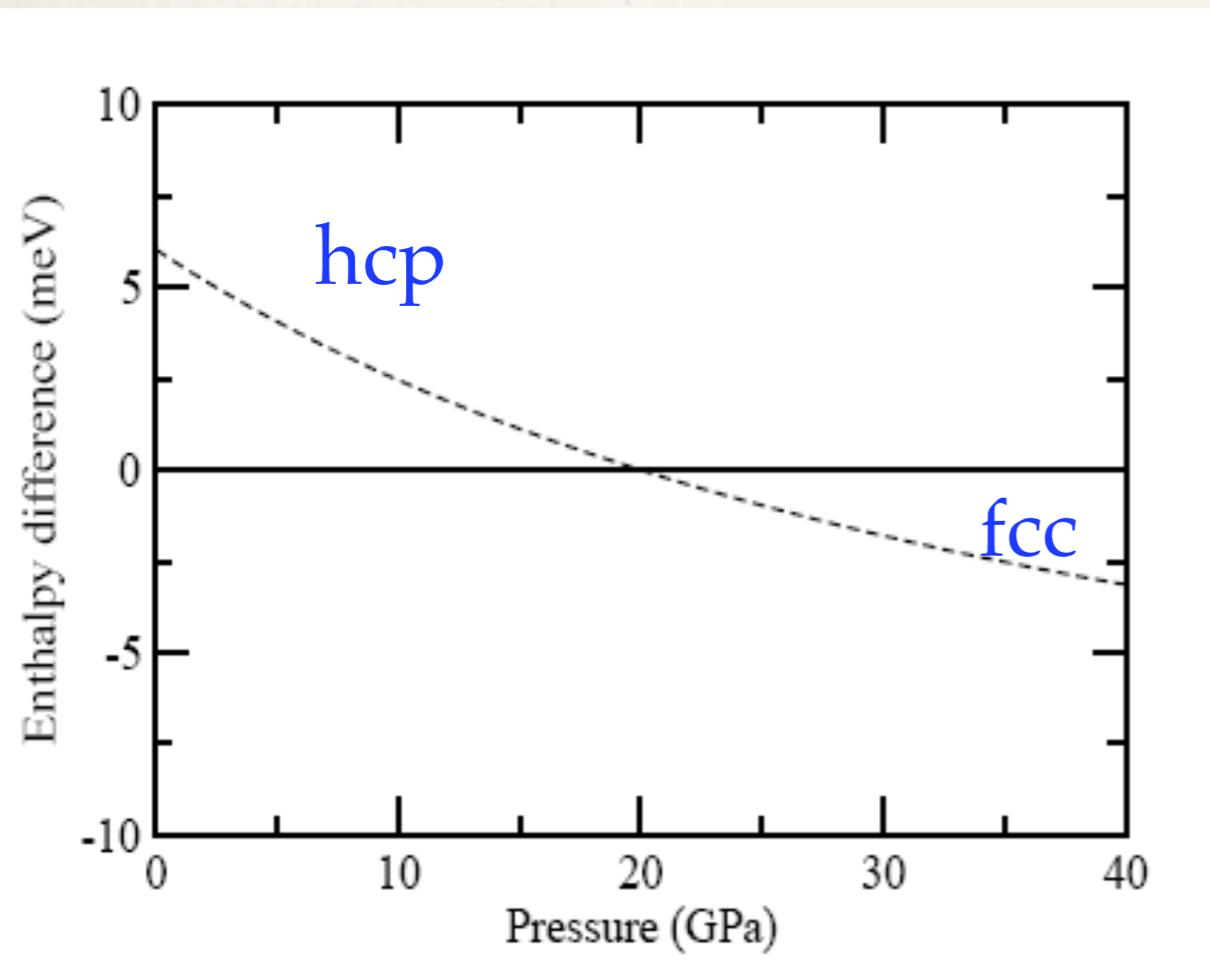
H(1) at tetrahedral site

H(2) at octahedral site

Y-H(1) (YH_2) forms a cage structure for H(2)

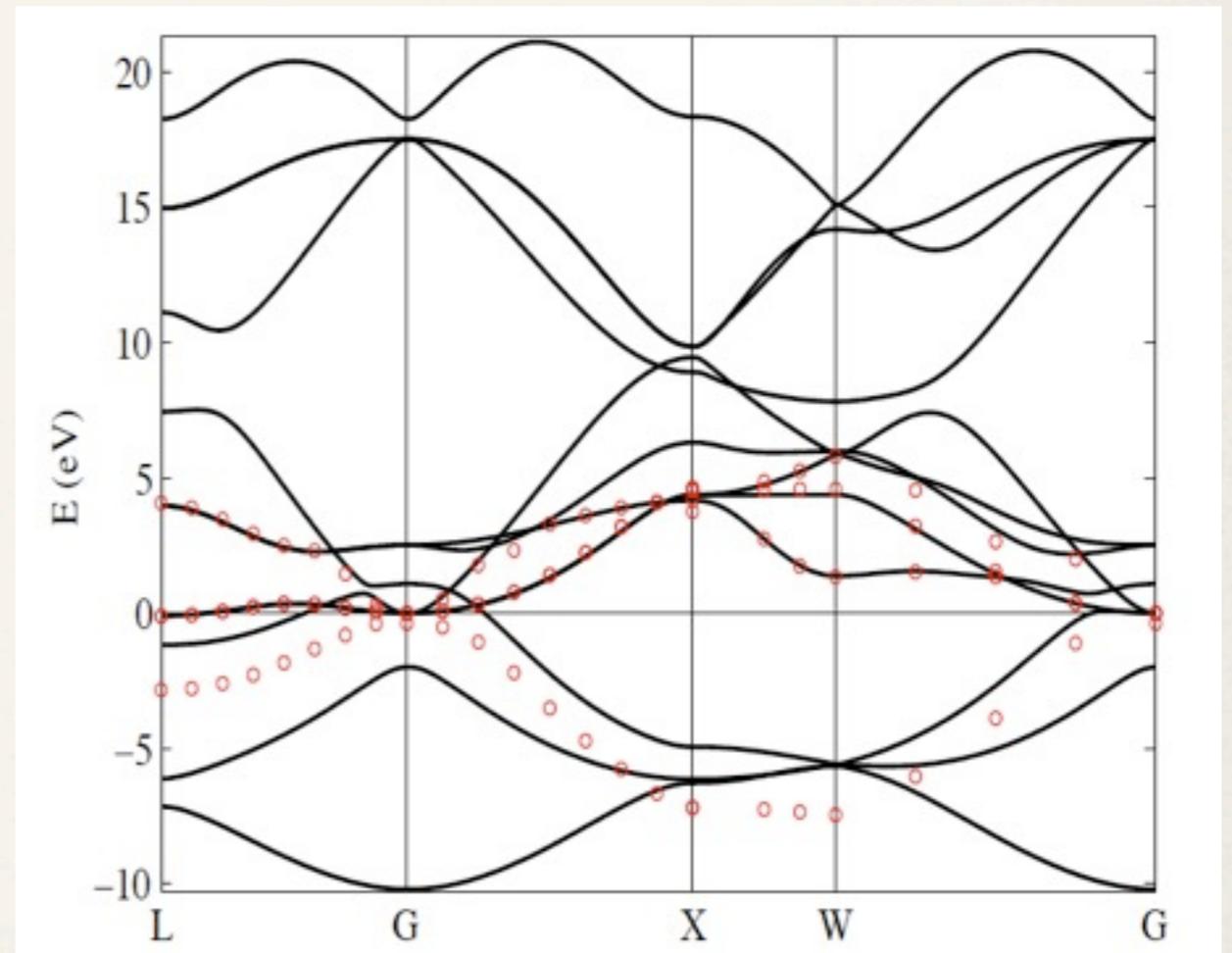
Enthalpy & Band dispersion (GW)

Enthalpy ($H=E+PV$)



transition @ 20 GPa

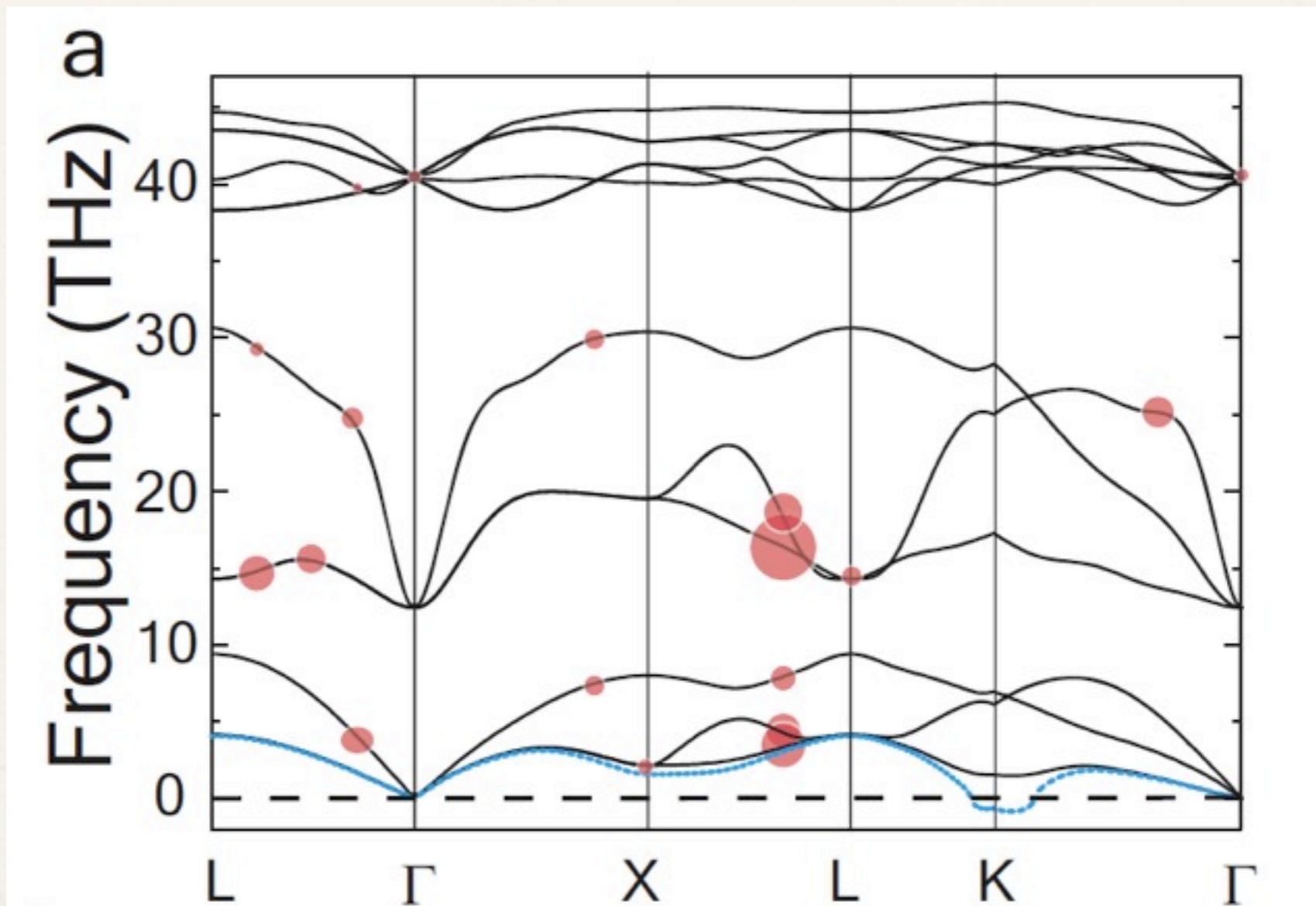
GW band dispersions



Metallic

J. S. de Almeida *APL* **94**, 251913 (2009)

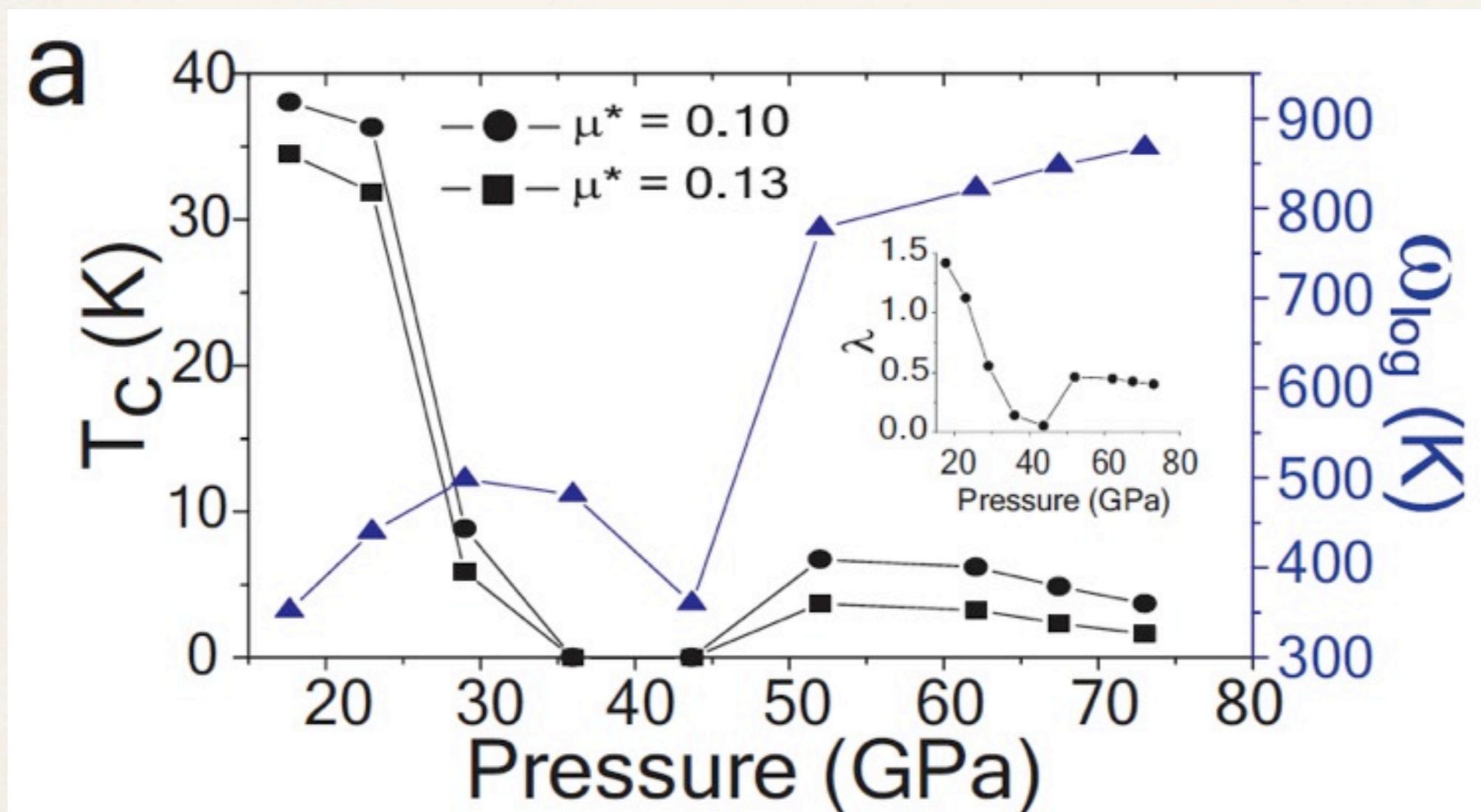
Phonon dispersions



Phonon dispersions are stabilized above 17.7 GPa

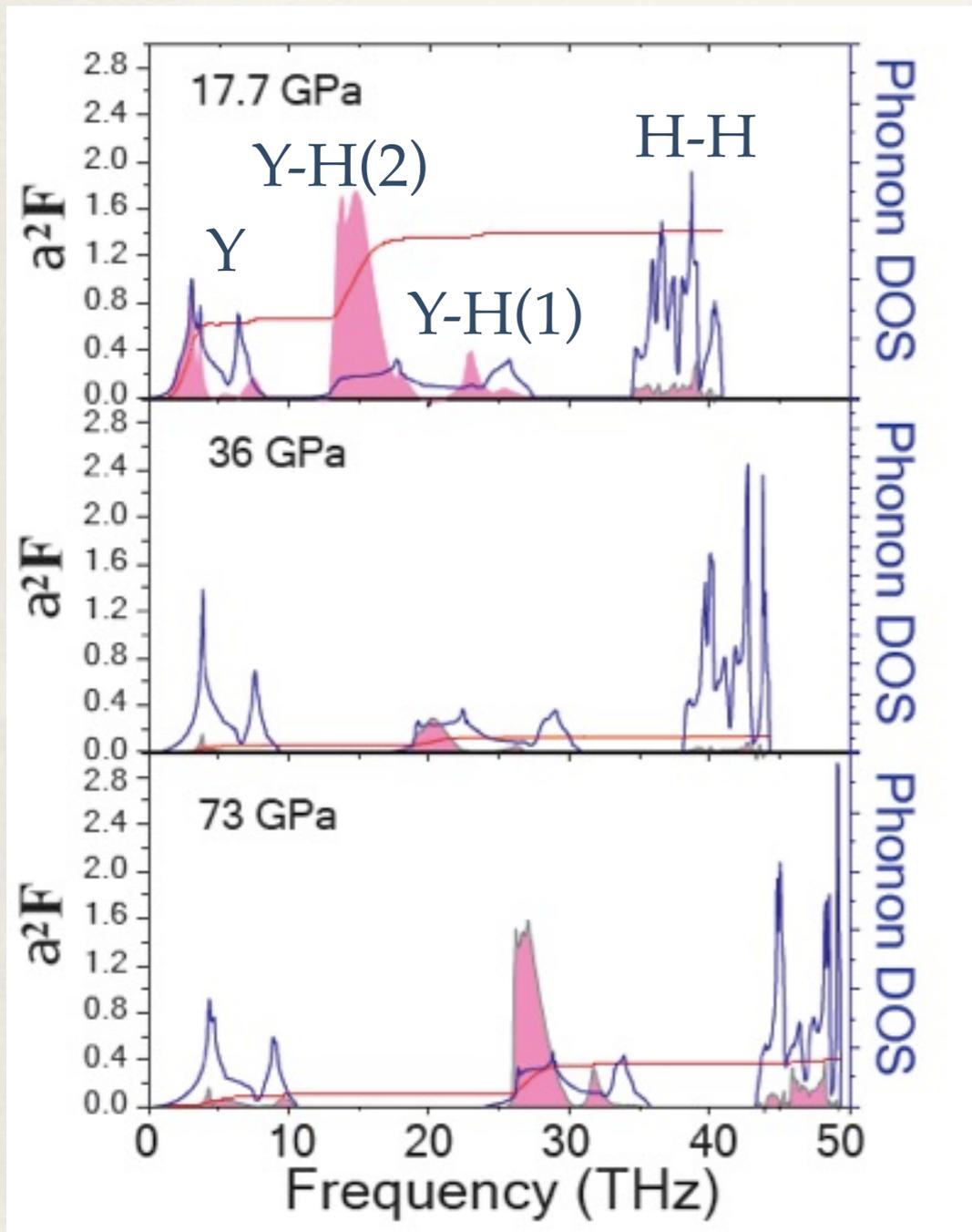
D. Y. Kim *PRL* **103** 077002 (2009)

T_c of YH_3 under pressure



D. Y. Kim *PRL* **103** 077002 (2009)

Spectral function

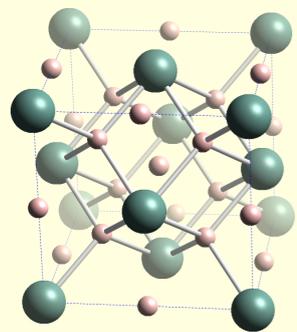


@ 17.7 GPa Y and Y-H(2) contribution are significant for EPC

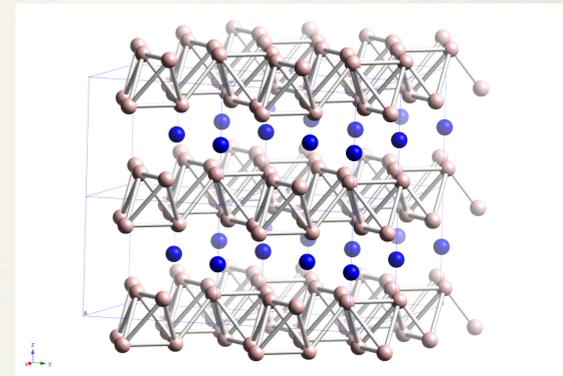
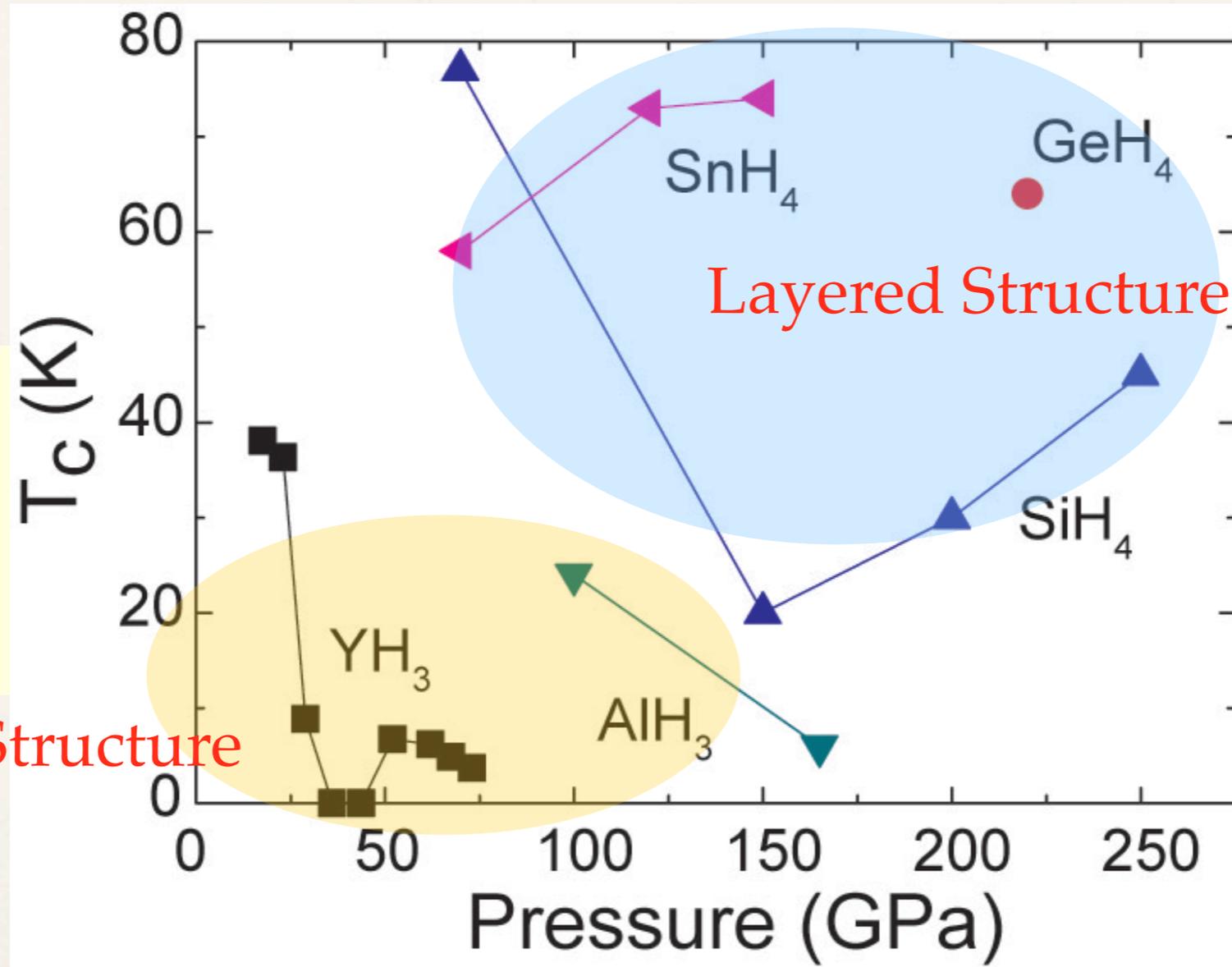
@ 36 GPa, normal metallic

@ 73 GPa, Y-H(2) is the dominant for EPC

Predicted superconducting T_c of Hydrogen-dense Materials

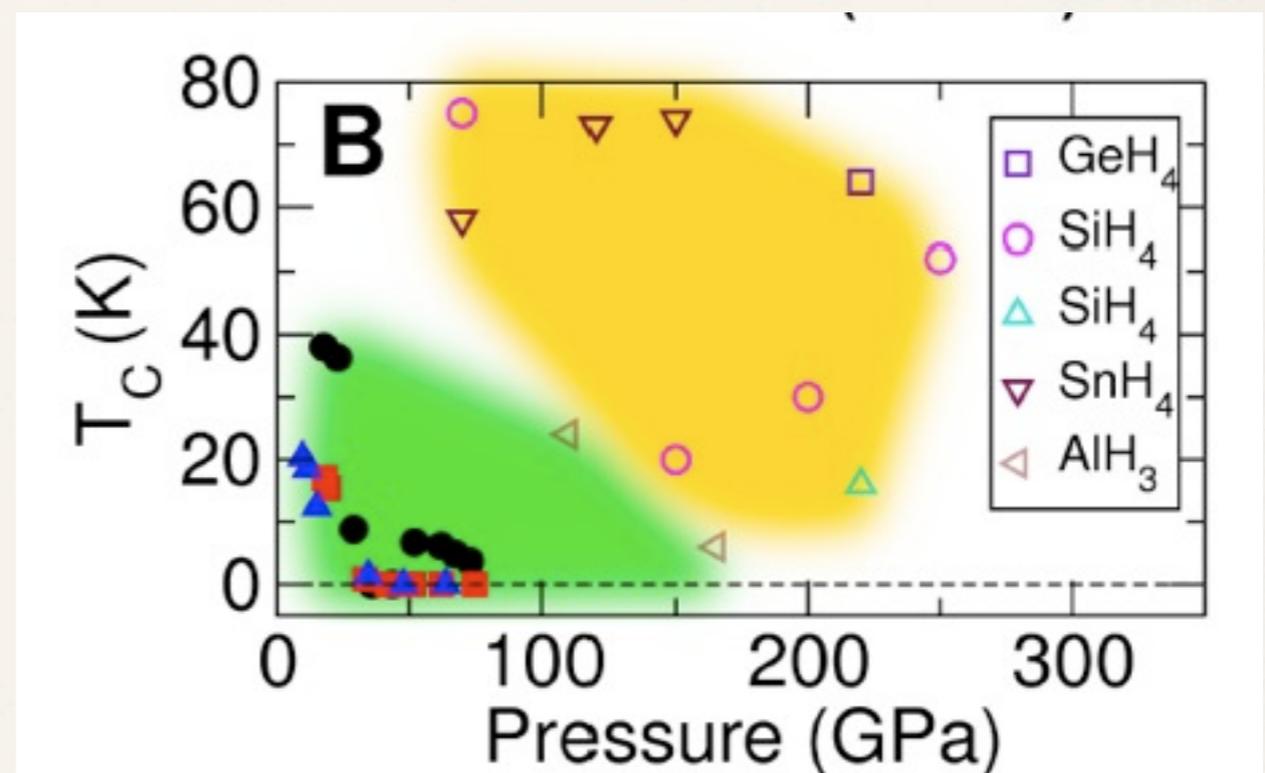
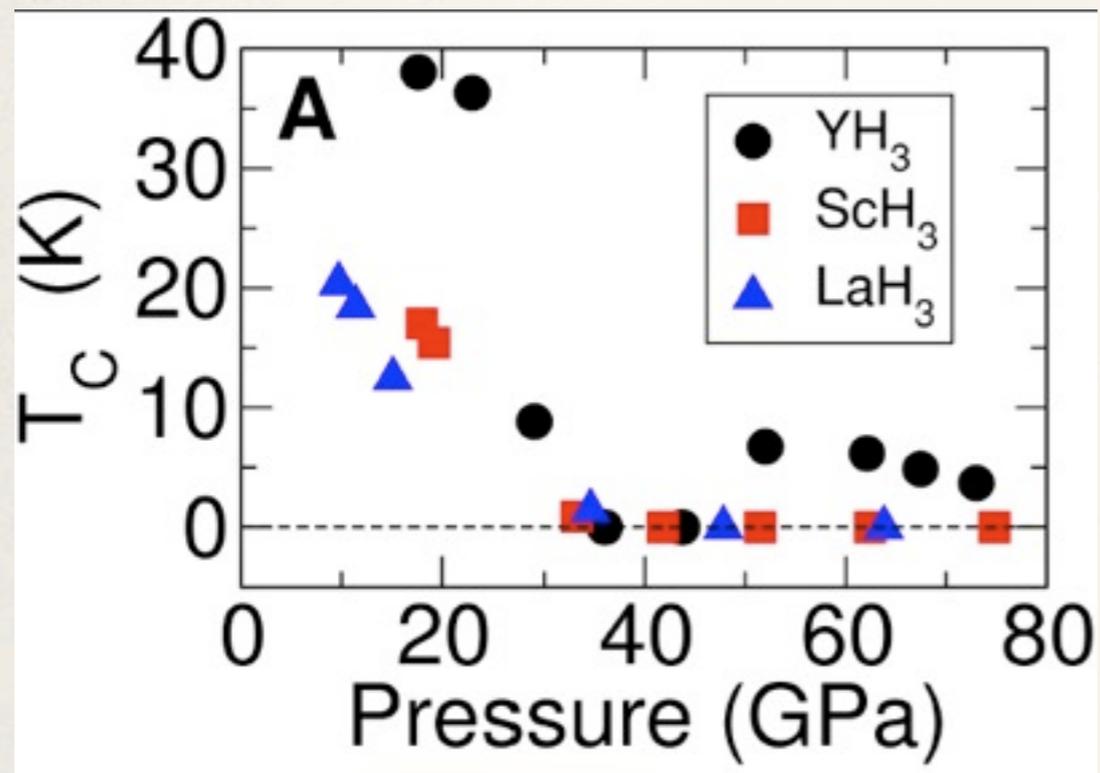


3D network Structure



GeH_4 : G. Gao *PRL* **101**, 107002 (2008) SiH_4 : X.-J. Chen *PRL* **101**, 077002 (2008)
 AlH_3 : I. Goncharenko *PRL* **100**, 045504 (2008), SnH_4 : J. S. Tse *PRL* **98** 117004 (2007)
 YH_3 D. Y. Kim *PRL* **103** 077002 (2009)

General trend of tri-hydrides



CONCLUSIONS

- ✱ MH_3 transforms into fcc phase near 10-20 GPa
- ✱ fcc YH_3 is metallic with GW calculations
- ✱ Near the structural transition, one can observe strong electron-phonon coupling
- ✱ Phonon-mediated superconductivity in fcc MH_3
- ✱ The secondary superconductivity region only for YH_3

Thank you for your attention

25-29 July 2010 - Uppsala, Sweden



EHPRG

European High Pressure Research Group Conference

