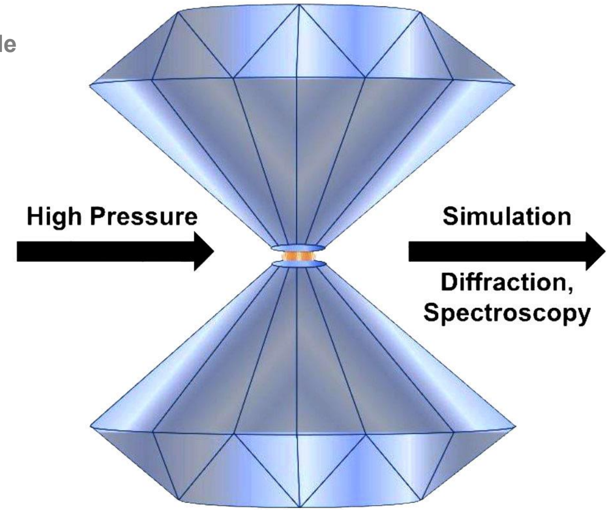
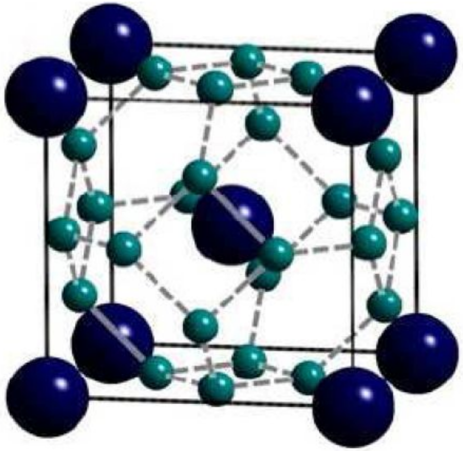
Calcium Hydride

Superconducting Phase in CaH_6 up to 215 K at 172 GPa

Authors: Liang **Ma** et. al.

2022





Presenter

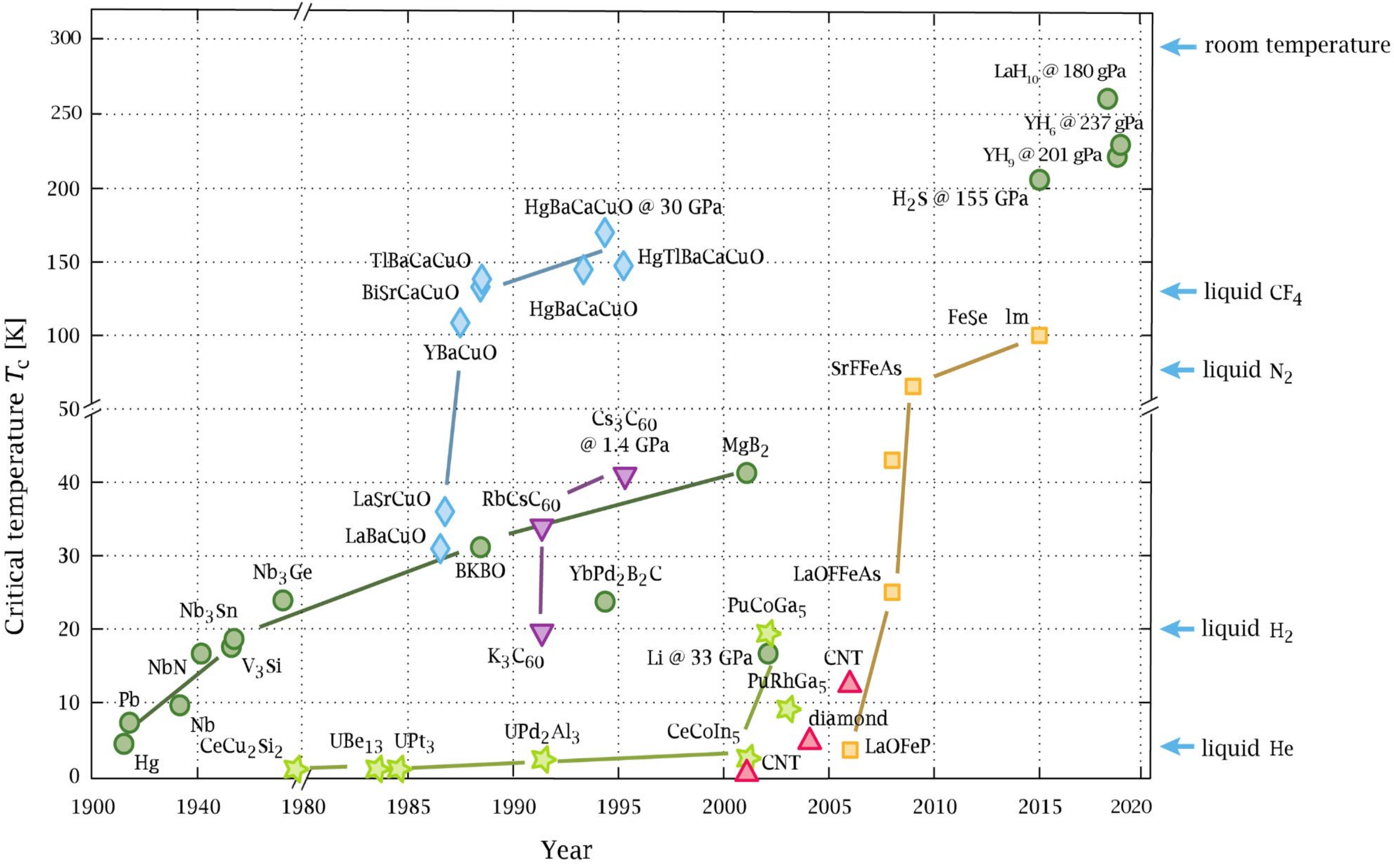
Jiyun Di

Stony Brook University

Thursday, April 6, 2023; 16:45–18:05

I. Intro

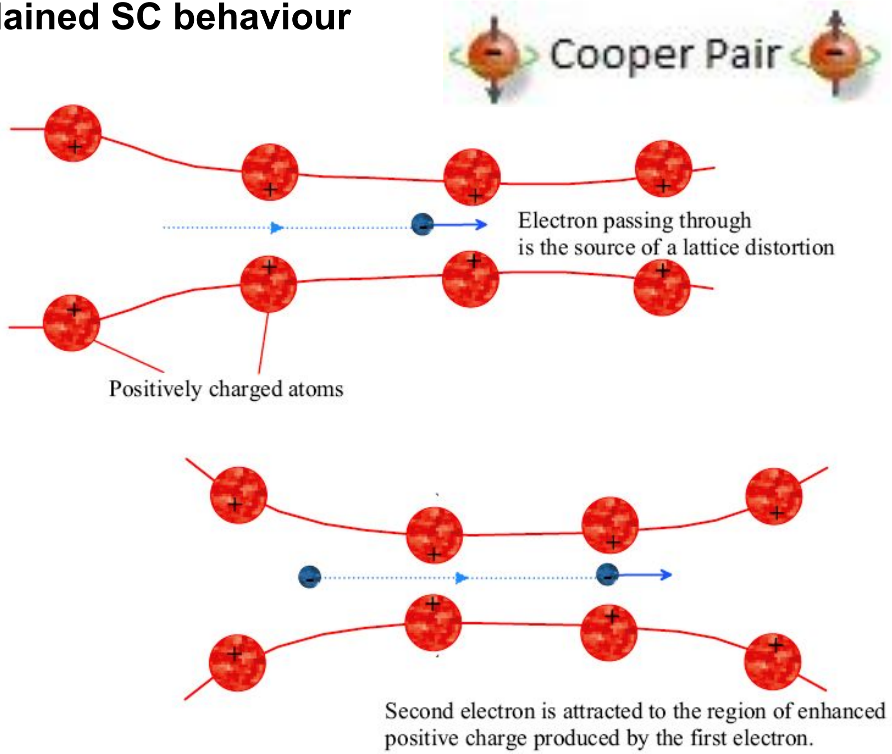
Discovery history of **s**uper**c**onductivity materials since 1911



I. Introduction

Bardeen-**C**ooper-**S**chrieffer **Theory** (1957): **explained SC behaviour**

1. Electrons inside are grouped in **Cooper pairs**
2. Coulomb **repulsion** of **e-** pairs → **attraction** of lattice positive region

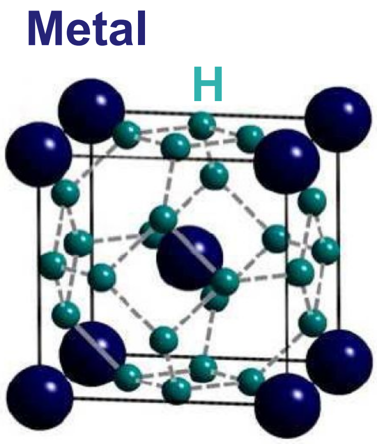


Strong electron-phonon coupling in **atomic metallic hydrogen**

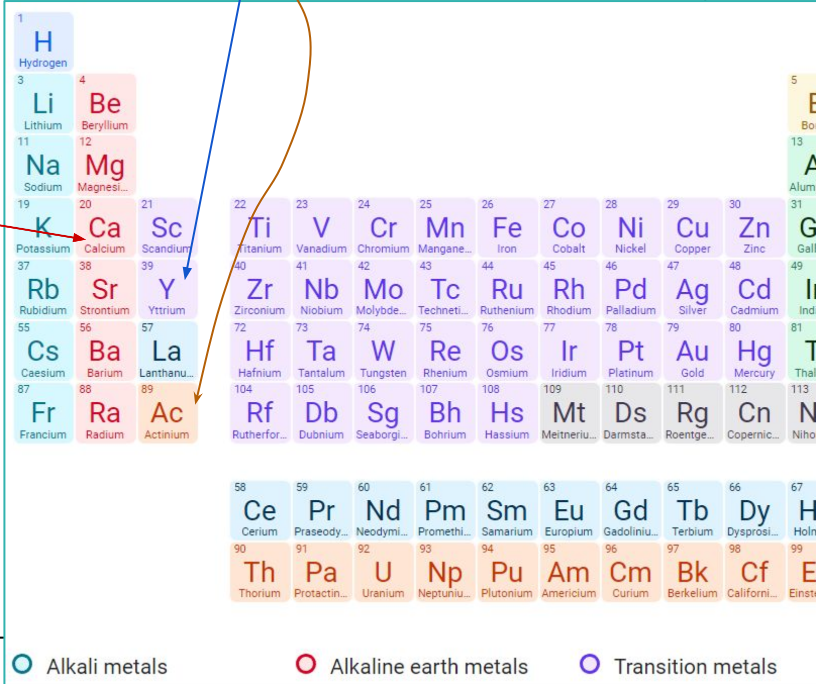
I. Introduction

Idea: “atomic metallic hydrogen”

- The current realized high-T_c super-hydrides contain rare earth (i.e. $_{21}$**Sc**, $_{39}$**Y**, $_{57\text{-}71}$**La**) and actinide ($_{89\text{-}103}$**Ac**) elements:
  - LaH_{10}: up to T_c=260 K and 180–200 GPa (Somayazulu et al. 2019)



alkaline-earth-metal



I. Introduction

Idea: Synthesis Attempts of CaH_6

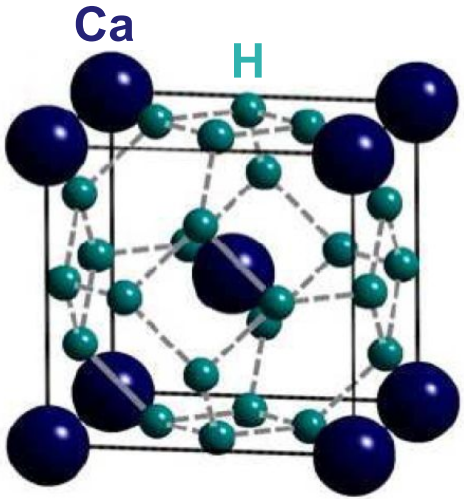
- Prediction (Wang et al. 2012):

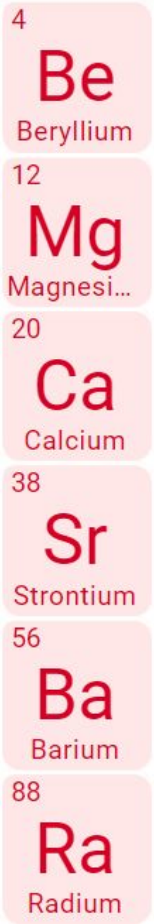
  Hydride with **alkaline-earth-metal** elements

  - CaH_6: **T_c~220–235K** at **~150GPa**
  - CaH_6: **Clathrate lattice**

Technical Difficulties:

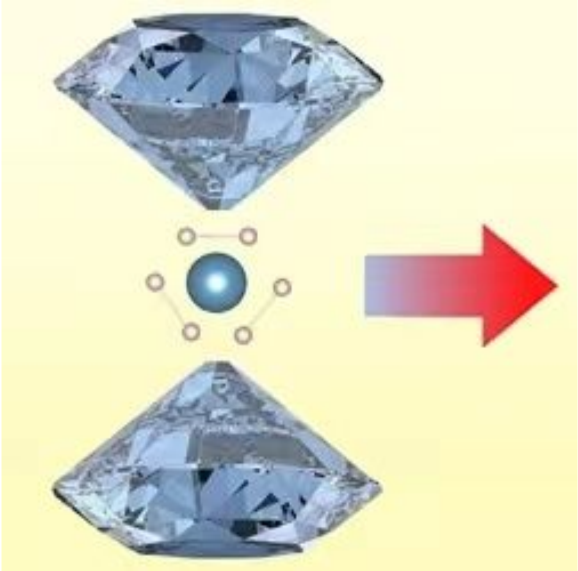
- **Lowest stabilization** among all the non-RE and -AC hydrides
- **Insufficient to synthesize** calcium hydride.

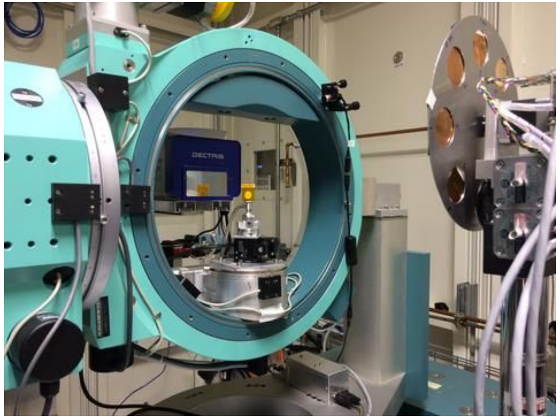




II. Experiments and Results

- 15 cells filled with **Ca** foil and Ammonia borane **(BH_3NH_3)**
  1. **Compress at room temperature** to 160–190 GPa
  2. **Heat** to about 2000 K with laser
- Cells differ from synthesizing pressures.
- X-ray Diffraction instrument **measures the crystal structures** of the products in cells





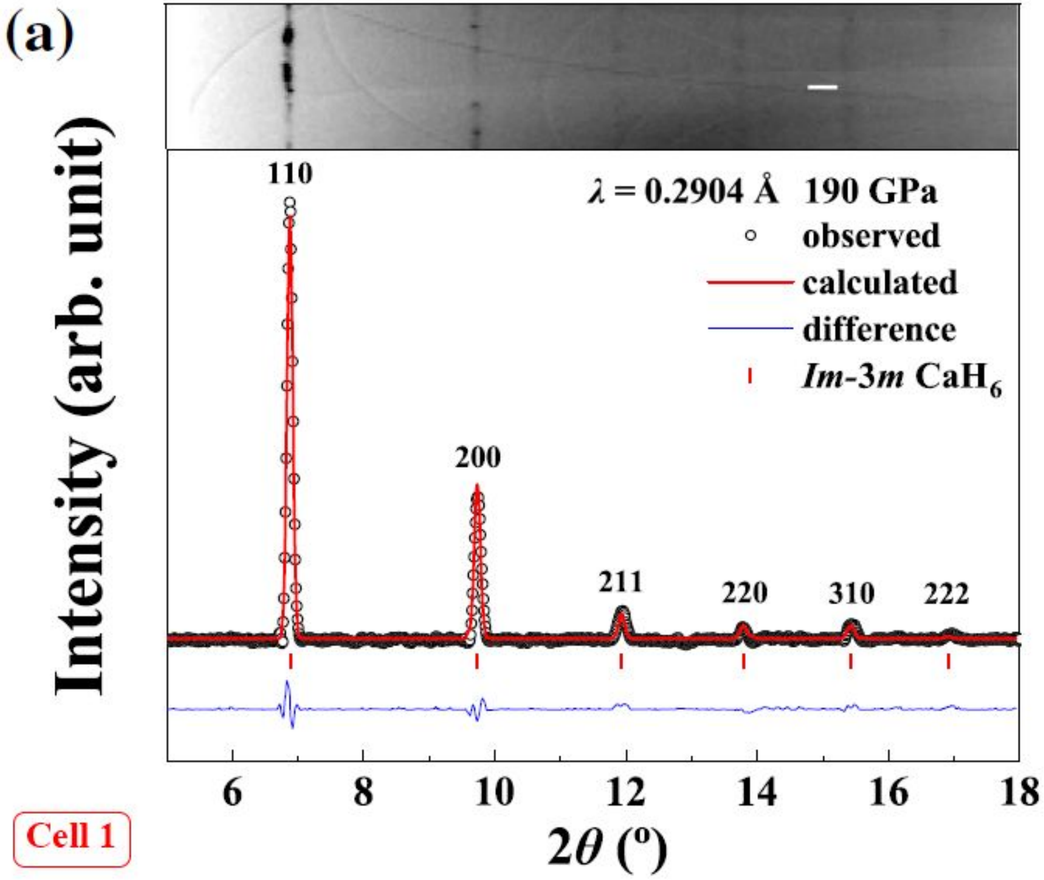
The X-ray diffraction is a foundational technique providing information on regularly occurring and well defined structures such as crystal lattices

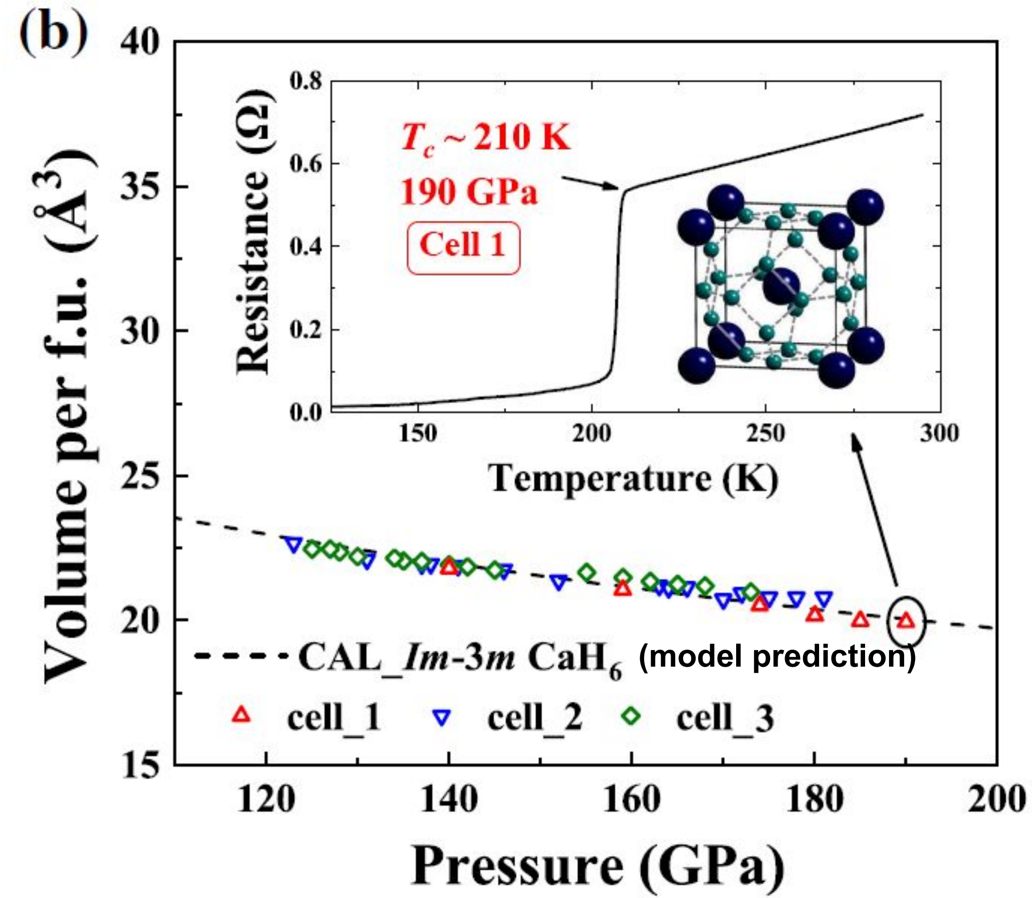
Example: X-ray Diffraction end station on the Beamline for Material Measurement at Brookhaven National Laboratory

II. Experiments and Results

(1/4) Products' Structures

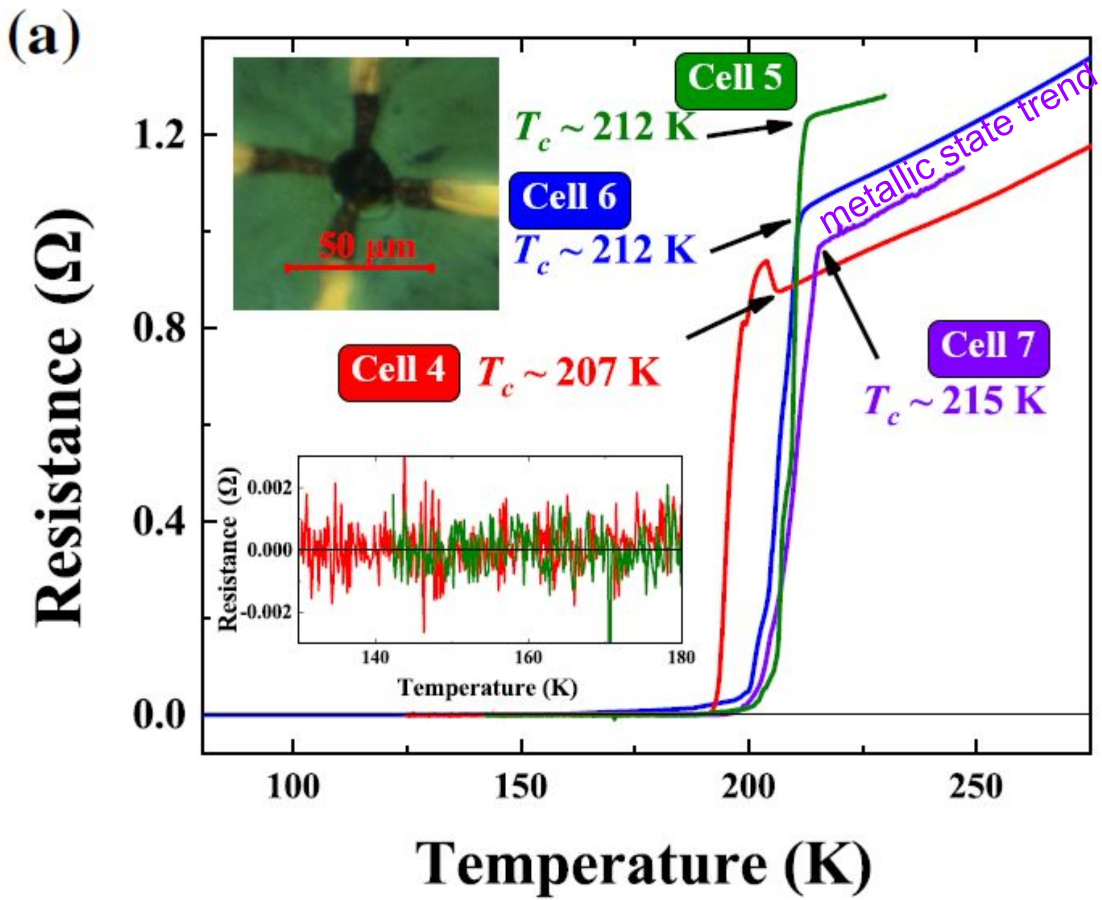
- **Known XRD patterns** of calcium hydrides such as CaH_2, CaH_4, and Ca_2H_5. Compare with experiment on right figure.
- Measured **unit cell volumes** → estimate **the stoichiometry (x)** of the hydrides (CaH_x).
    - $V = 40.07$ Å^3 at 190 GPa
    - Ca: 9.41 Å^3/atom x 2 atoms
    - H: 1.78 Å^3/atom
    - $x = 5.97 \sim 6$
    - **CaH_6**





- In-lattice voids are possible.
- Figure shows **compression is well-defined**.
- **Cell 1: a successful synthesis** of clathrate CaH_6 at 190 GPa pressure and 2000 K temperature.
- Critical temperature: T_c ~ 210 K

(2/4) Max. T_c of CaH_6



Cell 7 at 190 GPa pressure:

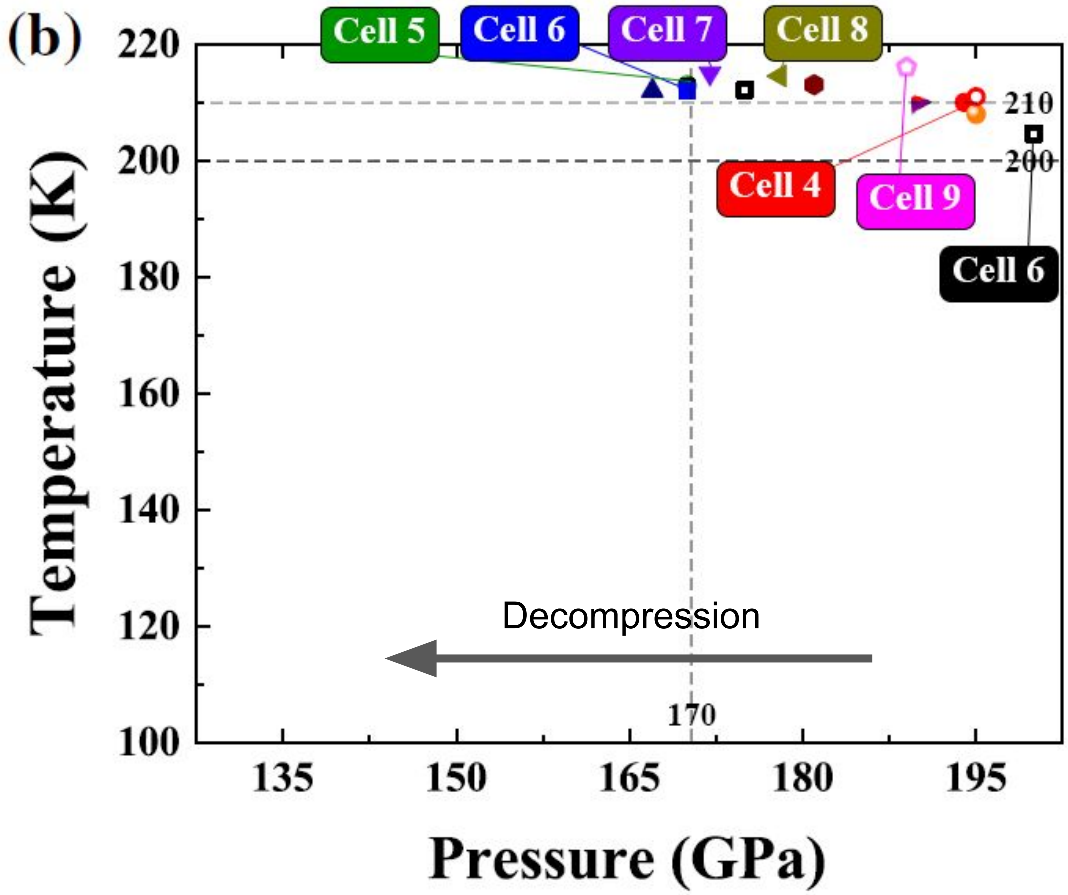
- **Critical temperature: T_c ~ 215 K.**
- Yes w/ prediction:

  dTc/dP = -0.33 K/GPa

  $T_{c,predicted}$ ~ 213 K

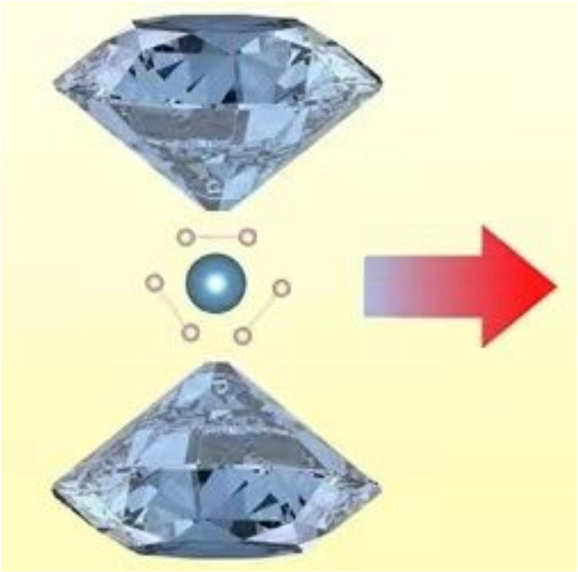
Cell 4 (181 GPa) Cell 5 (170 GPa)

- Zero resistance was observed on 150K–180K. (still there as low T.)

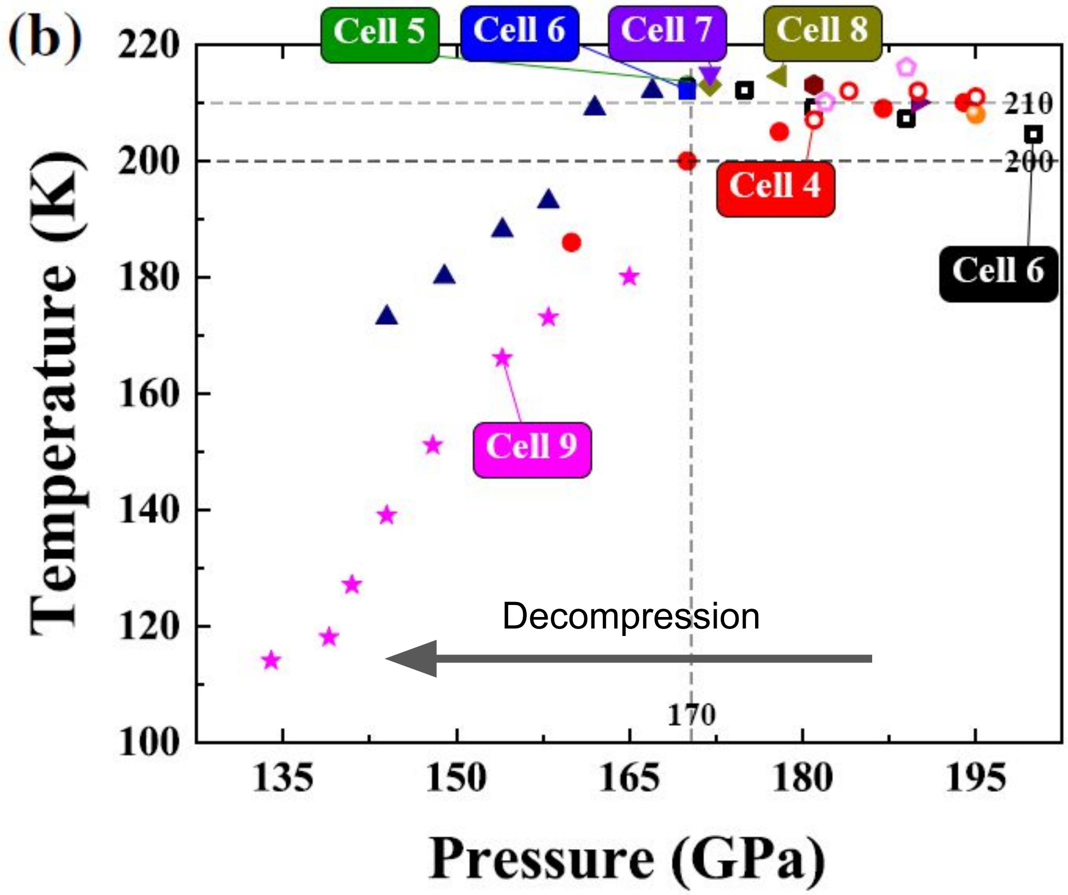


What if we:

- **Decrease pressure** of CaH_6
- Guess: CaH_6 may decompose → at what pressure?



(3/4) High-P-only Property

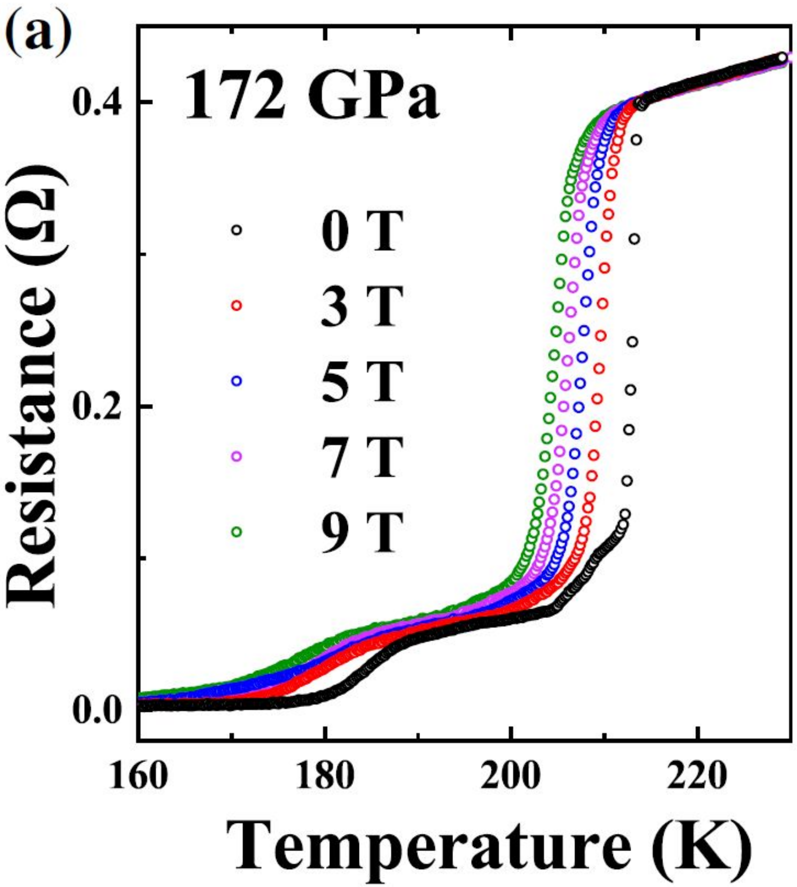


What if we:

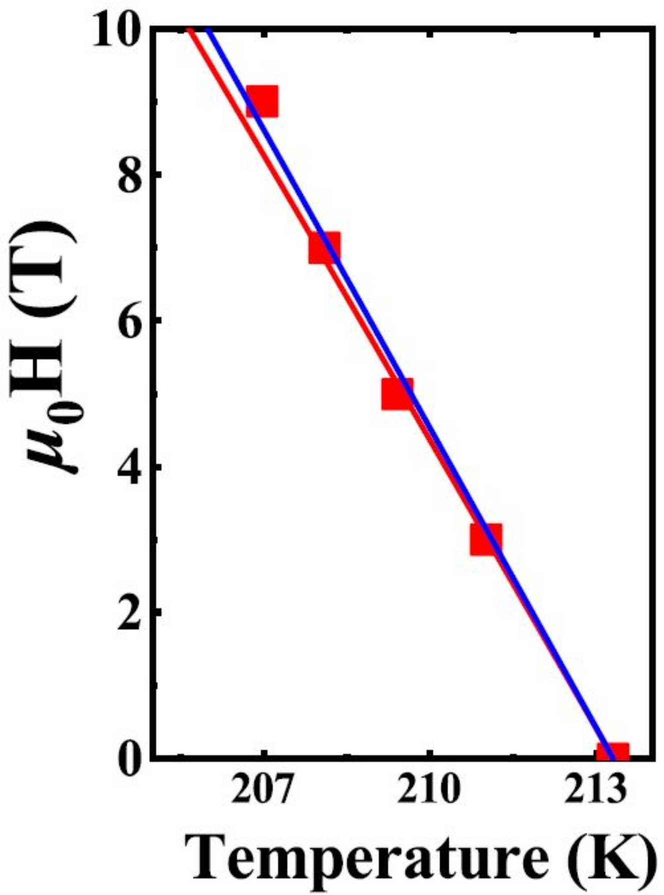
- **Decrease pressure** of CaH_6
- Guess: CaH_6 may decompose → at what pressure?
- Superconducting transition disappears on plot as P down.
- CaH_6 does not exist anymore at low pressure **<130 GPa** environment.

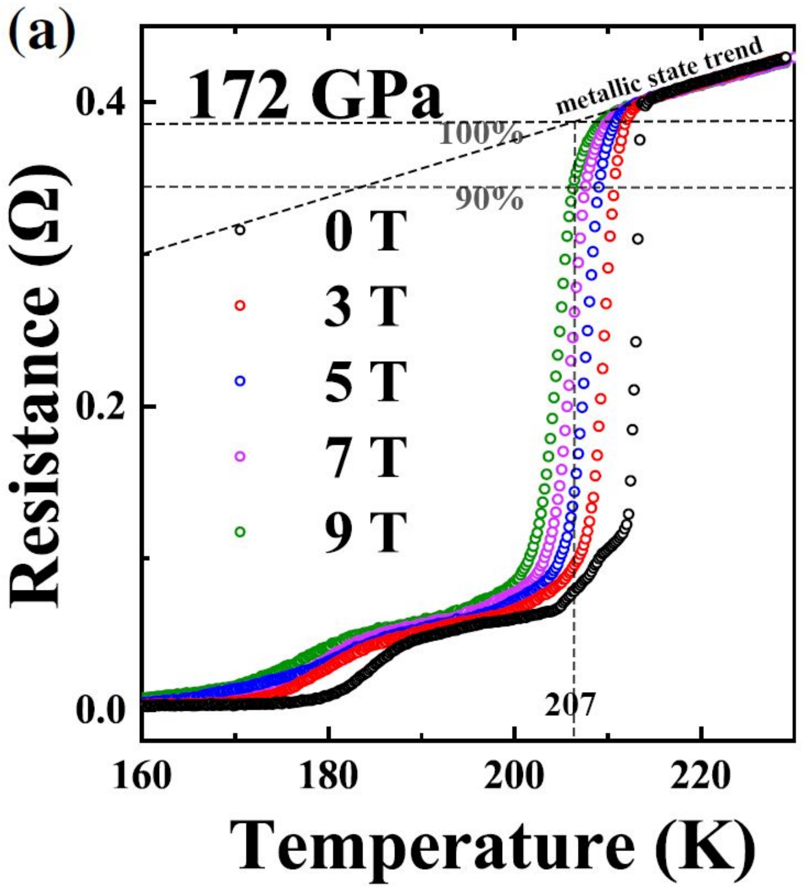
- **Magnetic flux expulsion effect** signal:
  - External mag. field strength
  - **Intense field breaks Cooper pairs**

    (due to Pauli effect of electron spin polarization and the diamagnetic effect of the orbital motion)
  - Thus **reducing the value of T_c**.
- Establish a resistance criteria to study **field-temperature relation** and models



(4/4) Field vs Temperature





Ginzburg-Landau (GL)

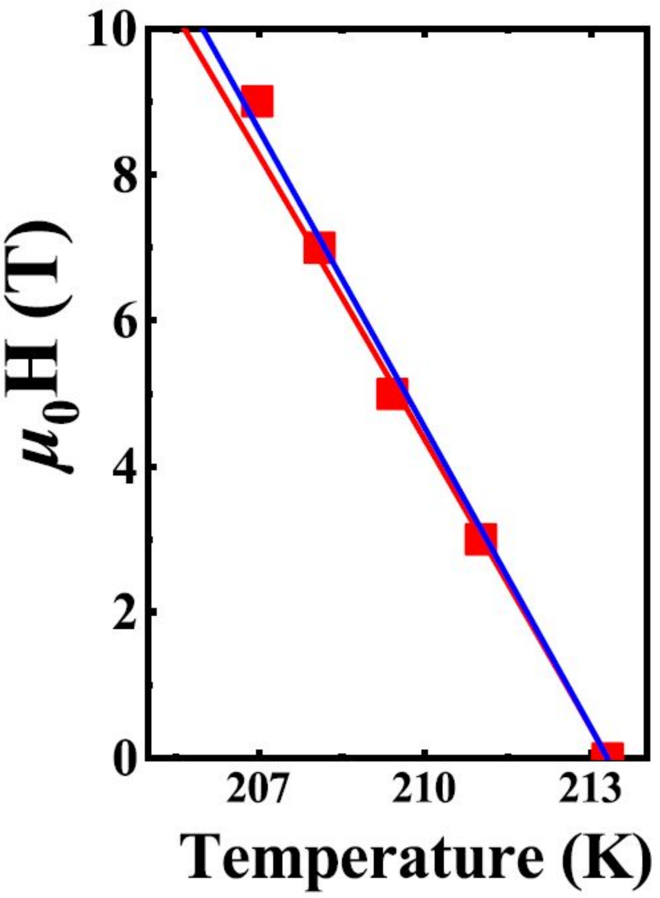
$$H_{c2}(T) = H_{c2}(0) * \left[\frac{(1-t^2)}{(1+t^2)}\right]$$

$$t = T/T_c$$

Werthamer-Helfand-Hohenberg (WHH)

$$B_{c2}(T) = \frac{B_{c2}(0)}{0.693} h^*_{\mathrm{fit}}(T/T_c).$$

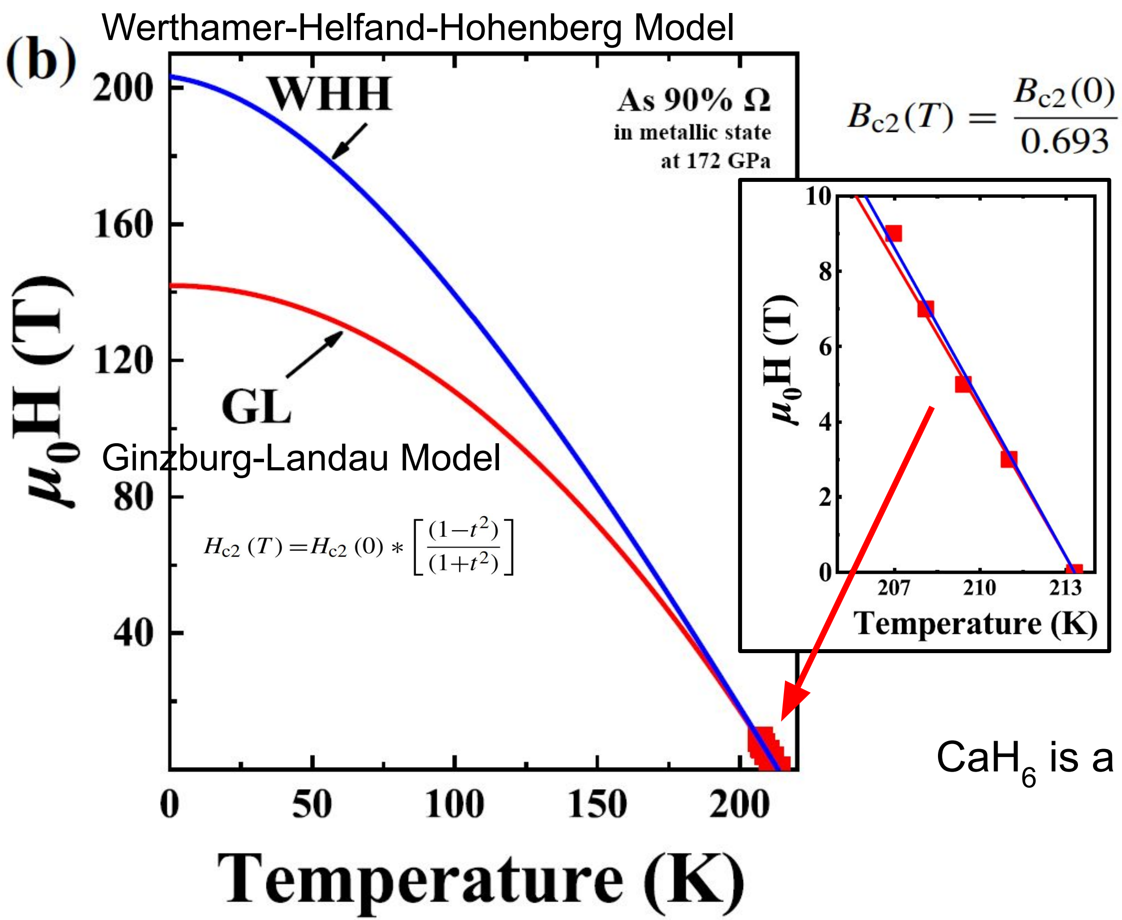
$$h^*_{\mathrm{fit}}(t) = 1 - t - C_1(1-t)^2 - C_2(1-t)^4$$



Equations cited from Baumgartner et al. 2014, Sultana et al. 2016.

II. Experiments and Results

(4/4) Field vs Temperature



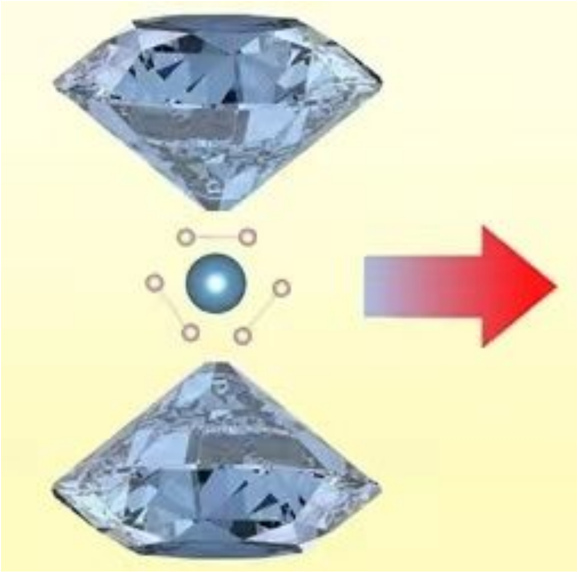
$$B_{c2}(T) = \frac{B_{c2}(0)}{0.693} h^*_{\mathrm{fit}}(T/T_c).$$

Type-II SC can be made for SC circuit under a stronger magnetic field environment, followed by applications e.g. MRI, NMR, and maglev trains.

CaH_6 is a **strong type-II superconductor**.

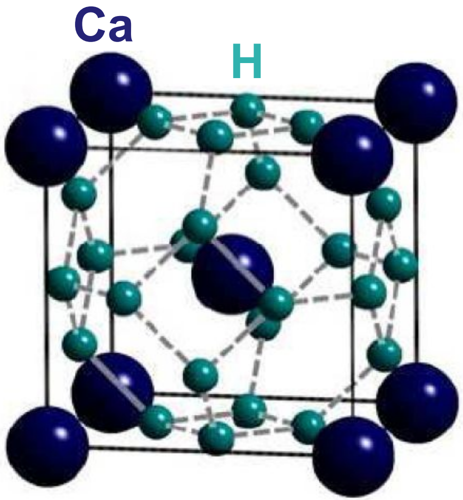
III. Discussion

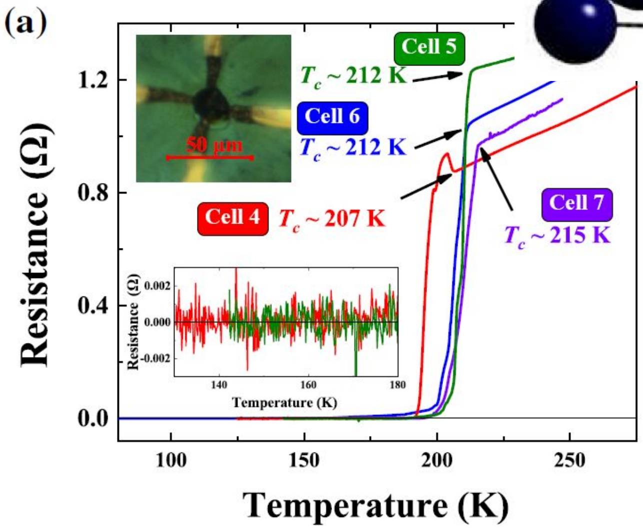
- Why we failed in the past?
  - Ca and **pure H_2** were used as precursors
  - CaH_x easily formed, but hard to **further react** with H_2
- Why successfully synthesized this hydride this time?
  - CaH_6 is H-rich
  - **Ammonia borane (BH_3NH_3)** can release H_2 **at higher temperatures.**



IV. Summary

- This result confirms the original theoretical prediction.
- CaH_6 discovery raises great prospects of expanding the **extraordinary class of high-T_c superhydrides** to a broader variety of compounds.
- Probably would develop <u>a new understanding</u> of the interactions between <u>electrons and other quasi-particles</u> (e.g. phonons). (Tao 2021)





Main Paper & Erratum

Ma L., Wang K., Xie Y., Yang X., Wang Y., Zhou M., Liu H., et al., **2022**, PhRvL, 128, 167001.
doi:10.1103/PhysRevLett.128.167001

Ma L., Wang K., Xie Y., Yang X., Wang Y., Zhou M., Liu H., et al., **2022**, PhRvL, 129, 269901.
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