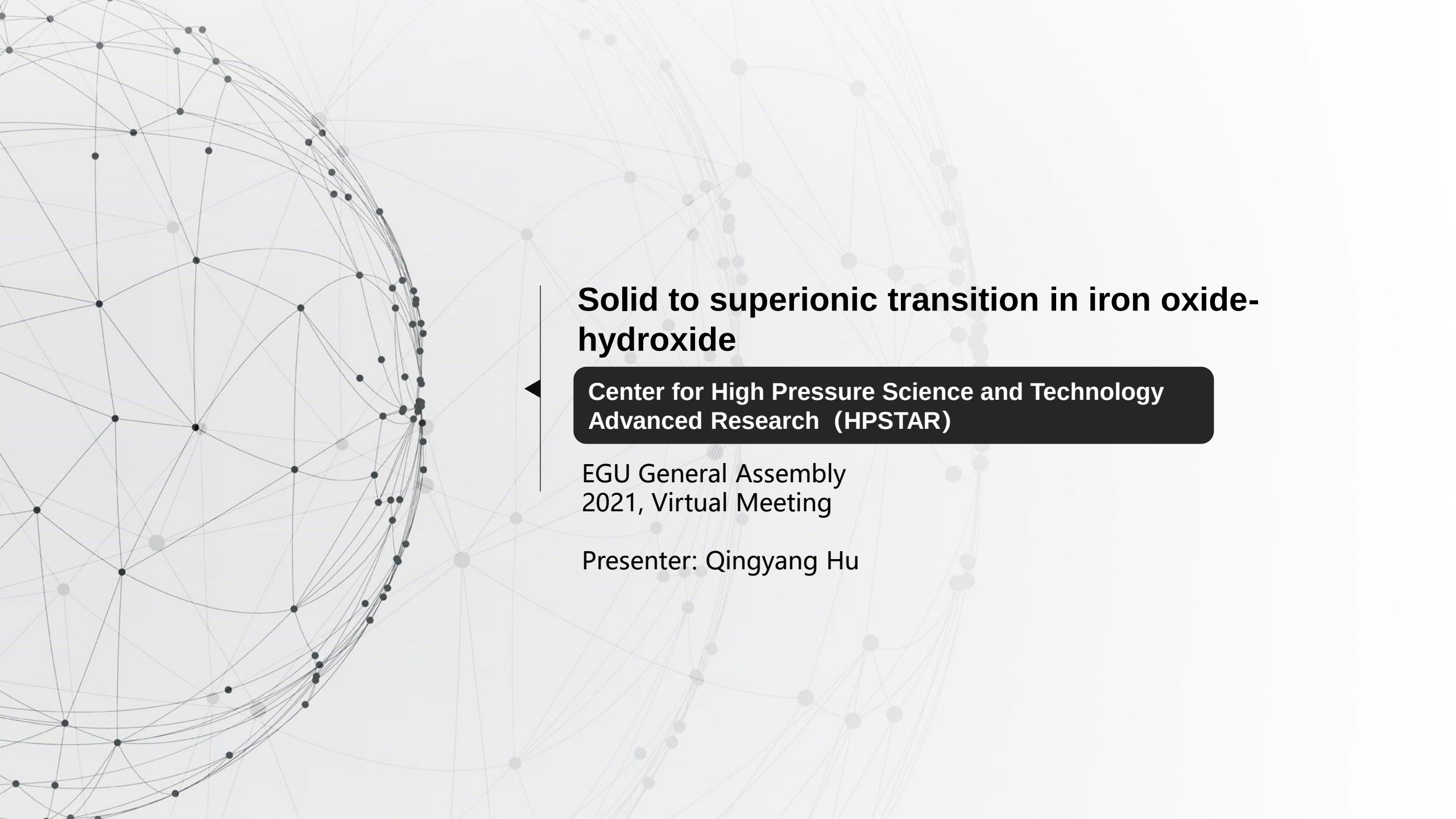


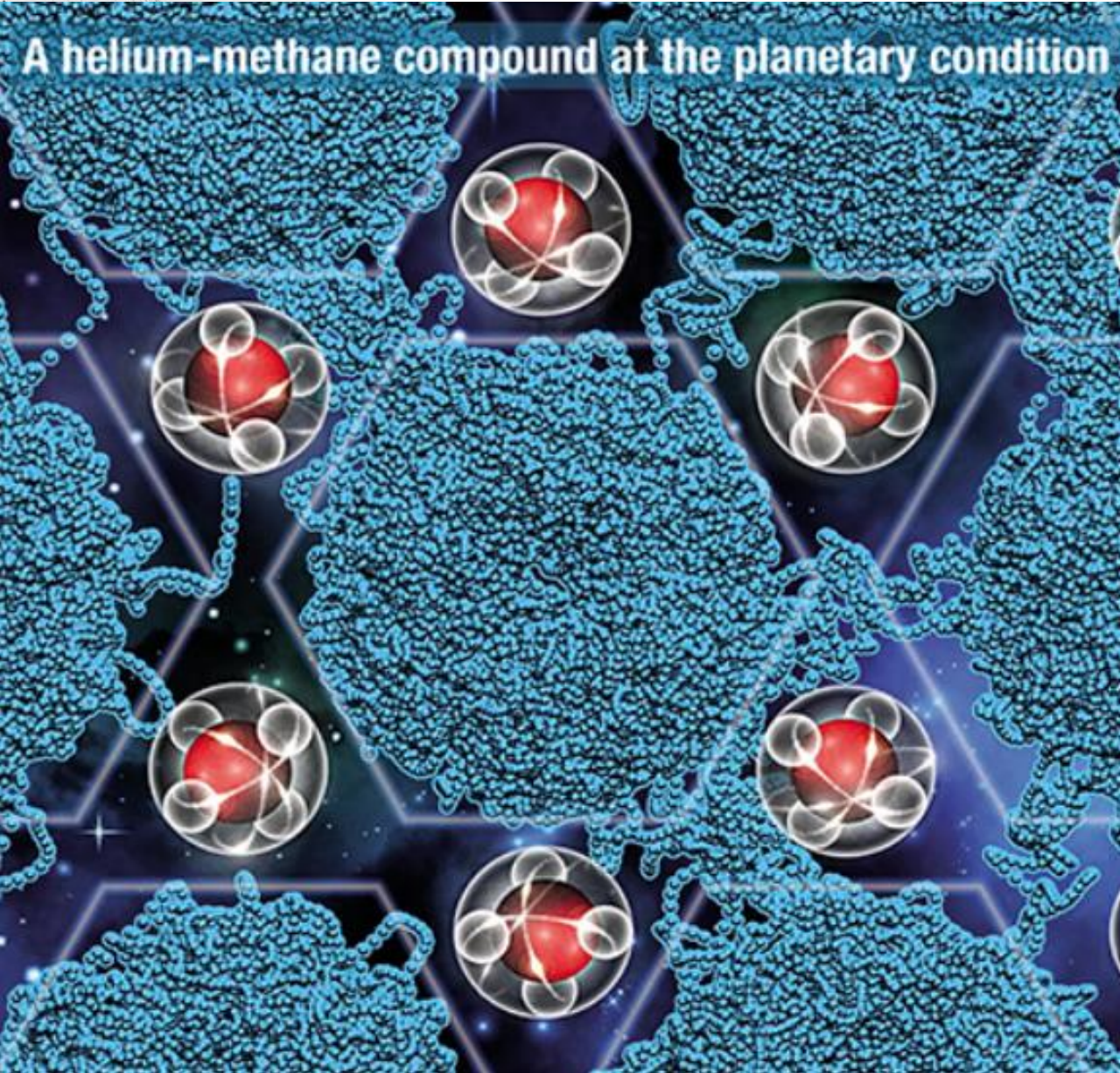


Solid to superionic transition in iron oxide-hydroxide

**Center for High Pressure Science and Technology
Advanced Research (HPSTAR)**

EGU General Assembly
2021, Virtual Meeting

Presenter: Qingyang Hu

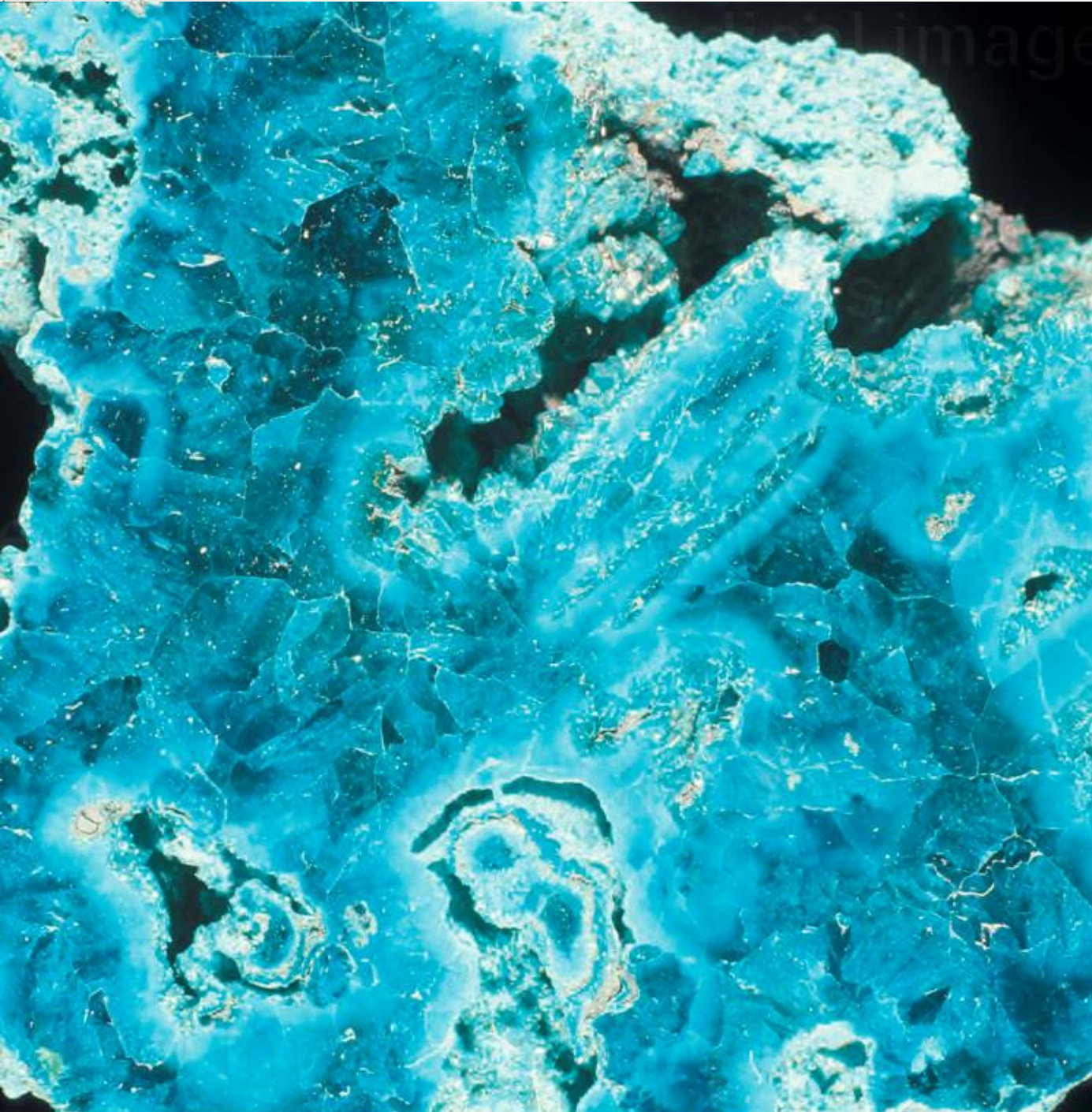


- **97%** of the universe are made of H and He.
- Most commonly seen H are found in **superionic phases**. For example:

Ice: *Science* 1999 (theory)
Nat. Phys. 2018, *Nature* 2019 (experiment)
He-Ice: *Nat. Phys.* 2019
He-CH₄: *Natl. Sci. Rev.* 2020
He-(NH₃)₂: *Phys. Rev. X* 2020
Hydride: *Phys. Rev. B* 2018, *Phys. Rev. Lett.* 2021

Caption:
Superionic He-CH₄ compound
Gao, *et al.*, *Natl. Sci. Rev.* 2020

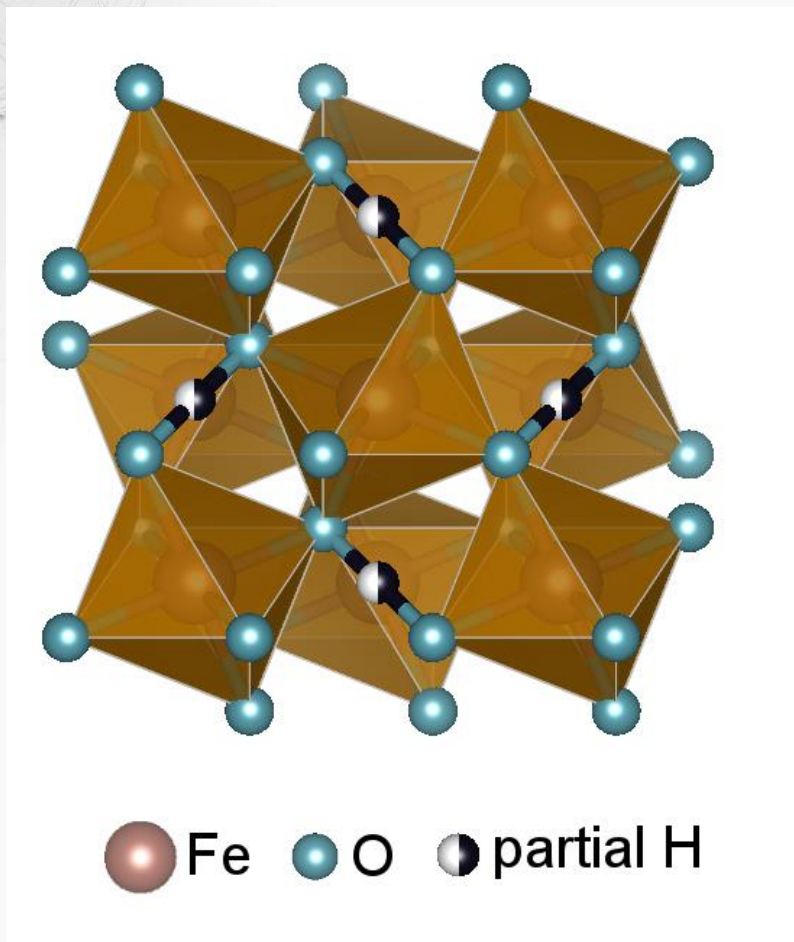




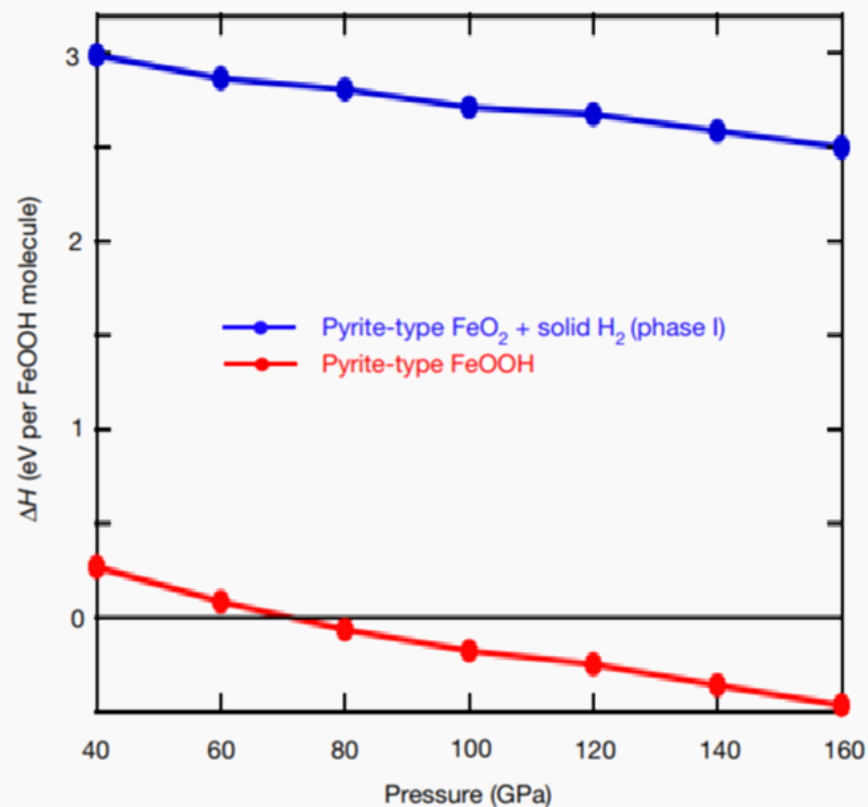
Superionic phase in lower mantle
hydrous mineral?

Caption:
Hydrous copper silicate mineral
www.medicalimages.com

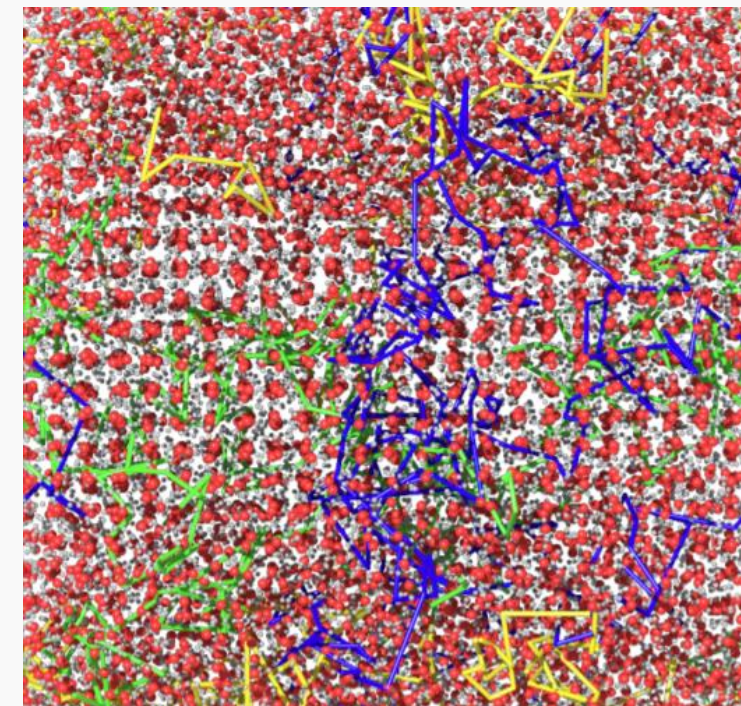




Dehydrogenation:
Fast H diffusion.
Hu, et al., 2017

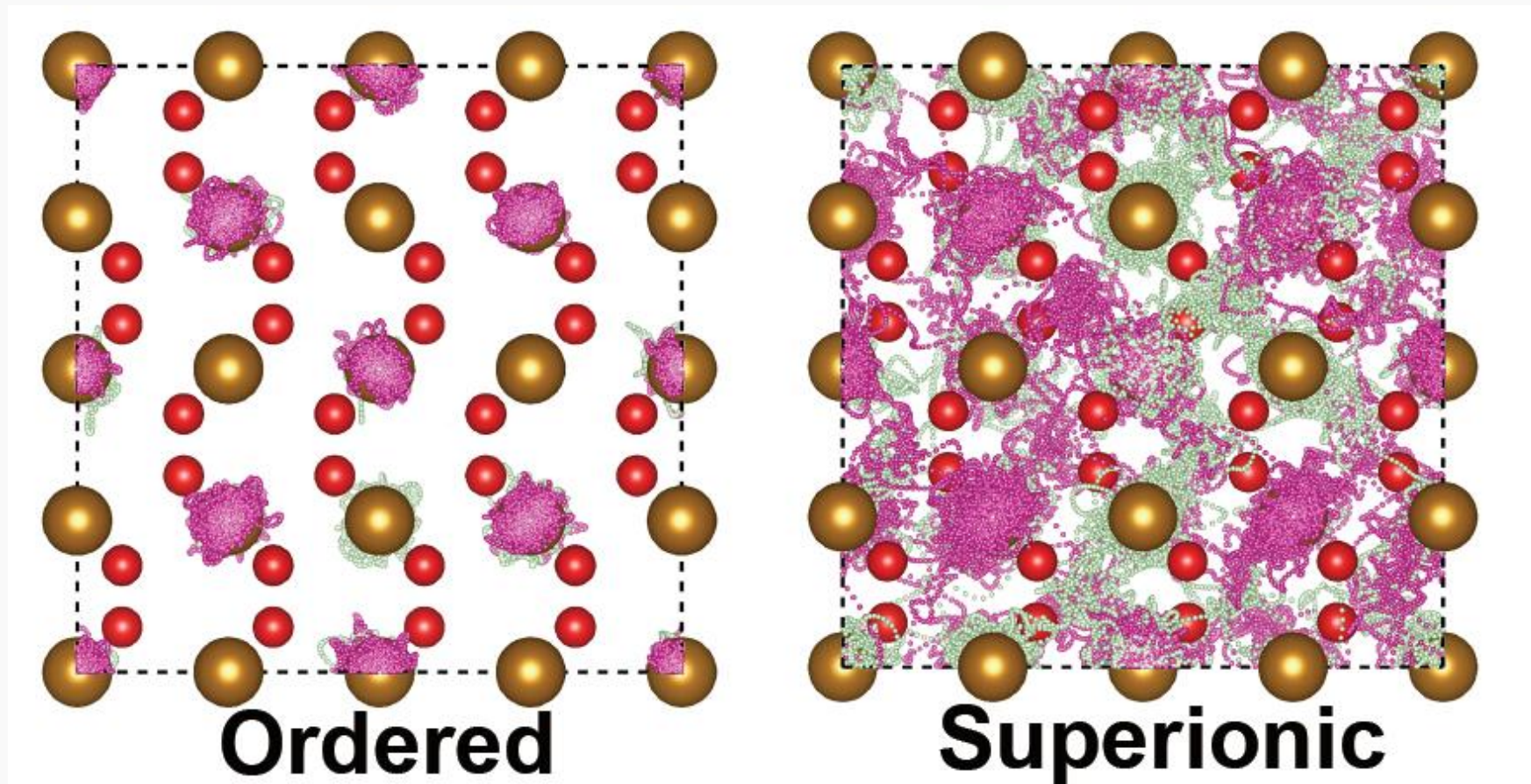


Whole FeOOH:
Classic hydroxyl.
Nishi, et al., 2017

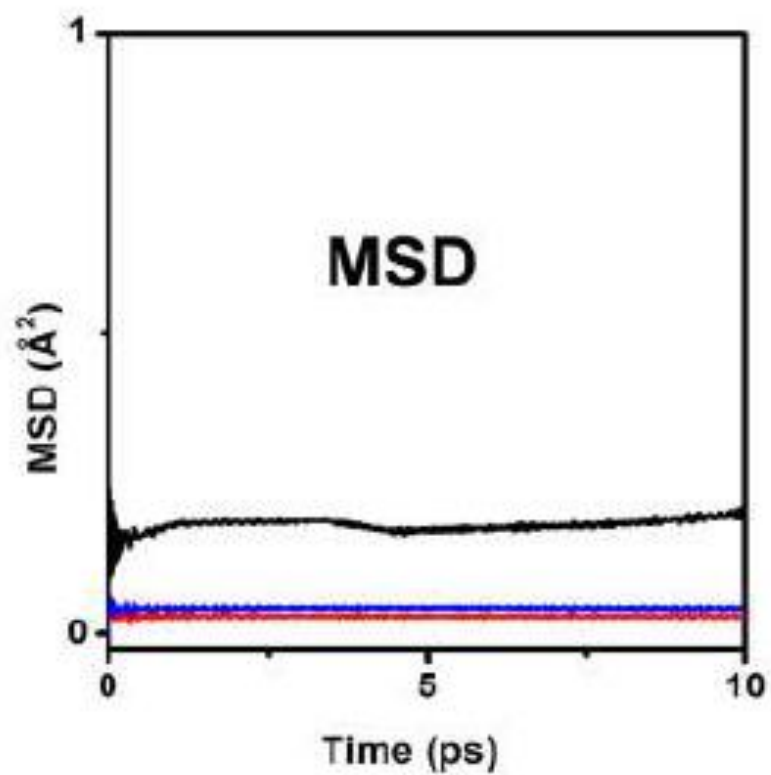


Cross-boundary H
diffusion in superionic ice.
Cheng et al., 2021

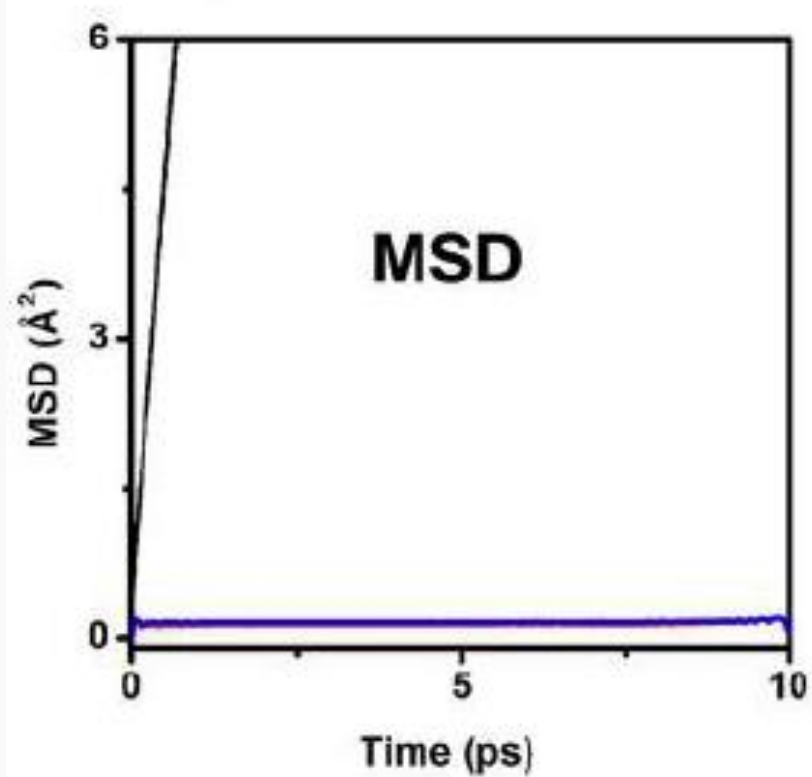
Trajectories of atoms



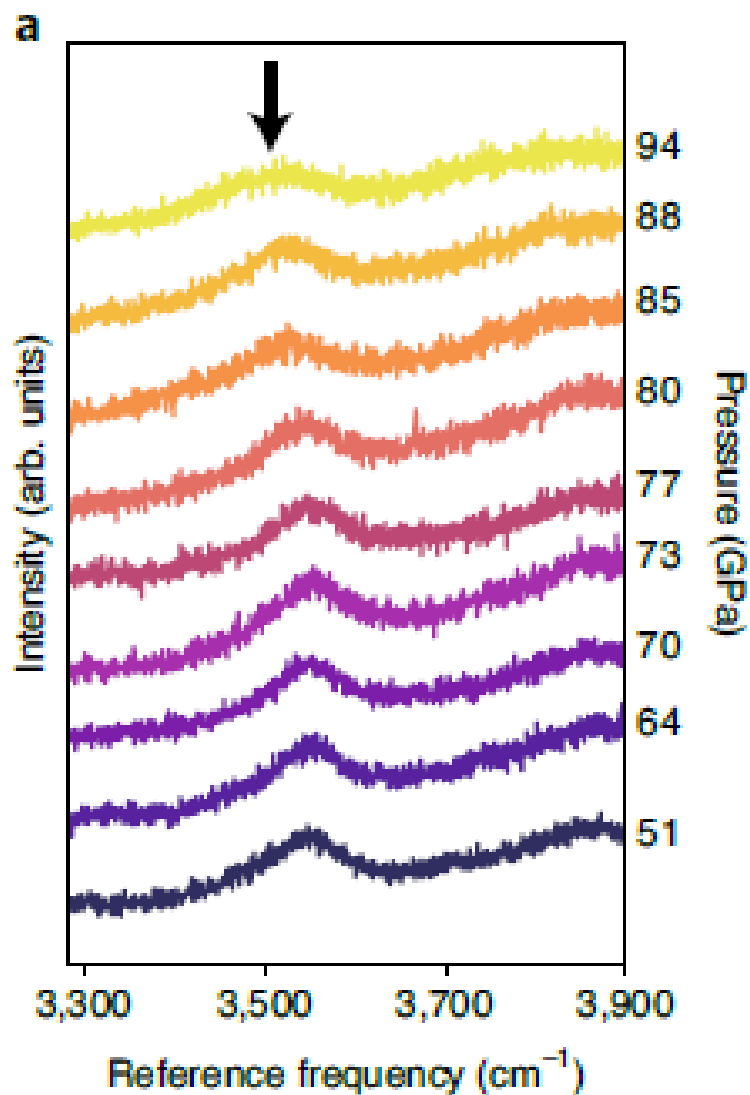
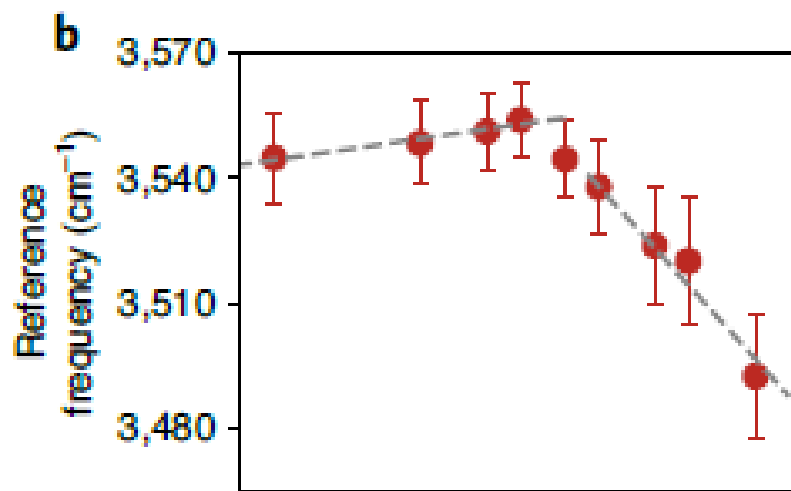
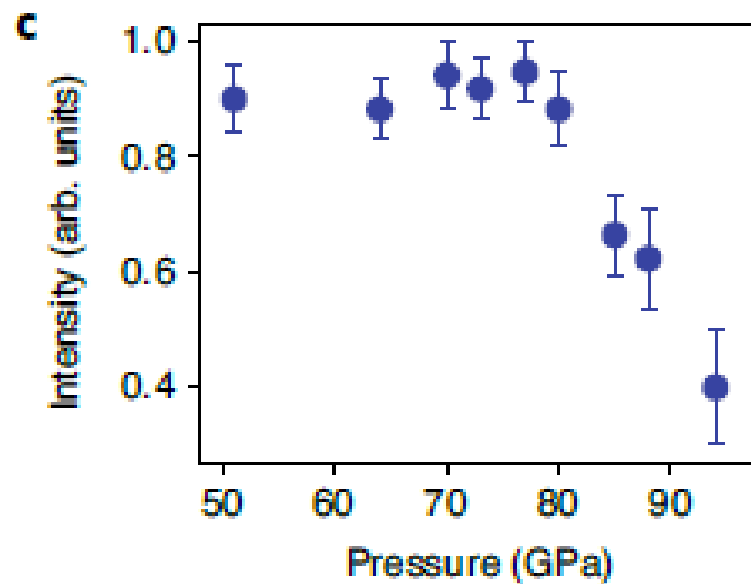
FeO₂H_{0.5} 124 (1) GPa 1500 (50) K



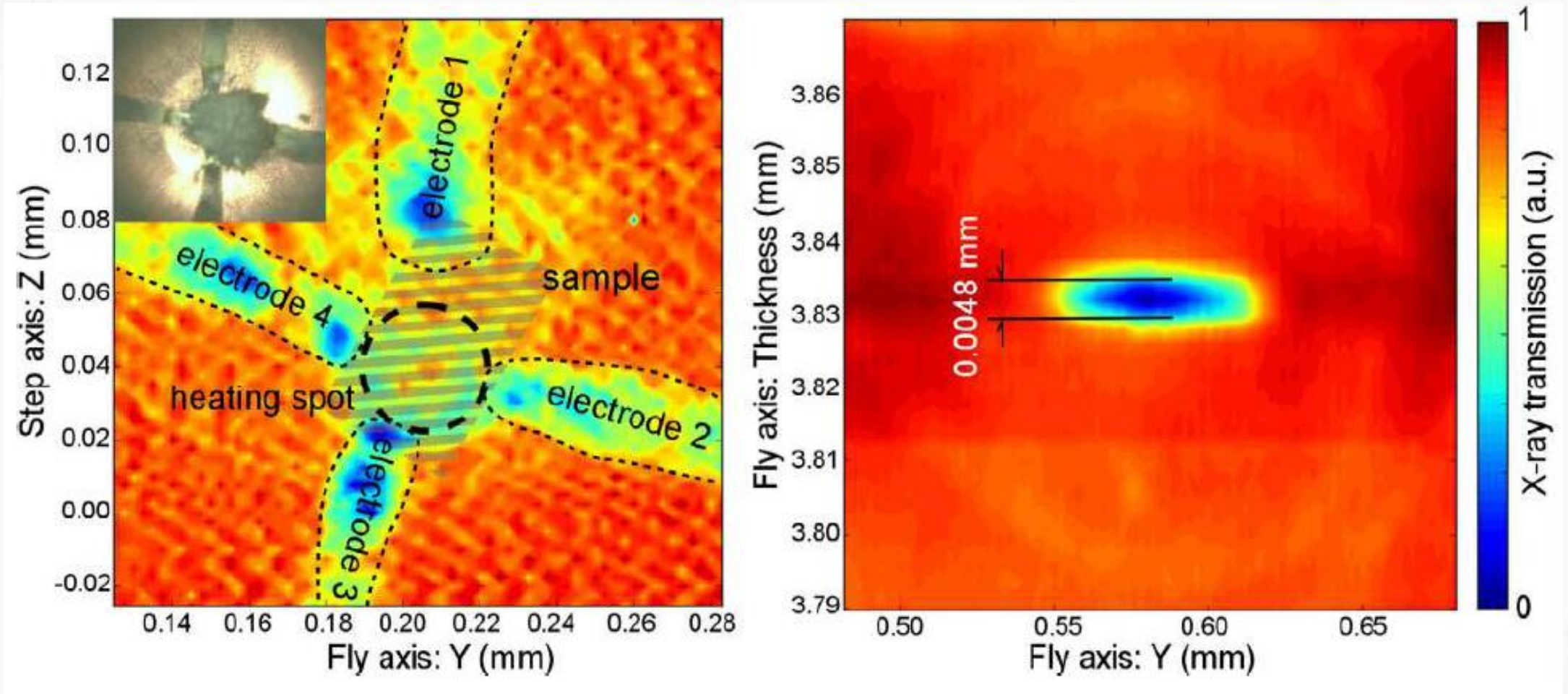
FeO₂H_{0.5} 139 (1) GPa 3000 (50) K



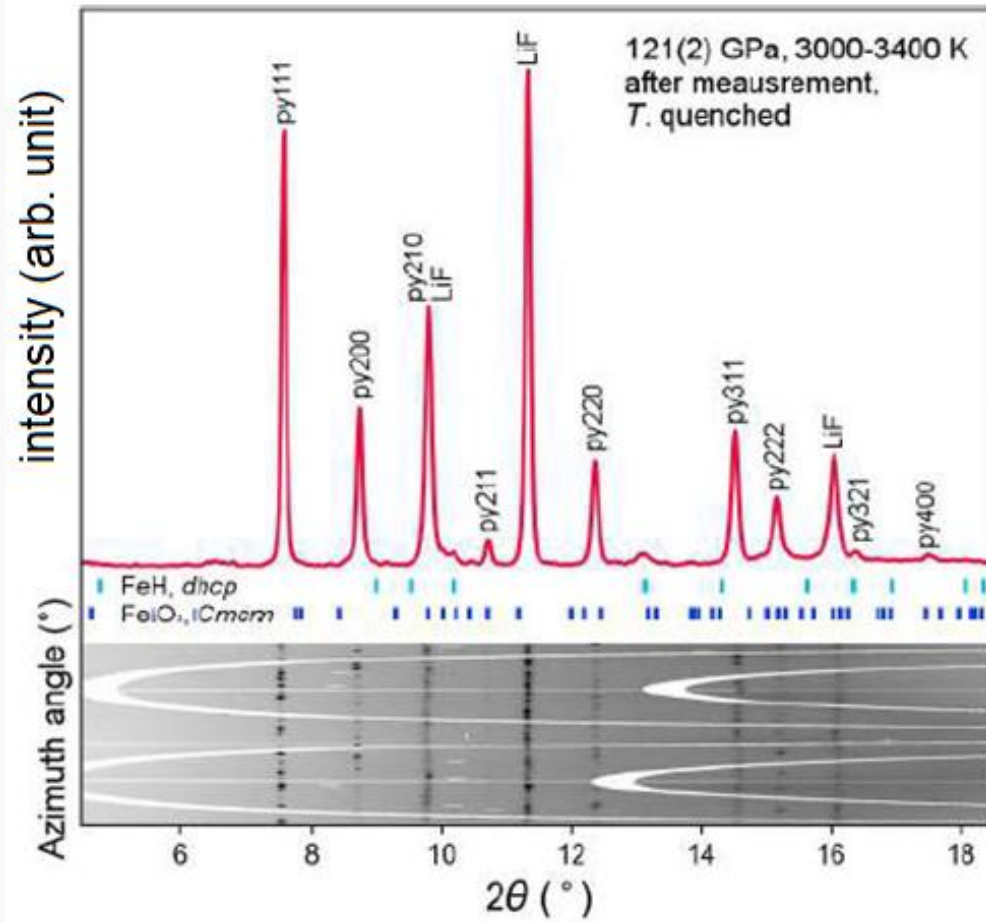
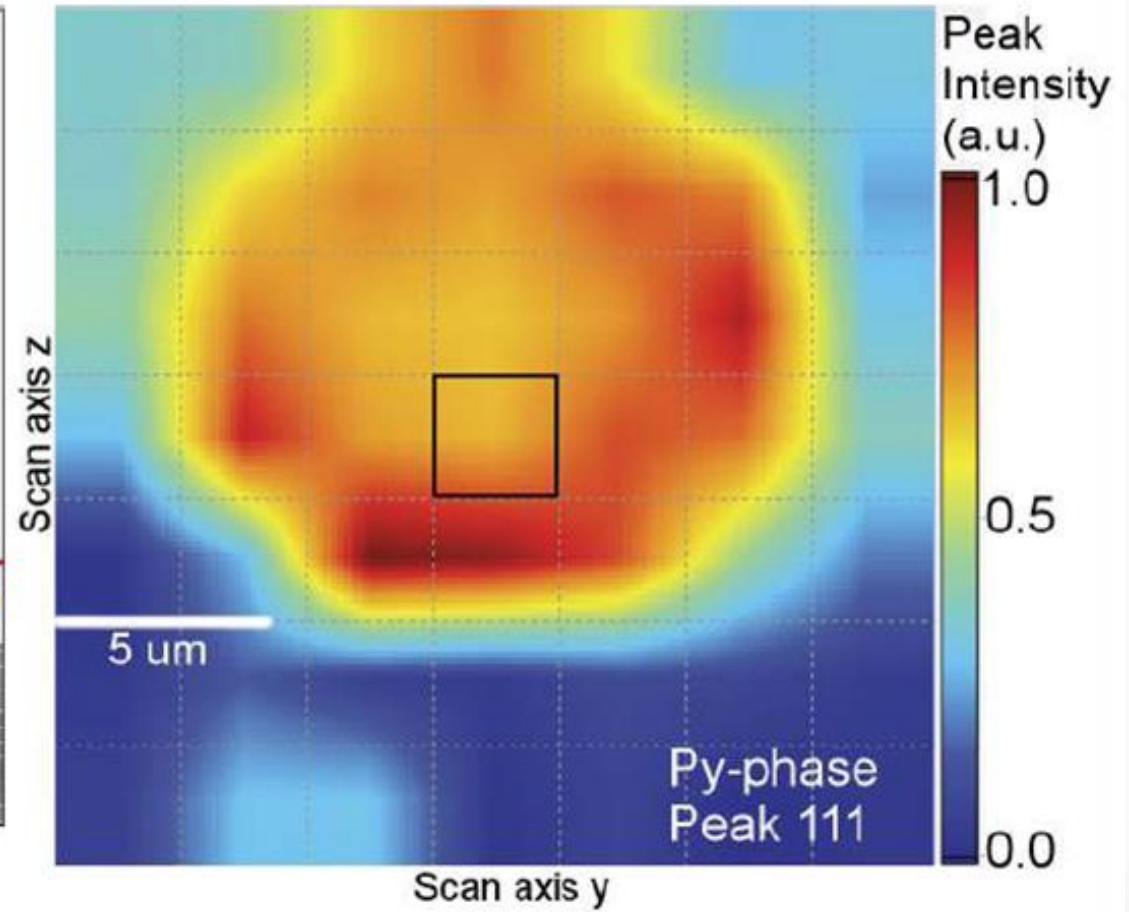
Softened O-H modes



Four-probe electrical conductivity measurement



XRD + laser heat: persistent pyrite-type phase



Electrical conductivity from MD + DMFT simulation

Ionic conductivity (IC):
$$\sigma_{IC} = \frac{f D c q^2}{kT}$$

Nernst-Einstein equation
MD simulation

Sharp increase with T

Electron mobility (EM):
$$\frac{1}{\sigma_{EM}} = \frac{1}{\sigma_{e-ph}} + \frac{1}{\sigma_{e-e}}$$

Kubo-Greenwood formula

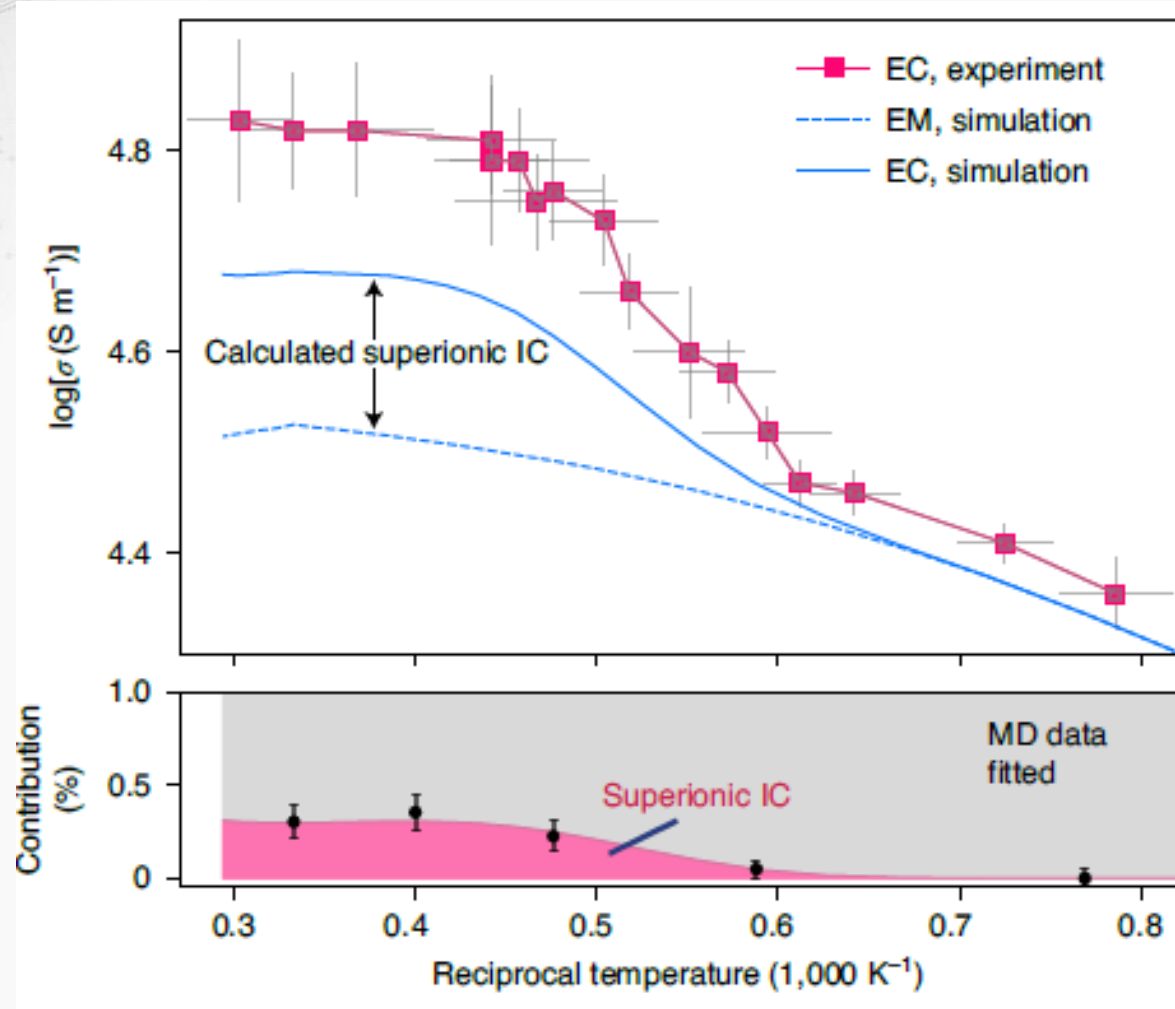
DMFT: e-e scattering

MD: e-ph contribution

Slow increase

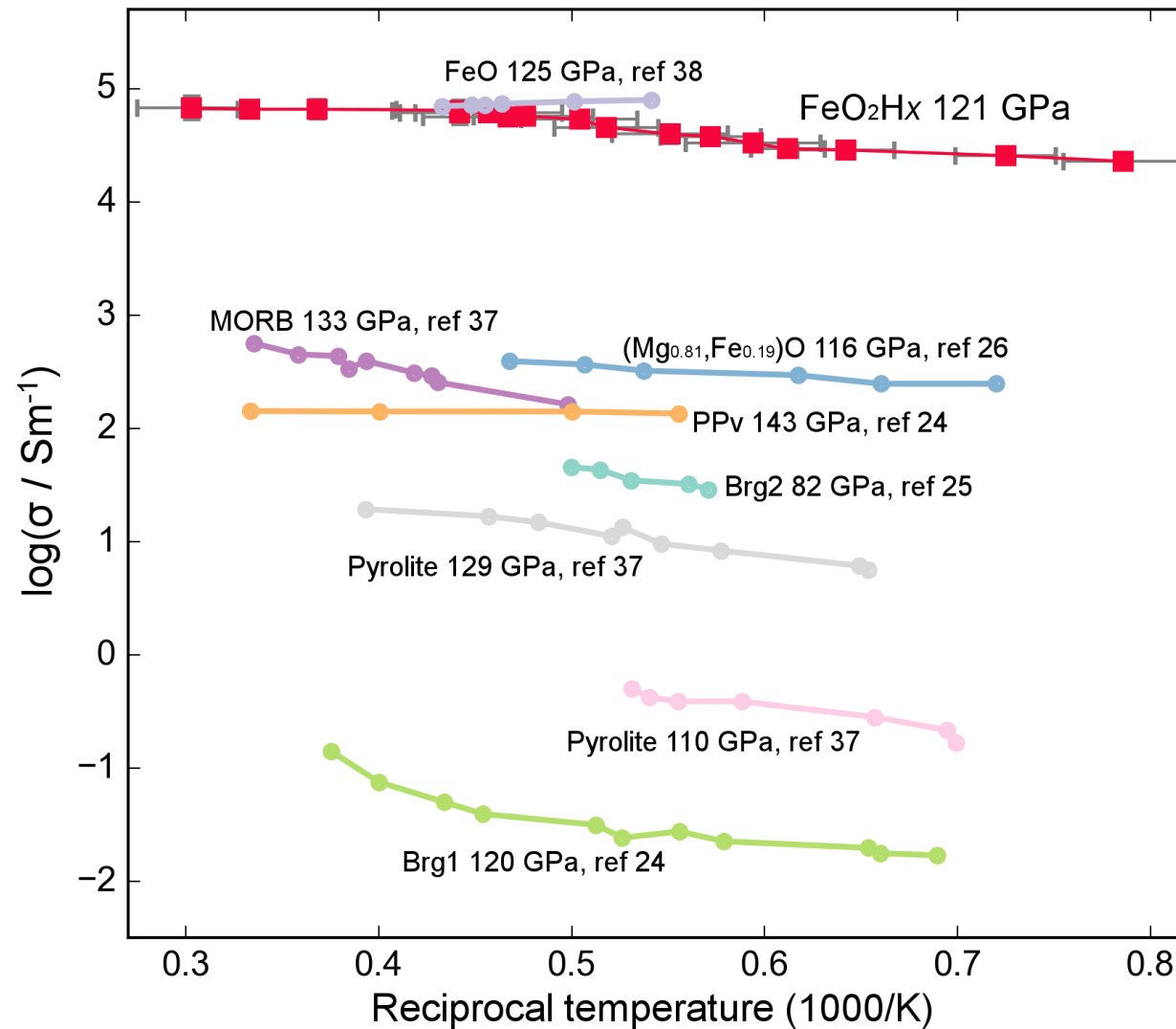
Total conductivity:
$$\sigma_{total} = \sigma_{IC} + \sigma_{EM}$$

EC results

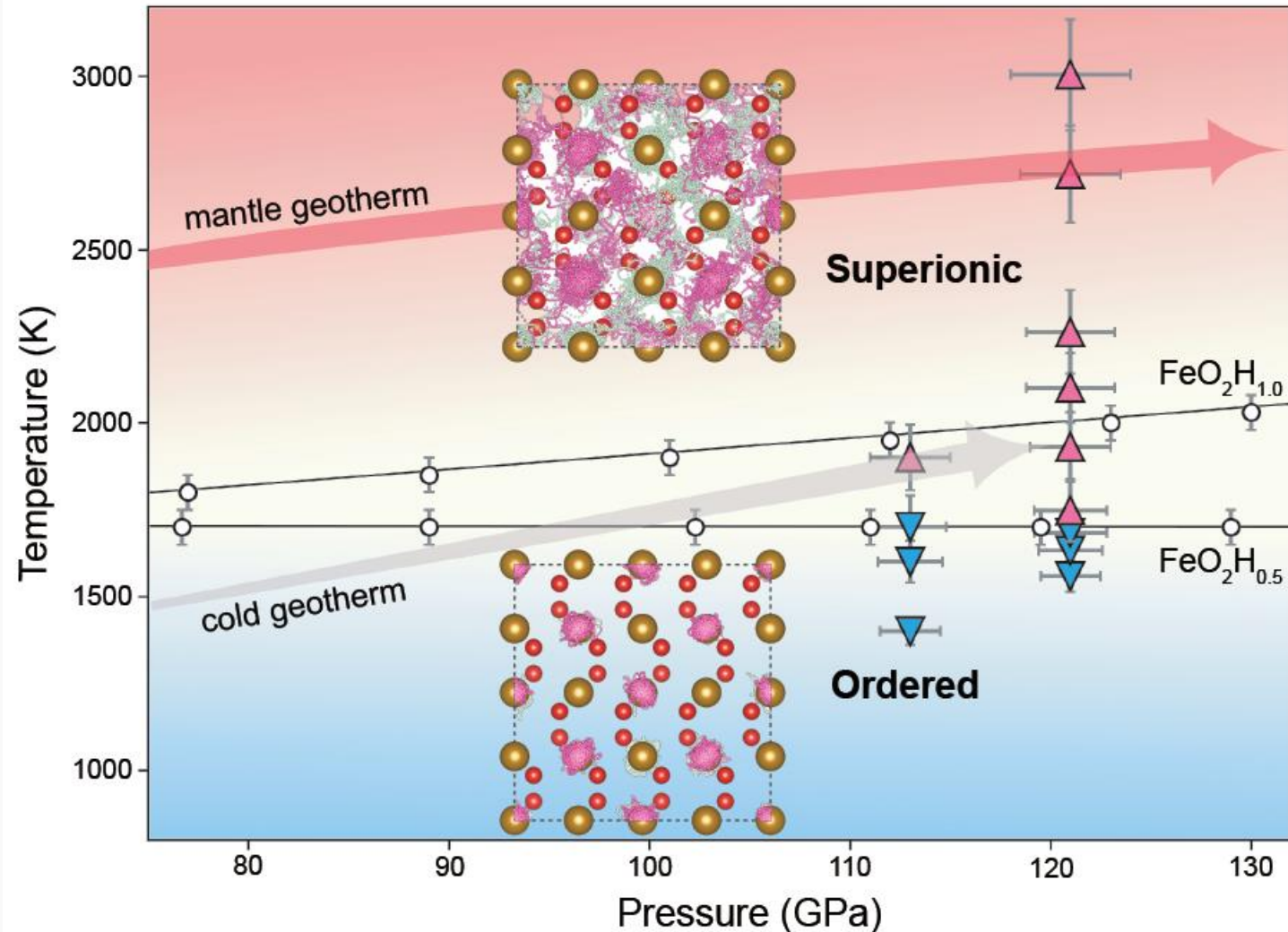


- Soaring EC in between 1600-1800 K.
- Experiment and theory are consistent in the trend of changing.
- Ionic conductivity contribute up to ~30% of total conductivity.

Compare with other lower mantle materials

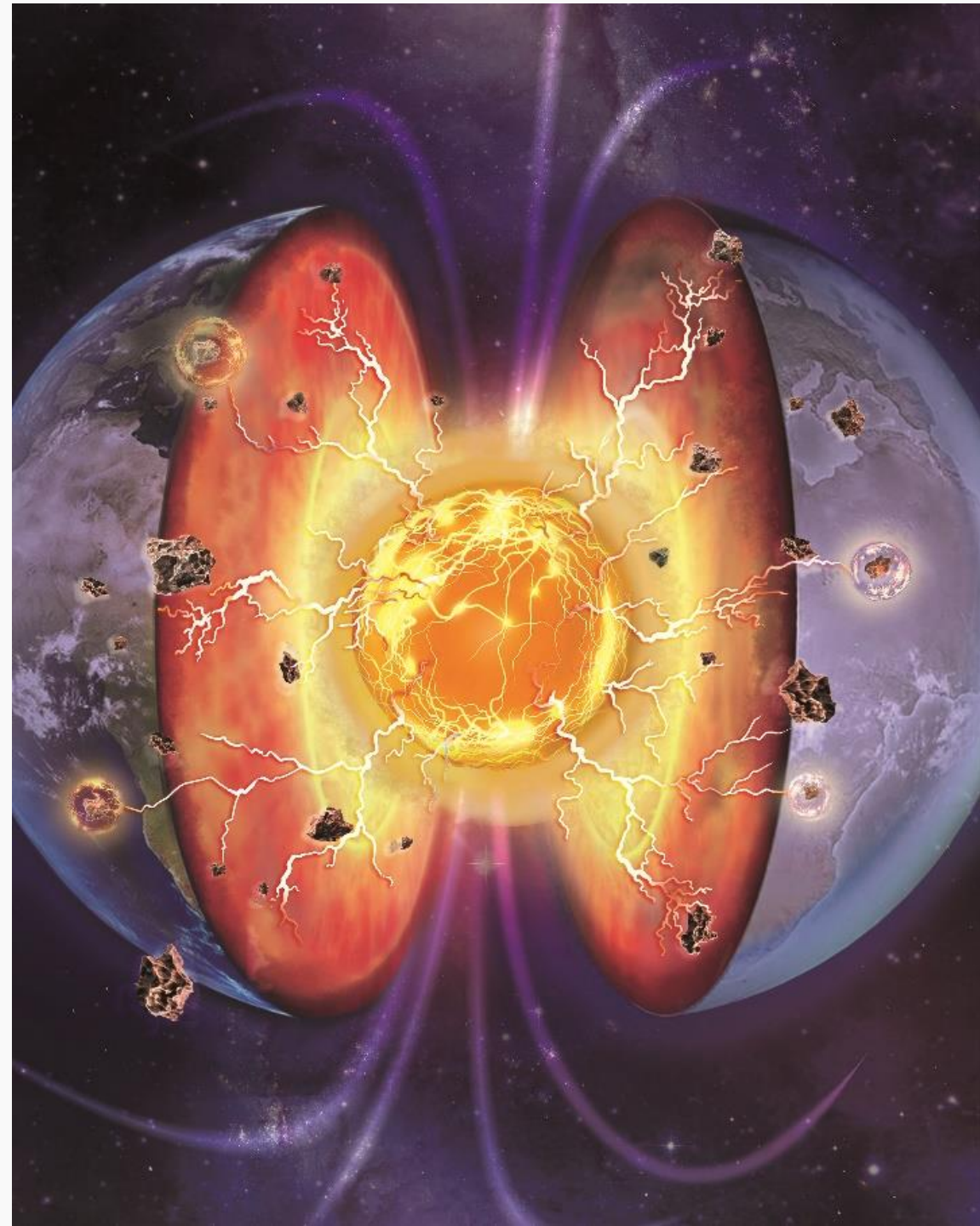


High-*P-T* Phase diagram



Take home messages

- In shallower mantle, normally anhydrous minerals like olivine can hold hydrogen and exhibit protonic current.
- Superionic phase is not only a measurement, but also a potential new form of solid in Earth's deep interiors and the major existence in icy giant planets.





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Yukai Zhuang, Ruilian Tang (Room T , *EC* experiment)

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Bo Gyu Jang, Ji Hoon Shim (DMFT simulation)

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