Superionic H-bearing iron alloys in the Earth's inner core

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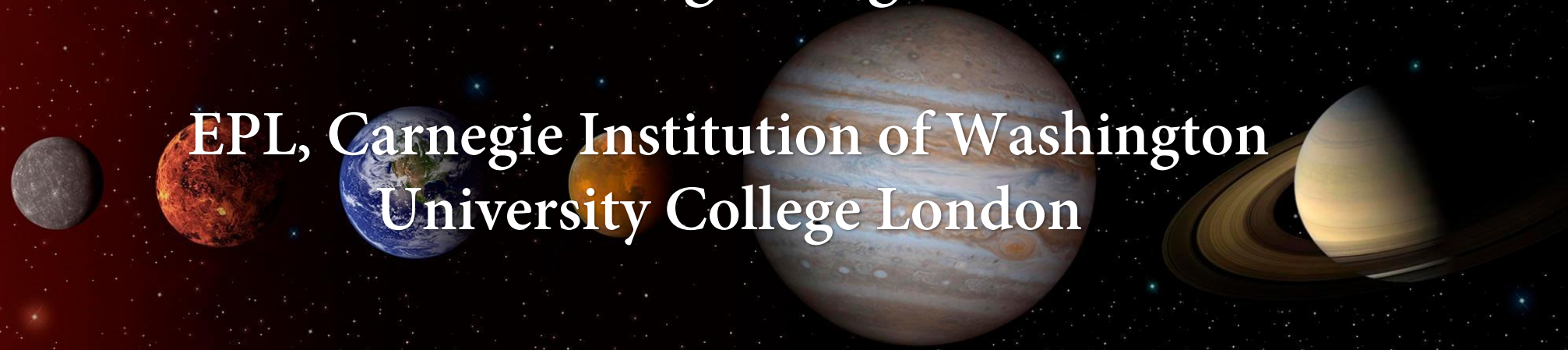
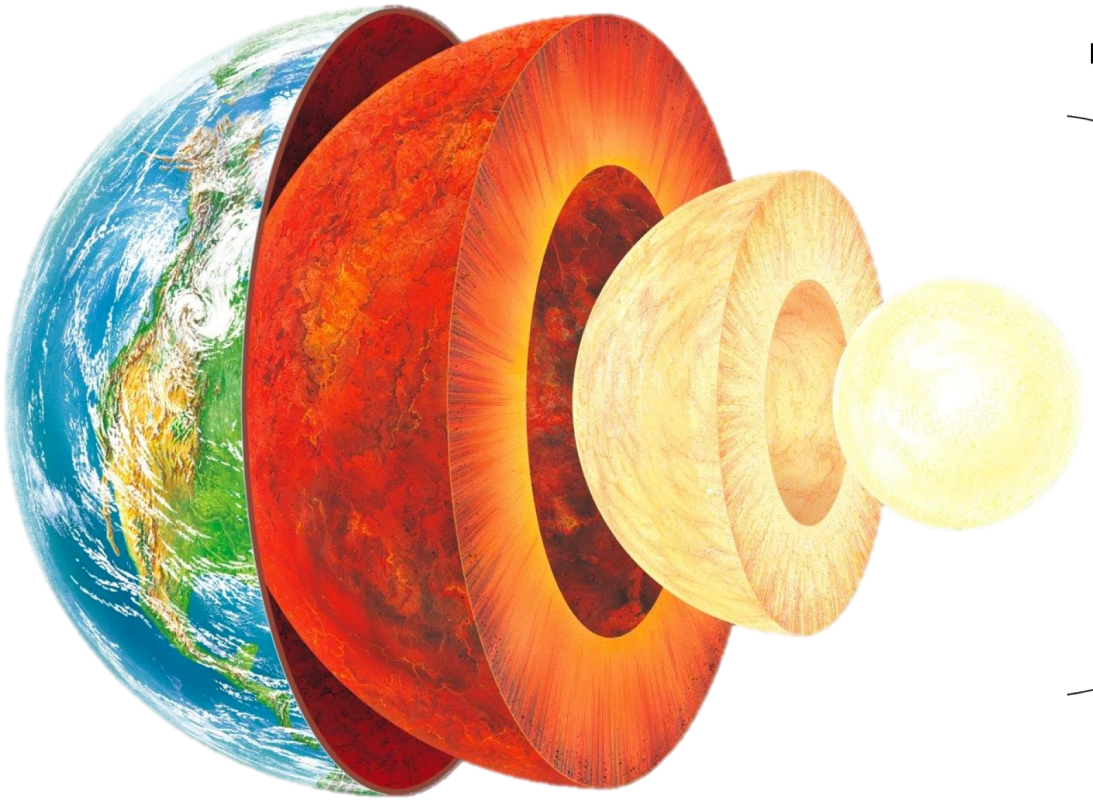


With thanks to: Yunguo Li, John Brodholt, Mike Walter, Lidunka Vočadlo

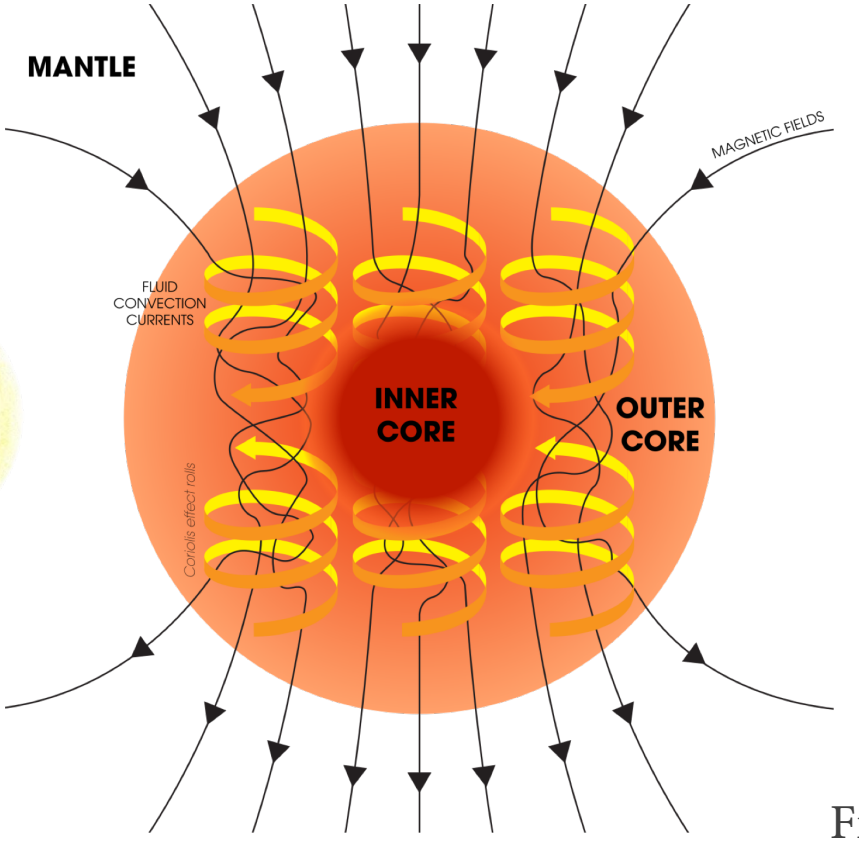
30-31, July, MMTE 2022

Earth's interior

Structure



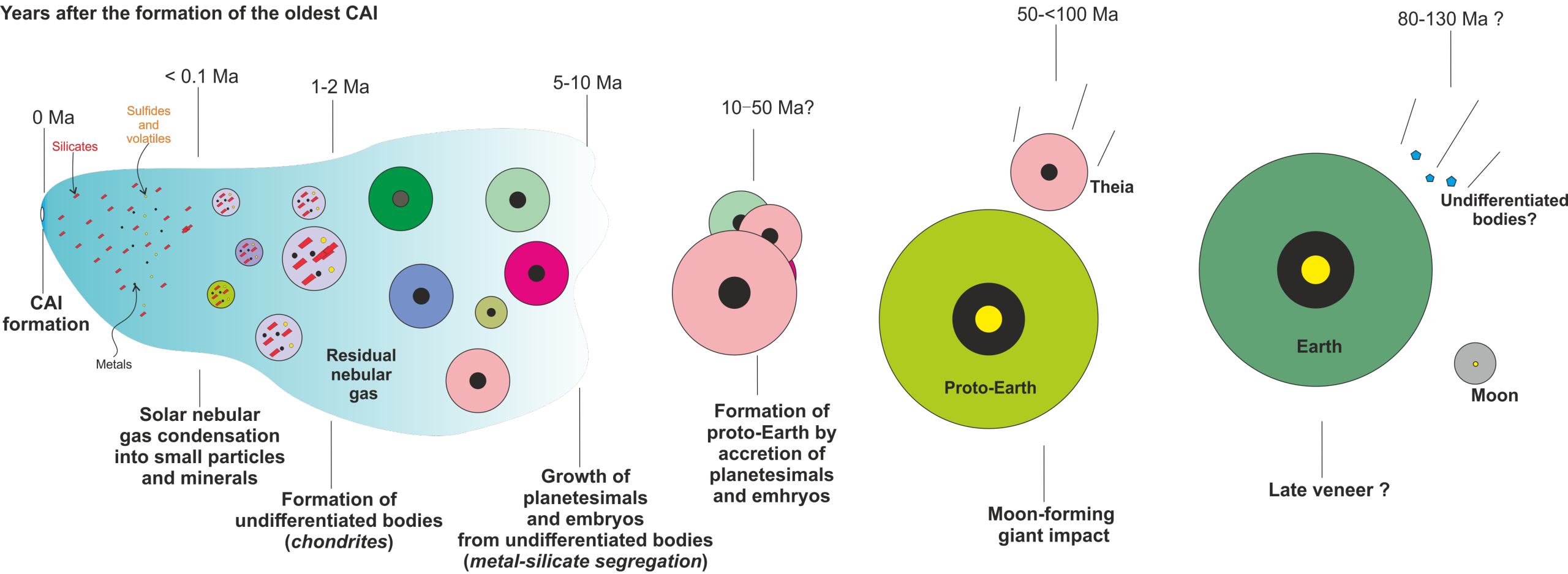
Geodynamo



From wikipedia

Earth's core is responsible for the generation of Earth's magnetic field, which is fundamental to Earth's habitability

Planetary Formation Processes



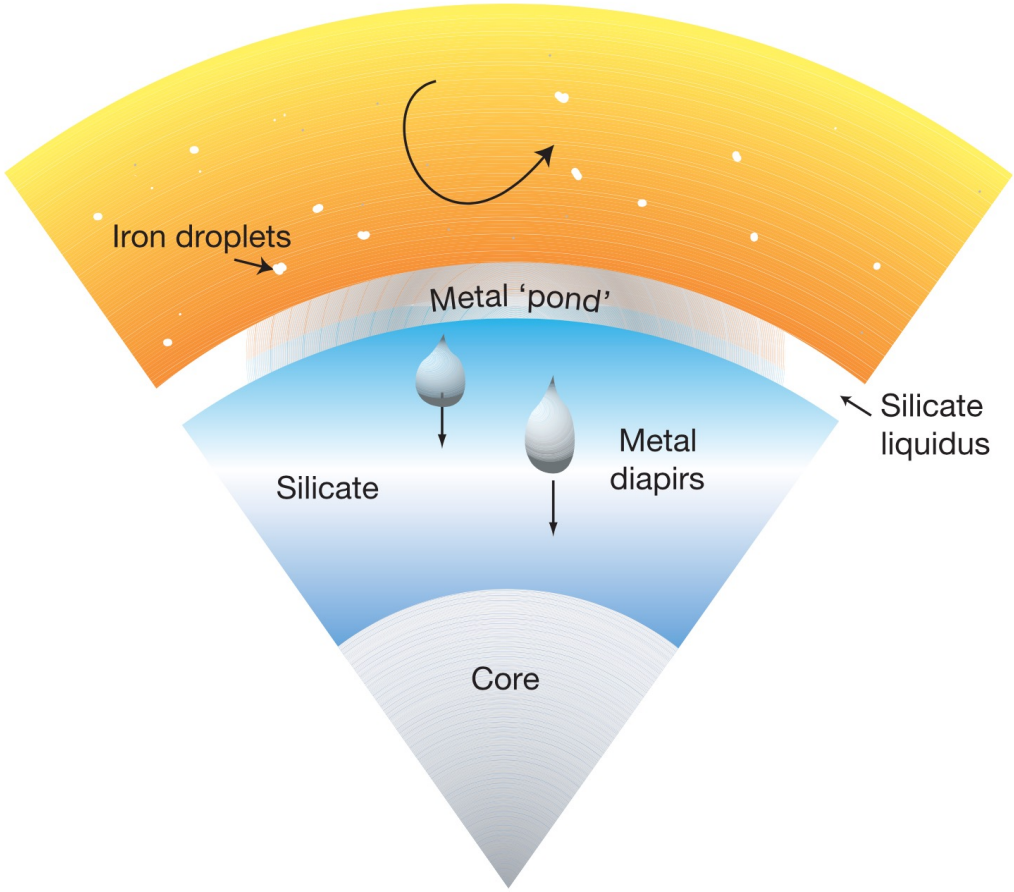
Vibrant stages of planetary formation

Collision, core formation, magma ocean, proto-atmosphere

Material and energy redistribution

Gain and loss

Core formation

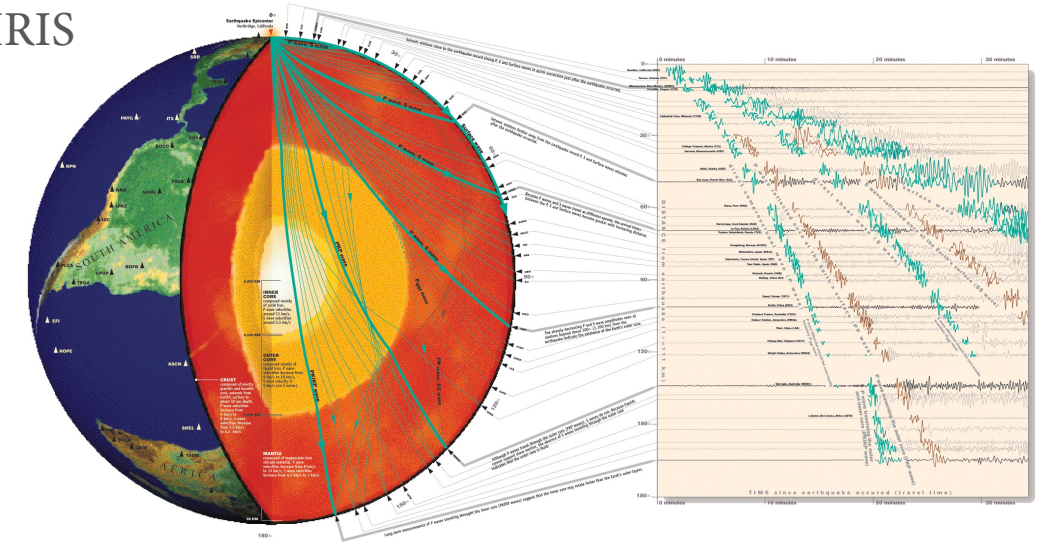


Wood et al. (2006)

Earth's core records important information regarding the history of Earth's accretion and influences the subsequent evolution of the mantle, crust, and atmosphere

Core composition – A multidisciplinary problem

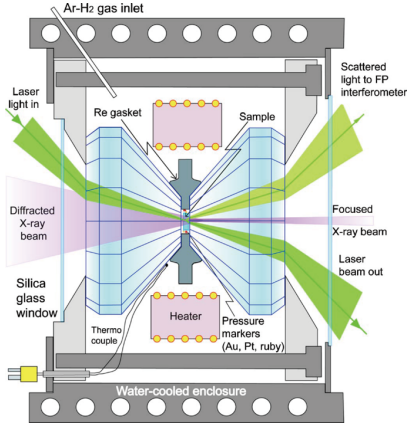
From IRIS

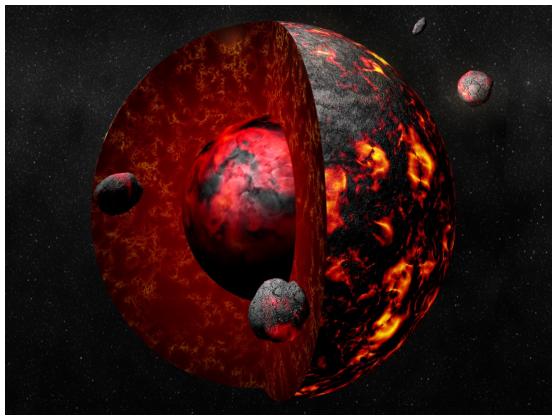


Earth's interior ← Seismology

- **Geophysical constraints:**

  wave velocities + density





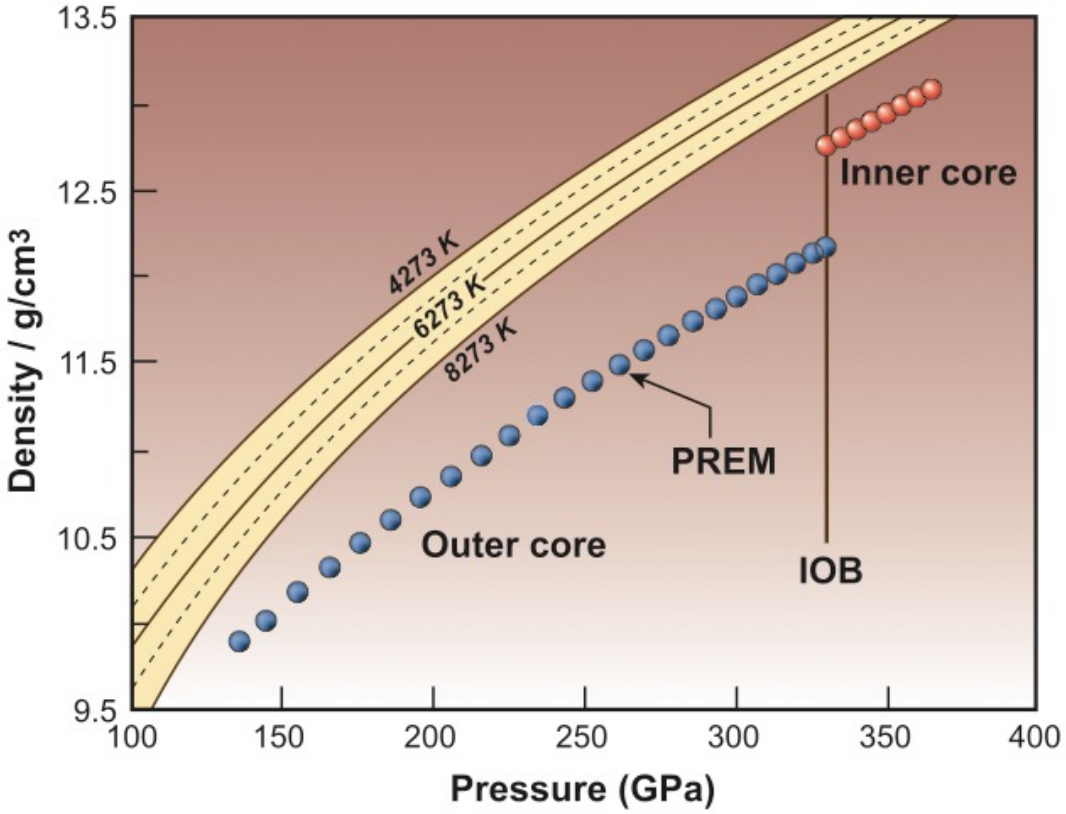
Experiments → Core formation

- **Geochemical constraints:**

  element partition + isotope fractionation

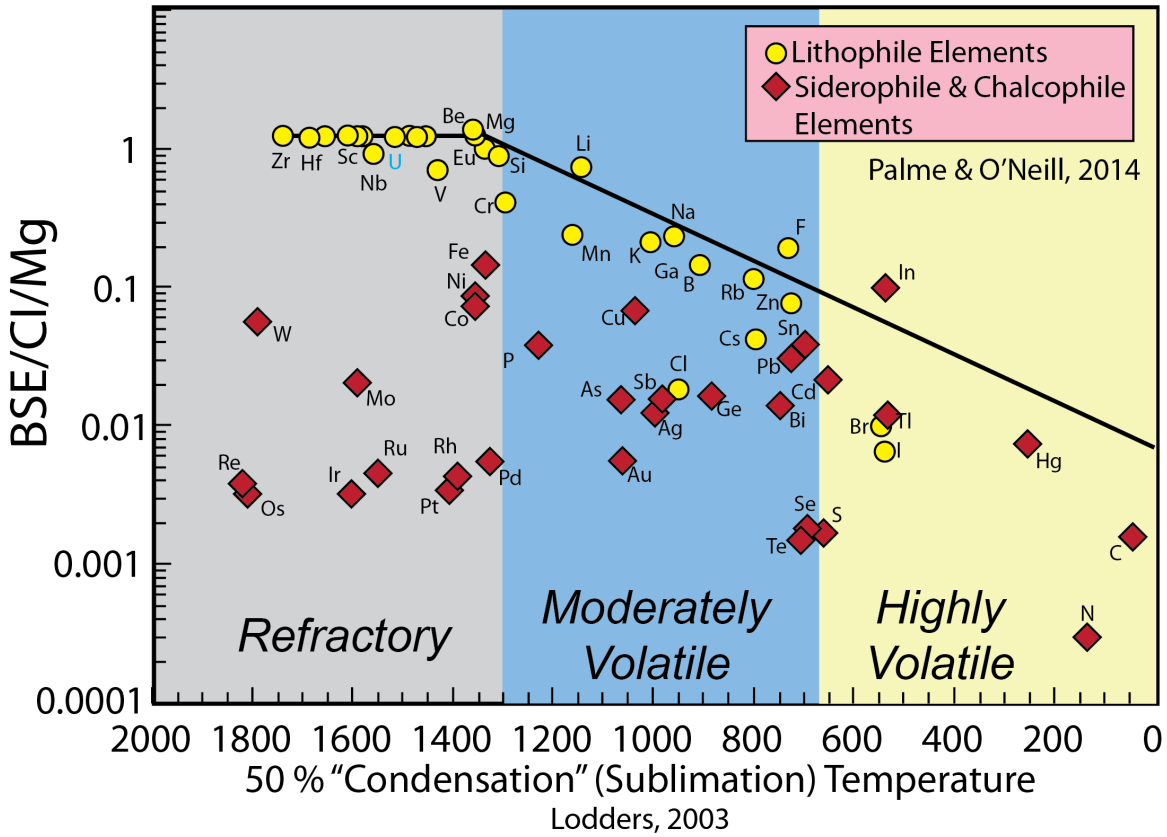
Core composition: Fe/Ni + "light elements"

James Badro after Uchida et al. (2001)



Density of Fe alloy

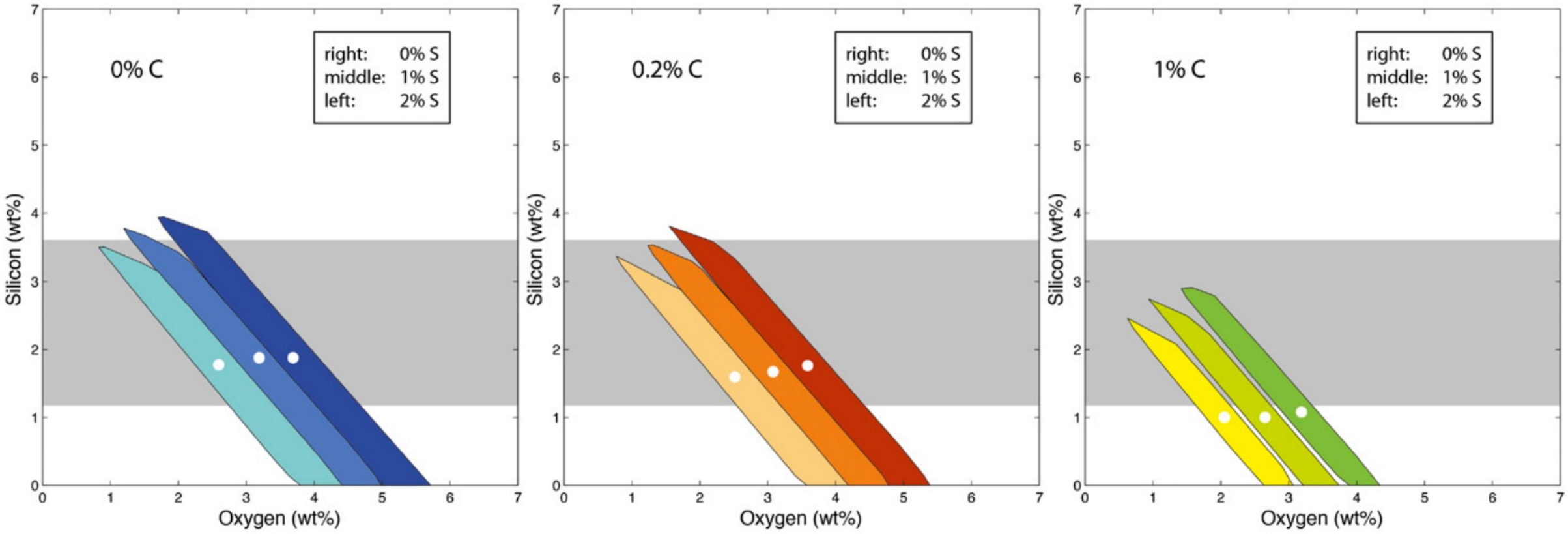
Image Credit: Marc Hirschmann



Siderophile light elements in the Mantle

Light elements are needed to match density +
Some have gone to the metal during core formation (Siderophile)

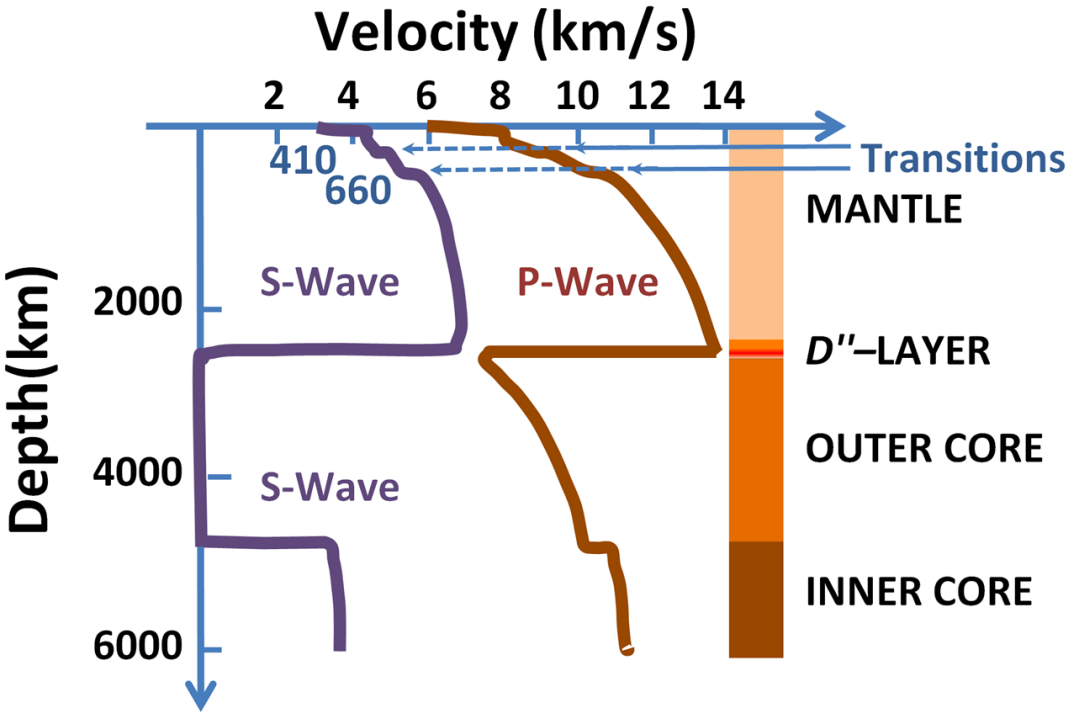
Outer core composition



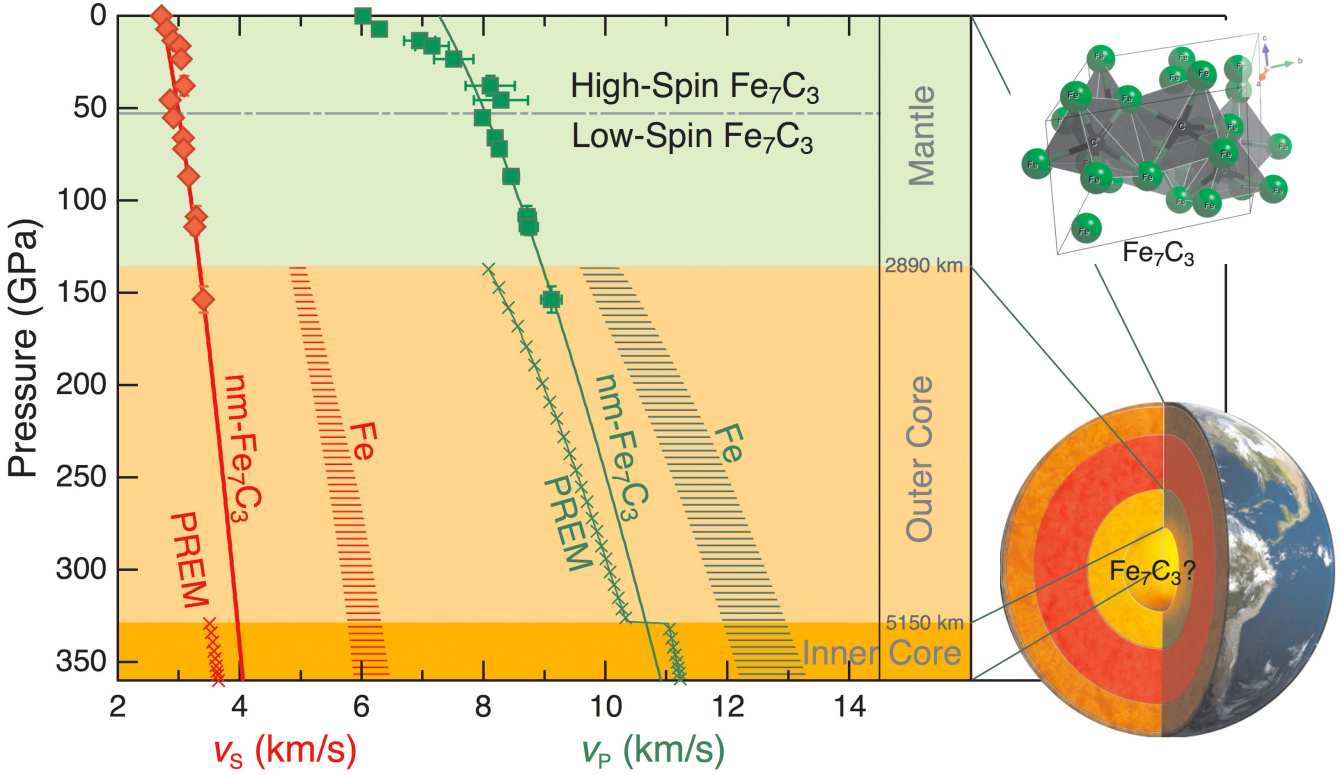
Badro et al. (2014)

A range of compositional models with O can fit the seismological data

Inner core



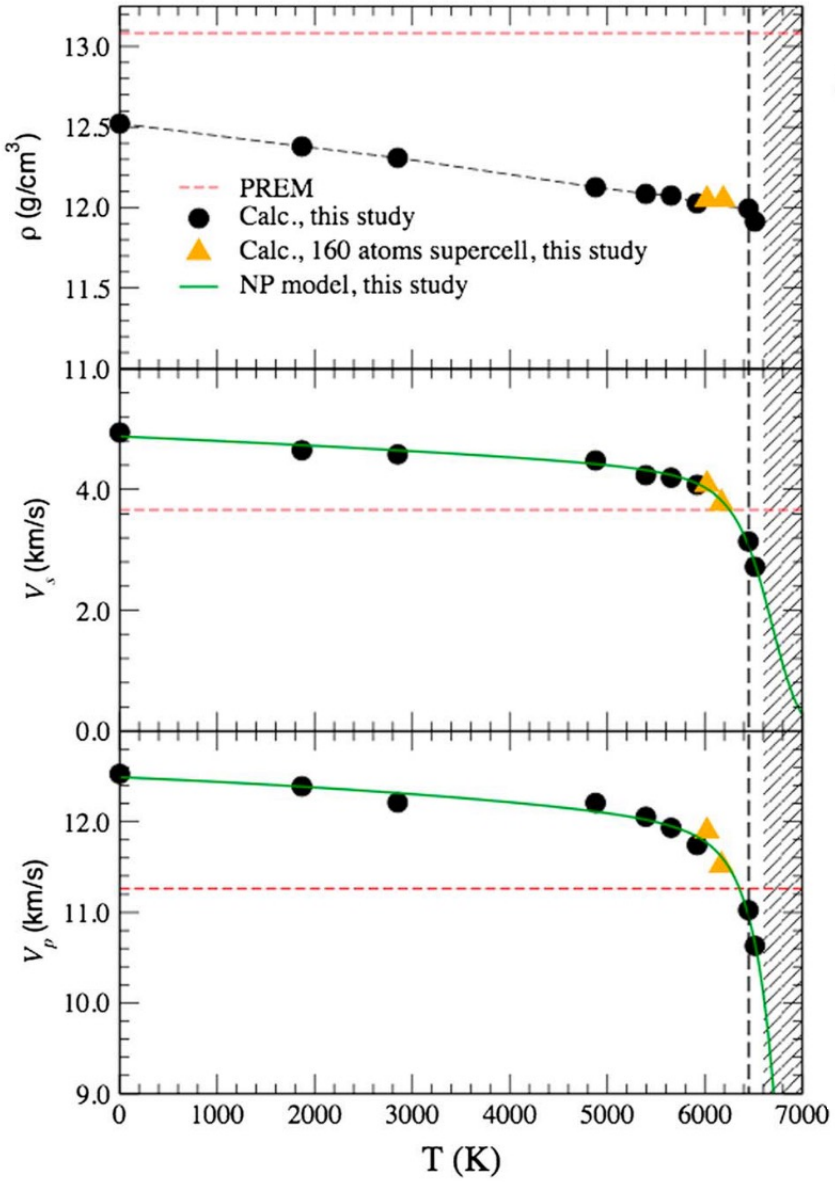
Carbon in the Earth's inner core?



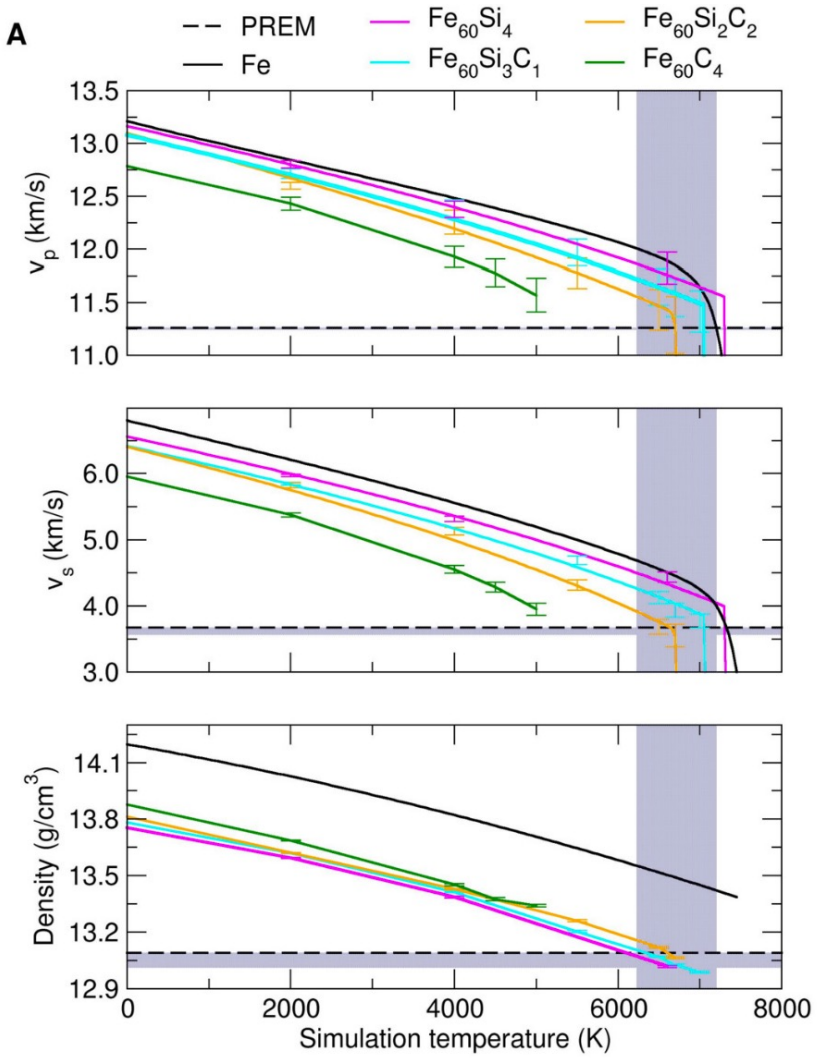
Low V_S + high V_P/V_S or Poisson's ratio

Chen et al. (2014)

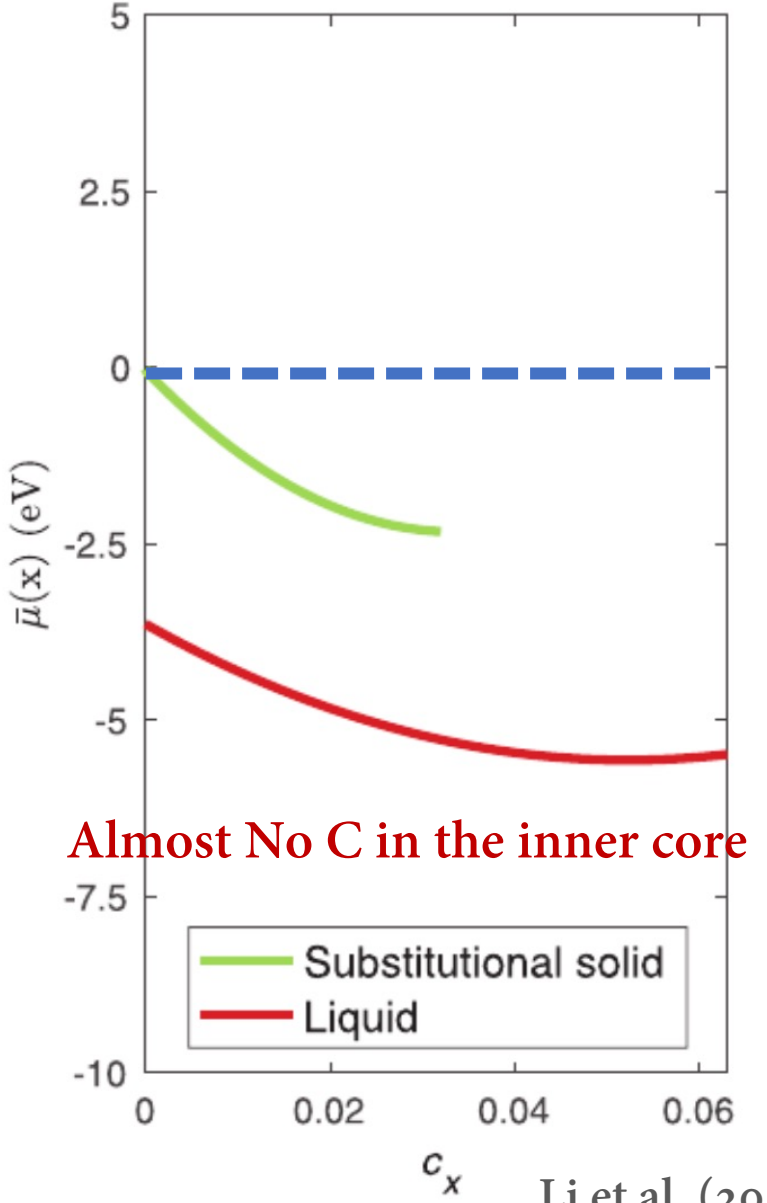
Carbon in the Earth's inner core?



Li et al. (2016)



Li et al. (2018)



Almost No C in the inner core

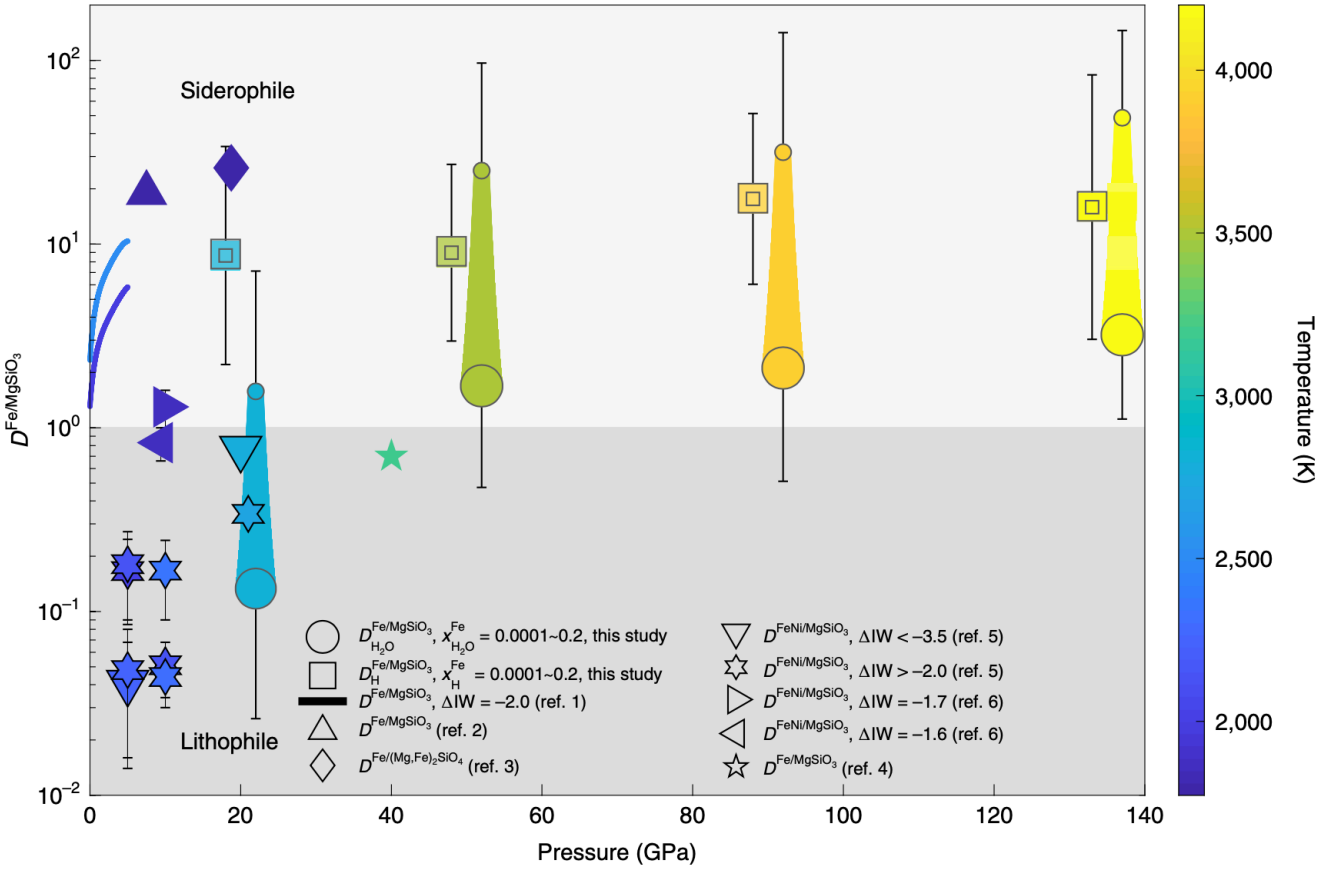
Li et al. (2019)

Partitioning of light elements between inner core and outer core

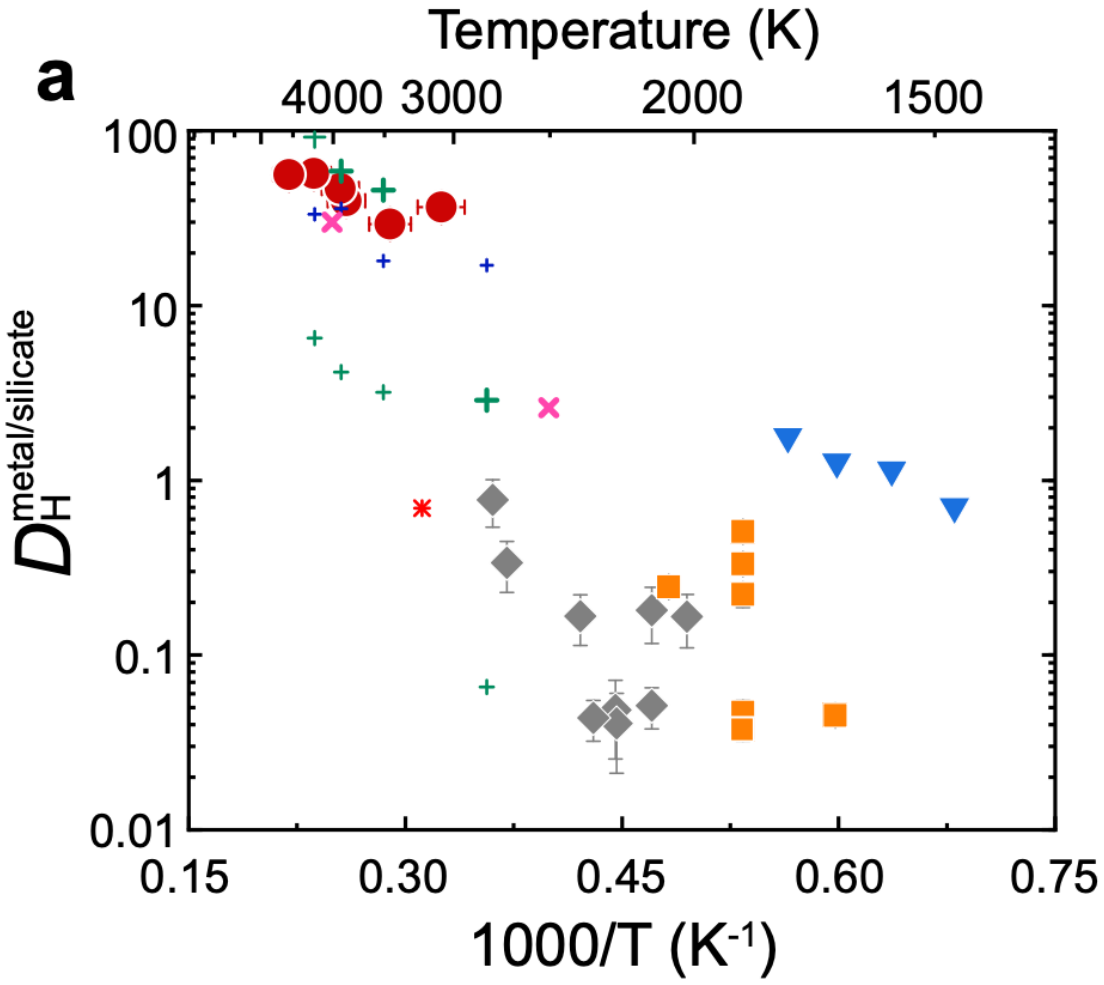
Solute	Chemical potential difference (liquid-solid)	Partition coefficient (solid/liquid)	References
S	-0.25 eV	0.63	Alfe et al. (2002)
S	-0.16 eV	0.75	Zhang et al. (2020)
Si	-0.05 eV	0.91	Alfe et al. (2002)
O	-2.6 eV	0.008	Alfe et al. (2002)
C	-3.6 eV	0.001	Alfe et al. (2002)

The inner core has negligible C and O concentrations
but substantial amounts of Si and S

Earth's core is a reservoir of water



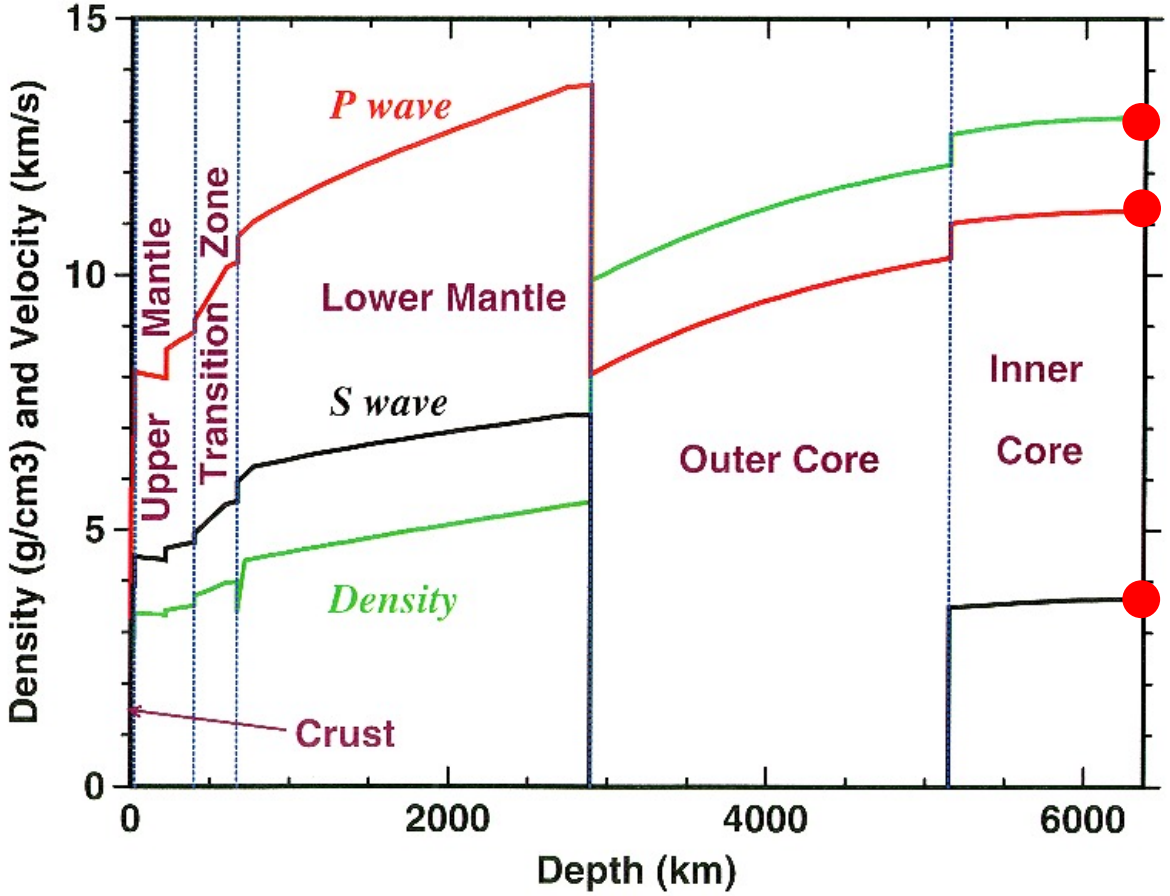
Li et al. (2020)



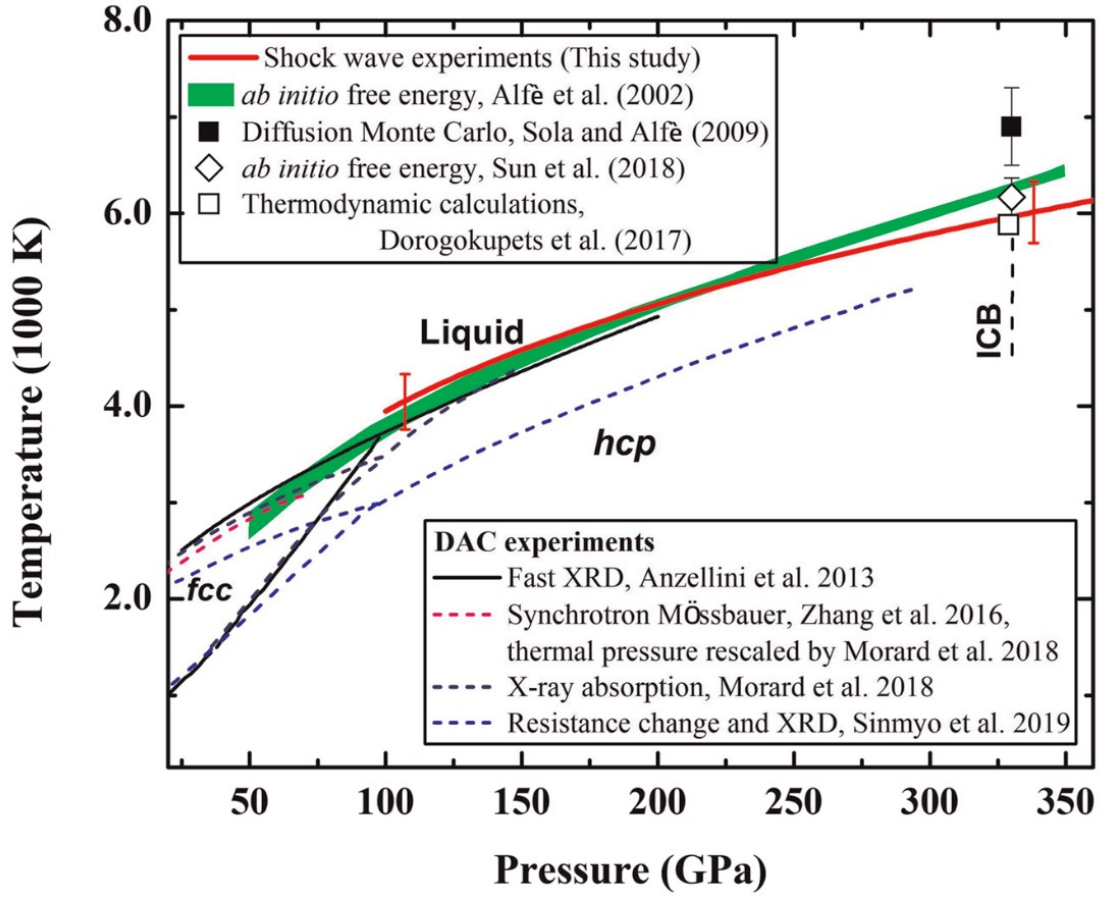
Tagawa et al. (2021)

Hydrogen in the inner core

Use *ab initio* molecular dynamics to calculate the density, elastic properties, and sound velocities of Fe-H and Fe-Si-H at ICB conditions

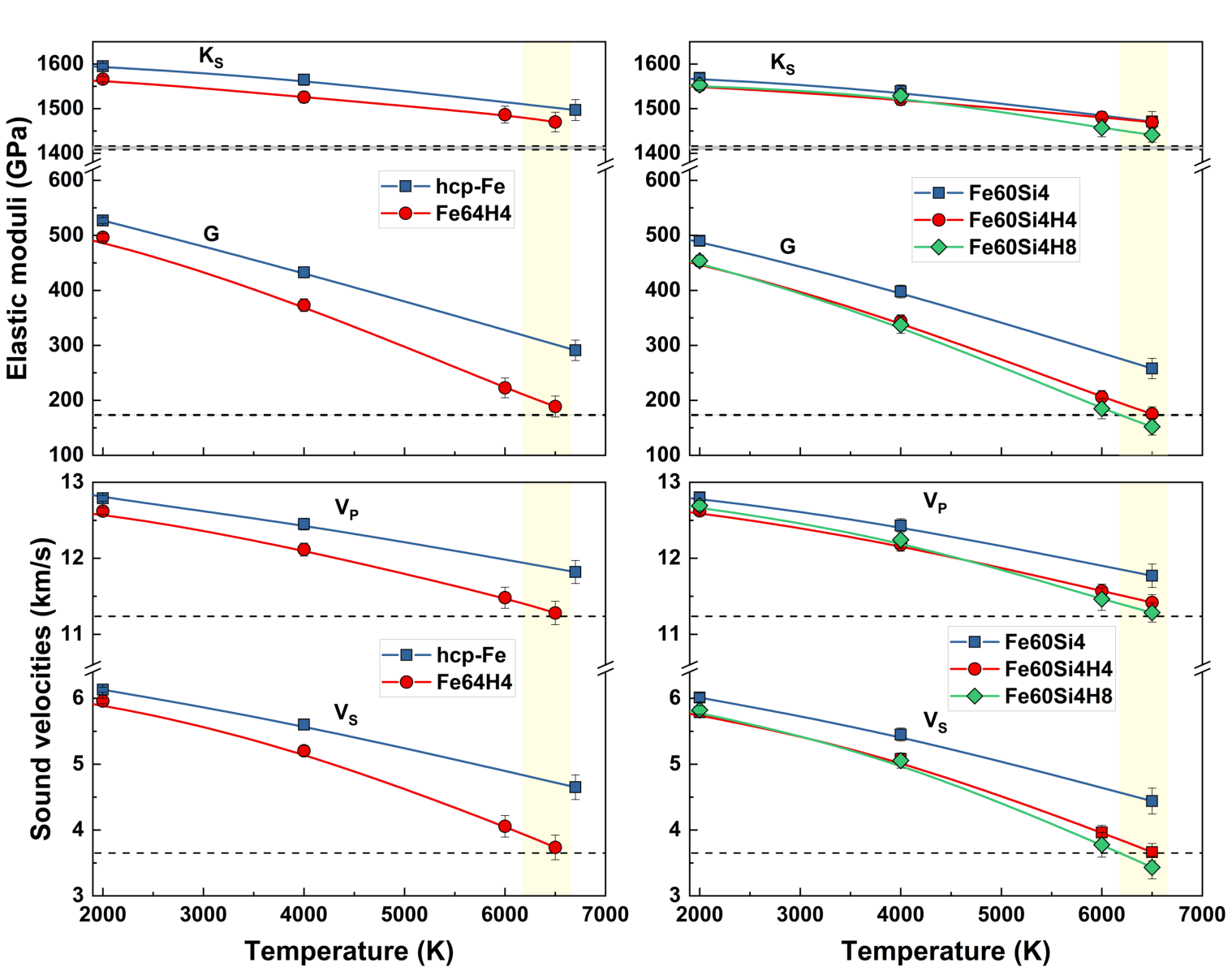


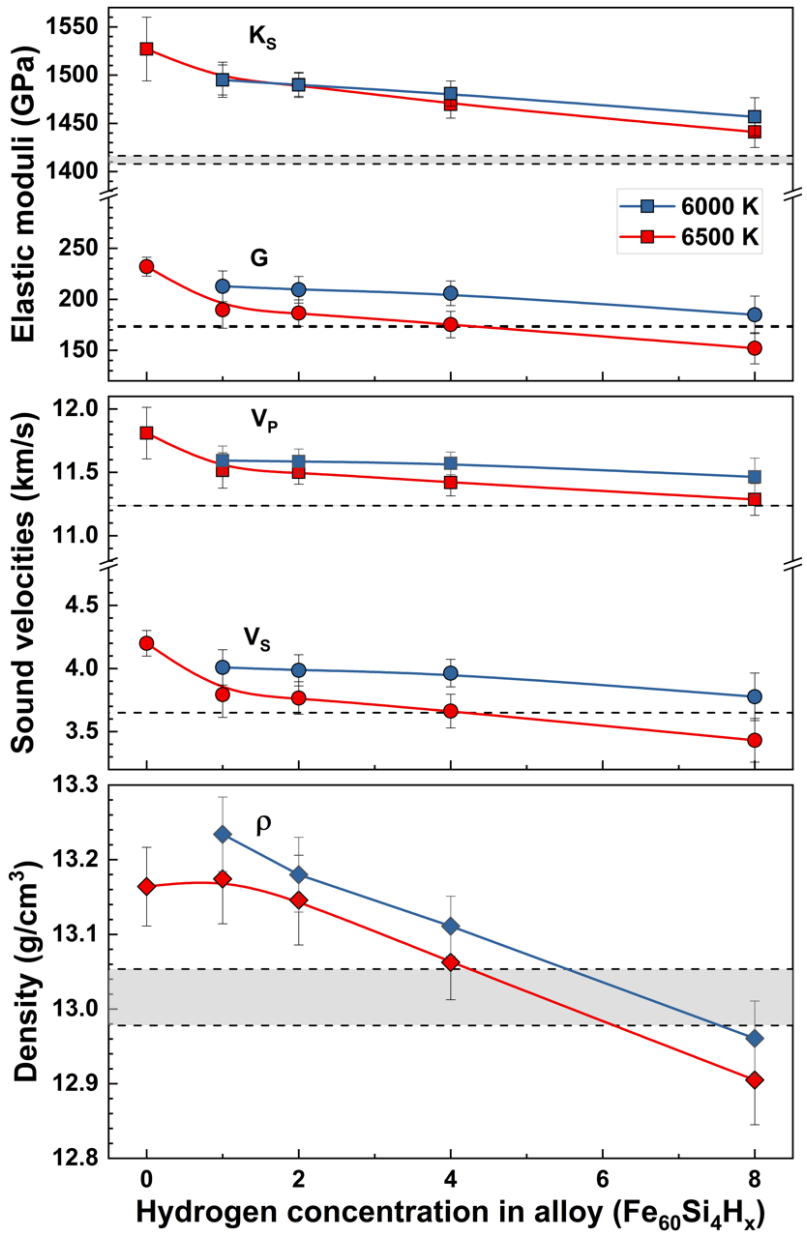
Dziewonski & Anderson (1981)



Jun Li et al. (2020)

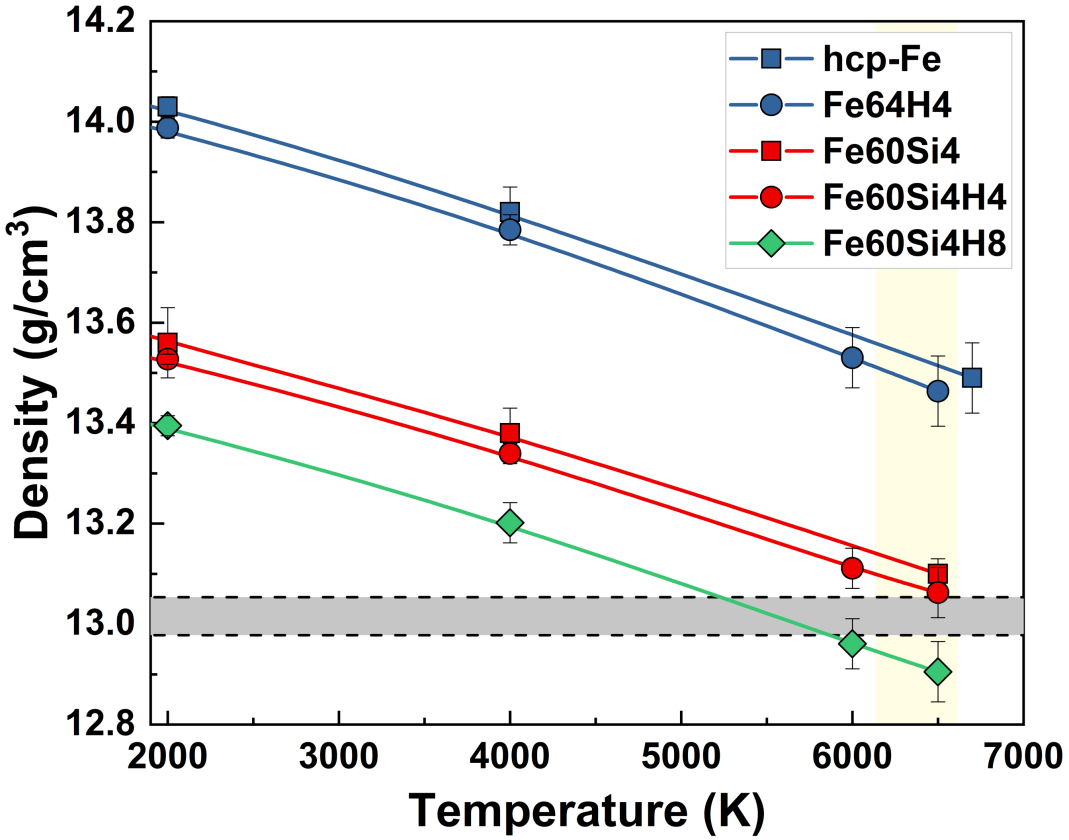
Low velocities of Fe-Si-H alloys

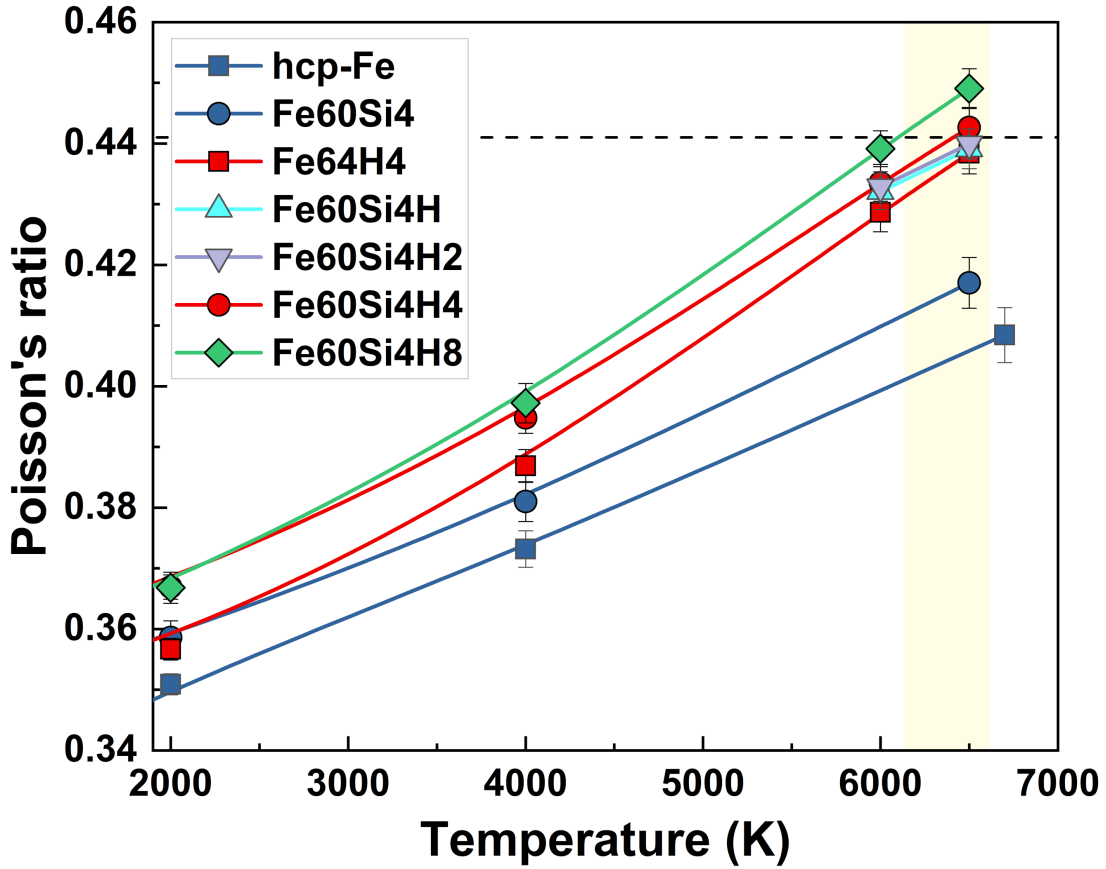




Wang et al. (2021)

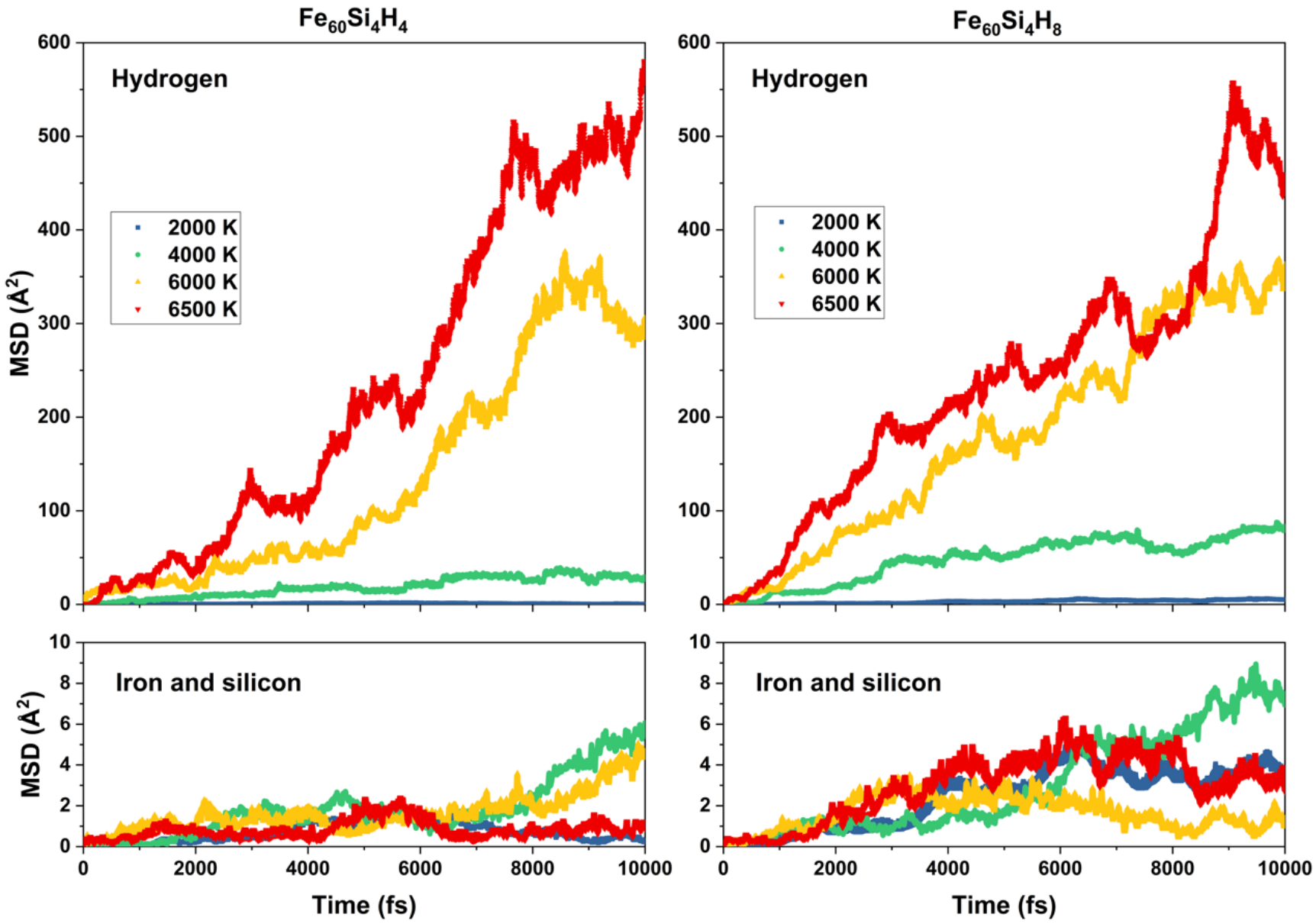
Density & High Poisson's ratio





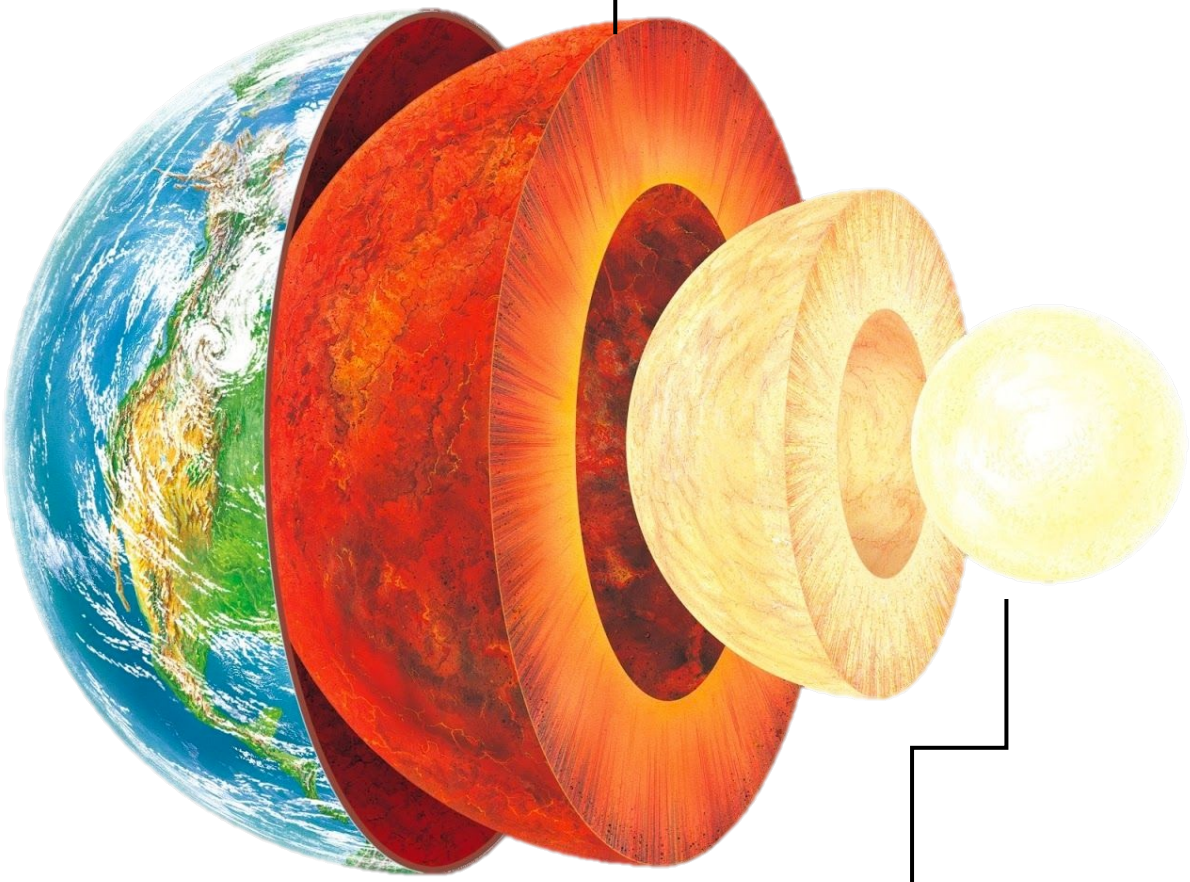
Wang et al. (2021)

Superionic Fe-Si-H alloys



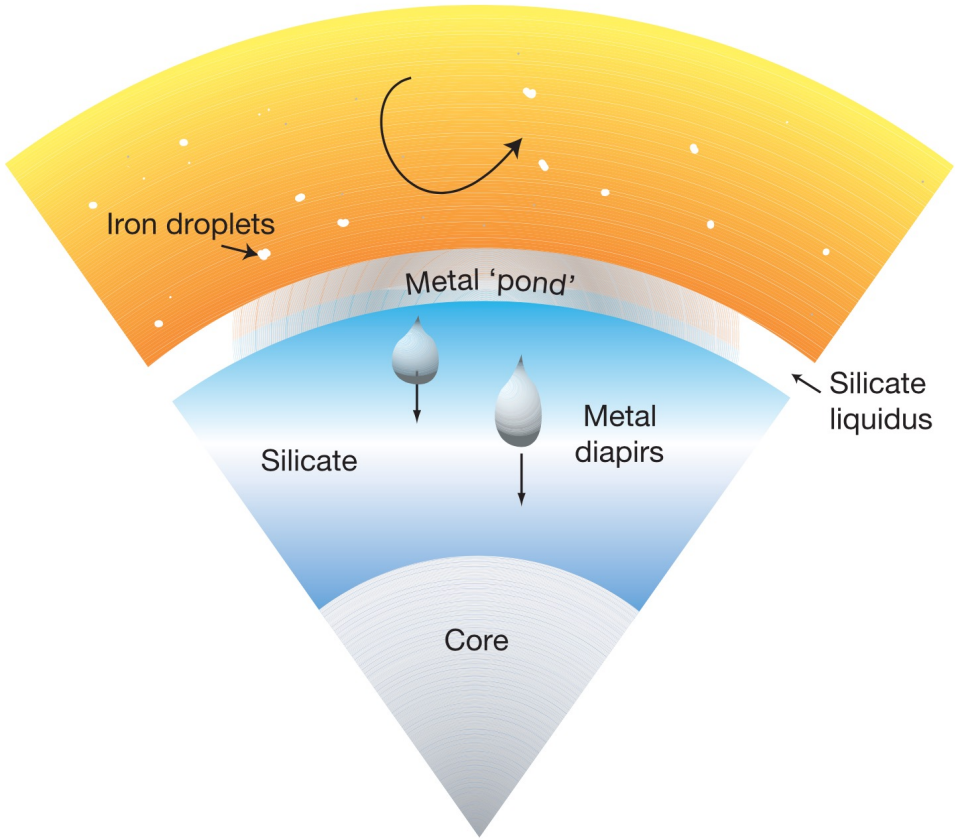
Wang et al. (2021)

1-2 oceans of water



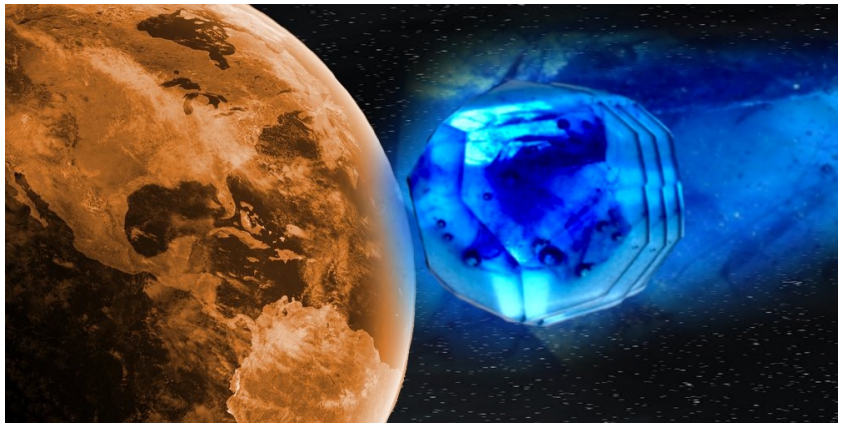
At least 5-28 oceans of water

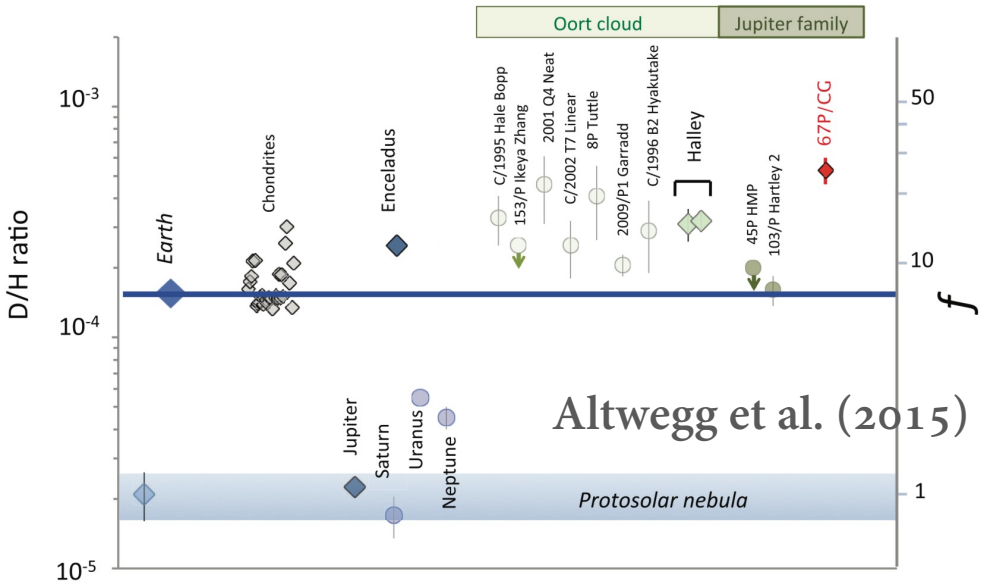
Proto-Earth had accreted lots of primordial water before core formation



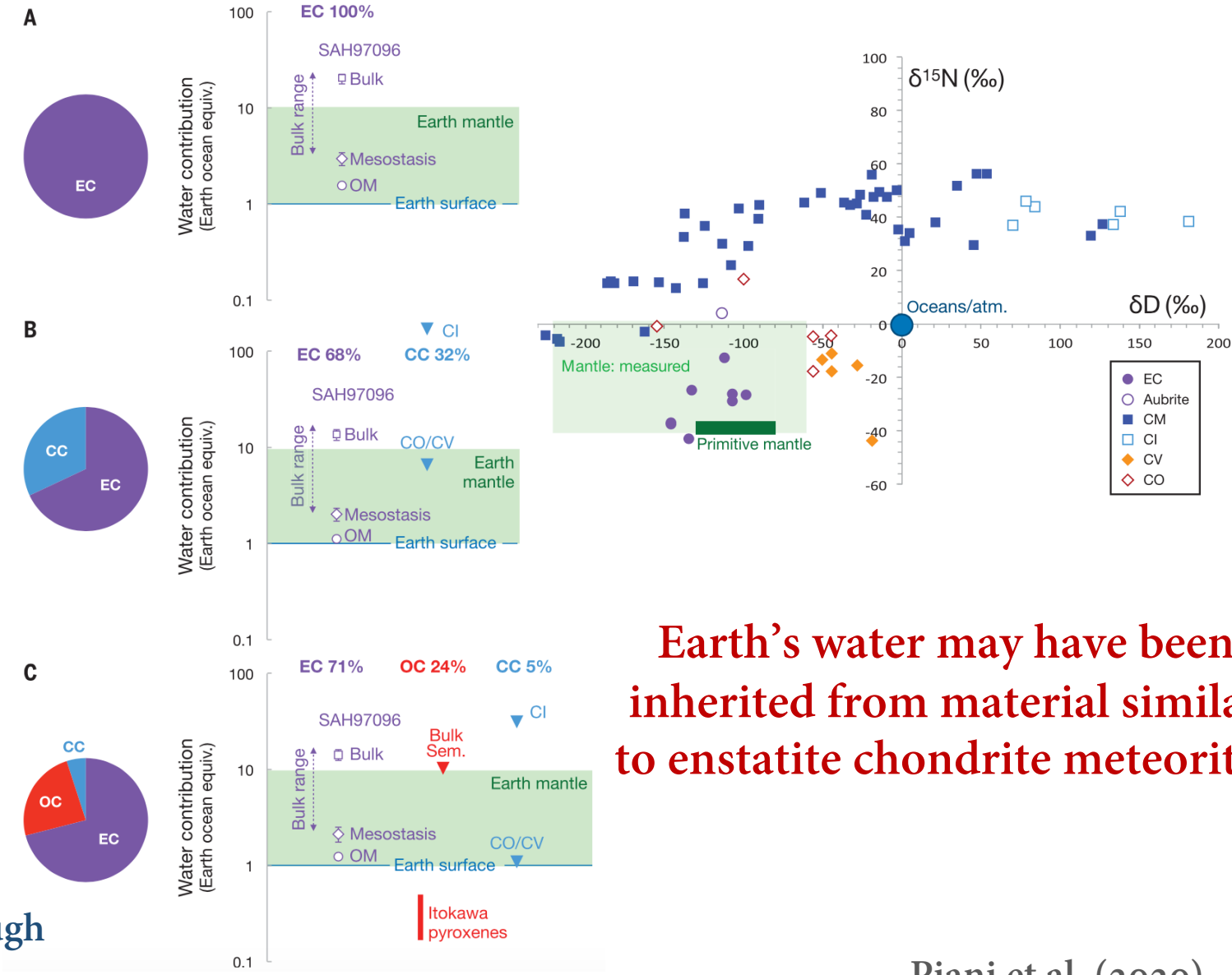
Wood et al. (2006)

Origin of Earth's water





Water might have been brought to Earth through water-rich asteroid/comets



Earth's water may have been inherited from material similar to enstatite chondrite meteorites

Piani et al. (2020)

Conclusions

- ✓ *Hcp* Fe-H and Fe-Si-H maintain a superionic state under inner-core conditions -- H diffuses rapidly but Fe and Si atoms remain in their equilibrium positions

- ✓ *Hcp* Fe-H and Fe-Si-H exhibit a strong shear softening due to the superionic effect, and several Fe-Si-H compositions can explain the observed V_P , V_S , and density of the inner core simultaneously

- ✓ H is a fundamental light element in the Earth's core, and the required amount of H corresponds to four to twenty-eight oceans of water

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