31st International Colloquium
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Hydrogen-water mixtures in giant planet interiors studied with ab-initio simulations.

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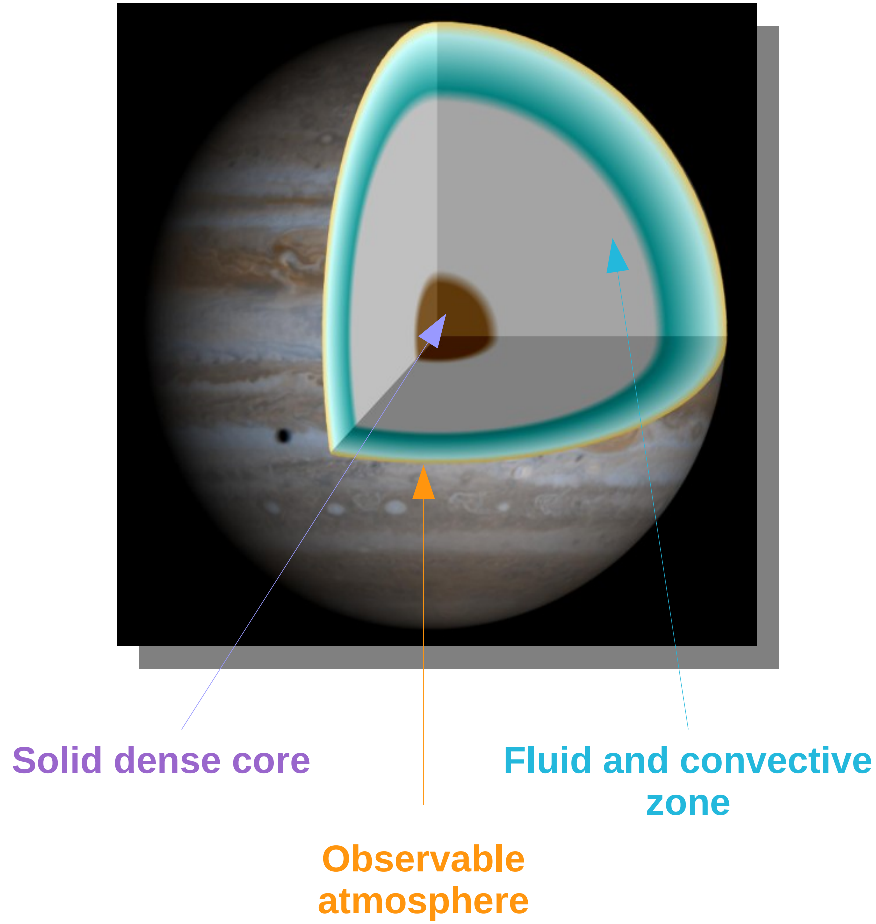
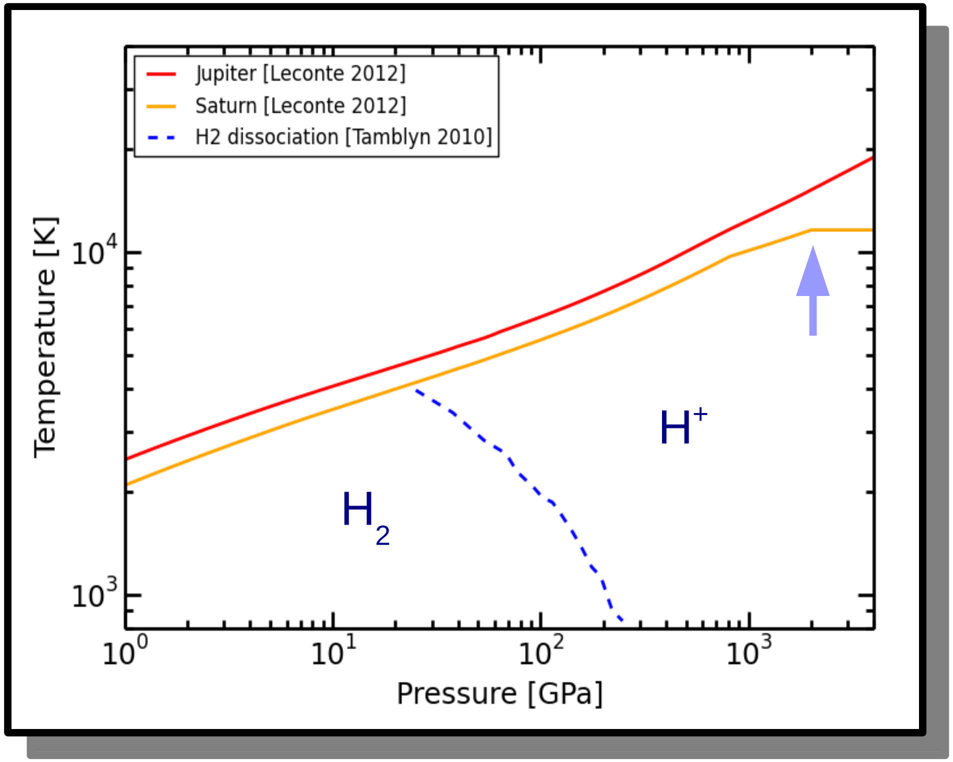
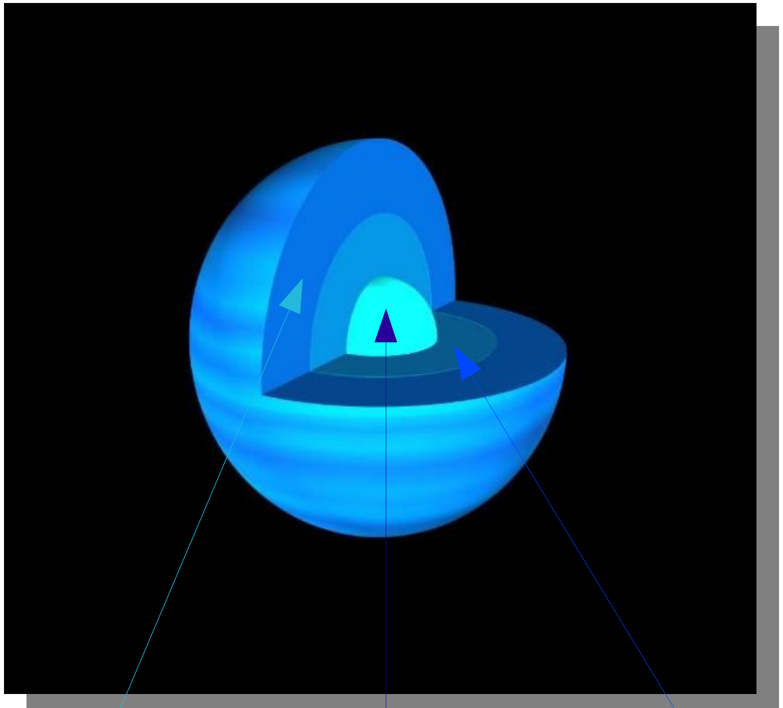
Gaseous Giants





- Observable atmosphere made of atoms and molecules.
- Fluid and convective zone of H/He
  → partially ionized
- Solid dense core with water, ices, rocks

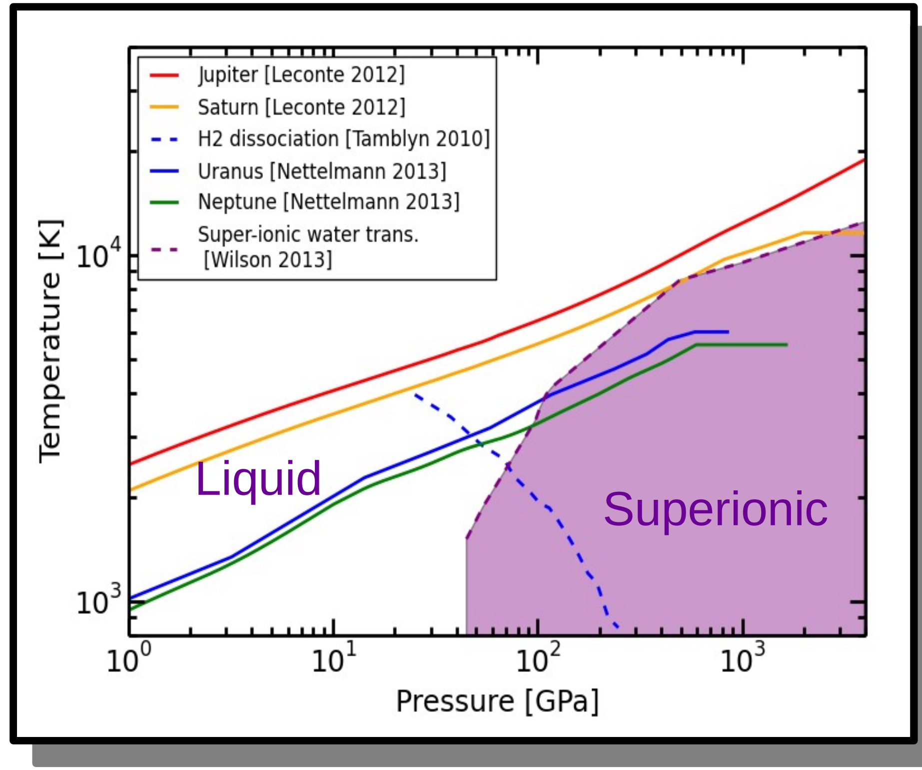
Water in Icy Giants



Fluid and convective zone

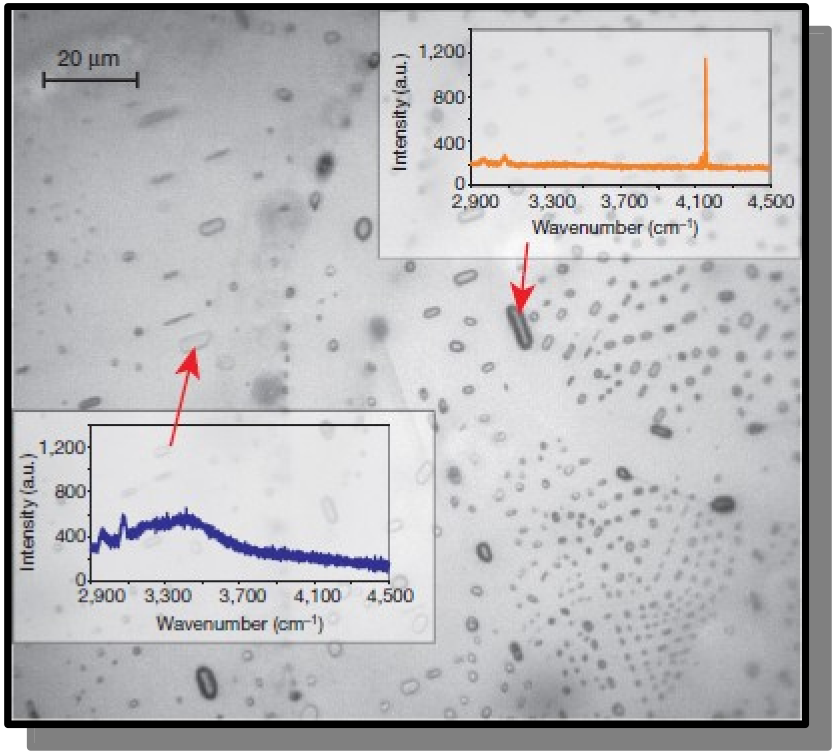
Partially fluid zone

Solid dense core



- Fluid upper mantle made of H, water, ices
- Partially fluid lower mantle with high metallicity mainly composed of water
  → superionic water
- Solid dense core of ices and rocks

Water-Hydrogen phase separation

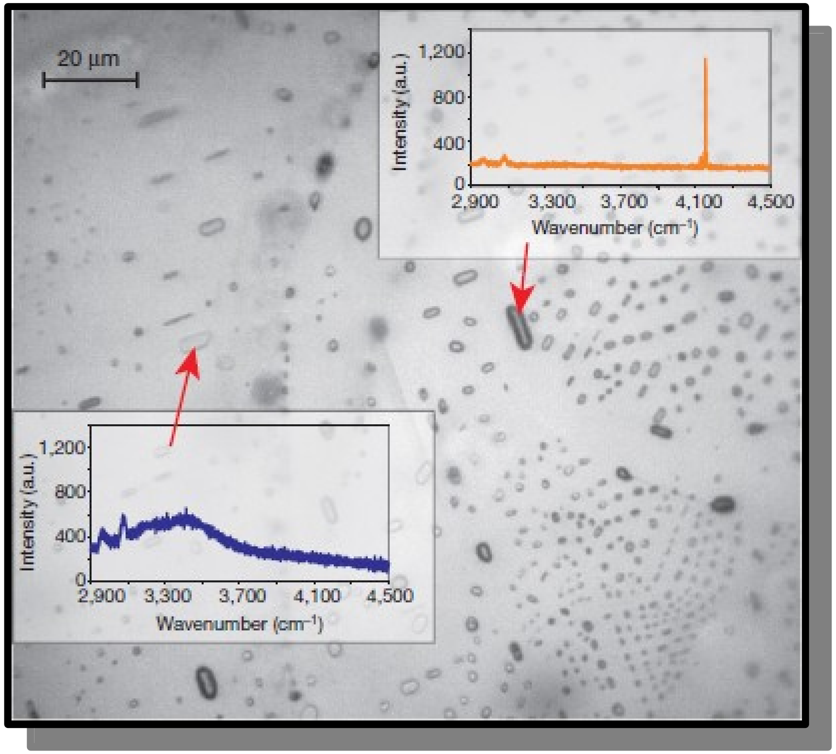


Synthetic fluid inclusions in olivine formed at 1,000 °C and 2.6 GPa at Fe–FeO buffer conditions. Three different types of fluid inclusions are visible. [...] These observations suggest that under run conditions, a hydrogen-rich fluid phase coexisted with an immiscible water-rich fluid phase.

Bali *et al.*, Nature 2013

- Static experiments on synthetic minerals
- Observation of inclusions
- At low temperature: two separated types of inclusions:
  - →water rich inclusions
  - →hydrogen rich inclusions
- **Phase separation** of the mixture

Water-Hydrogen phase separation



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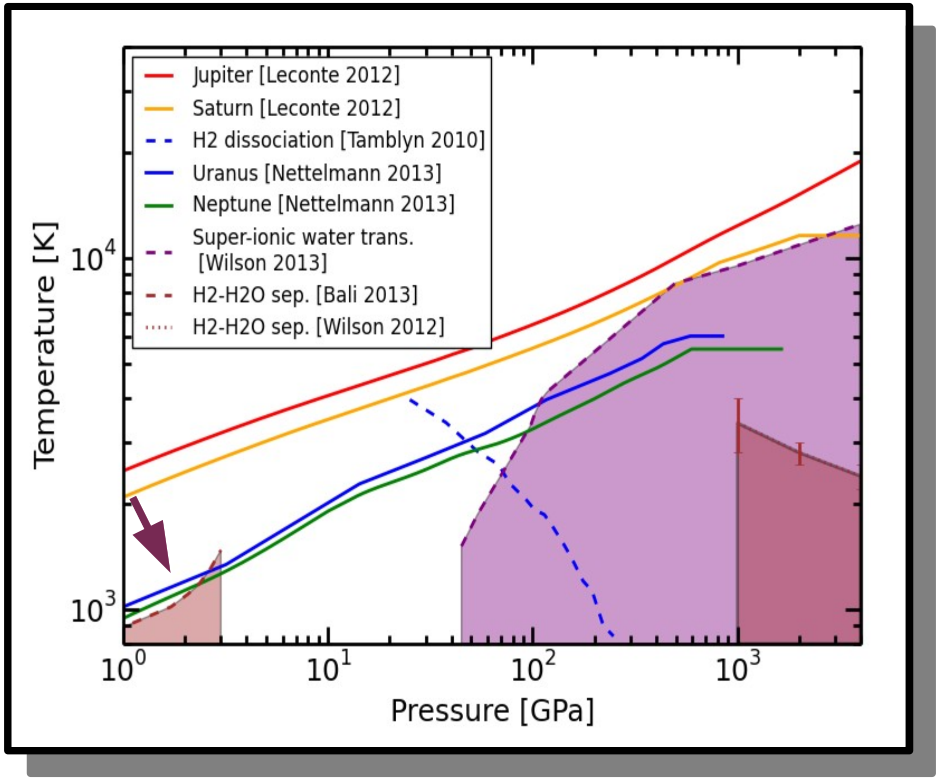
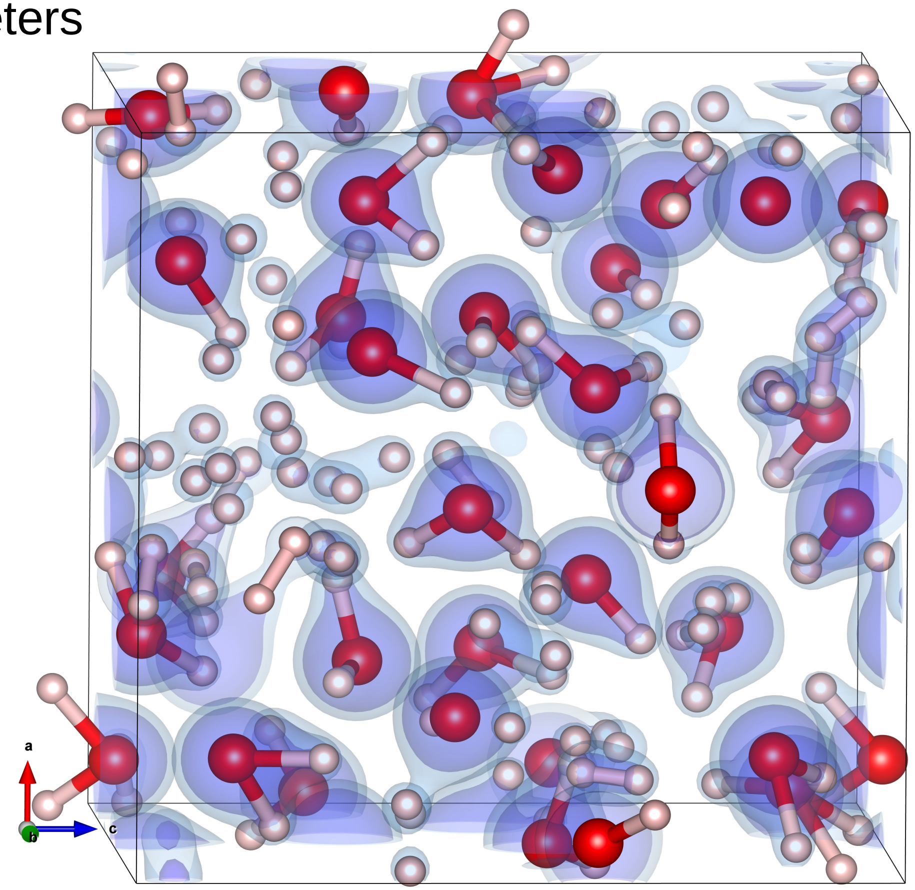


- May change the structure of the icy giant planets

- **What is the phase diagram for intermediate pressures?**

MD-DFT and EOS

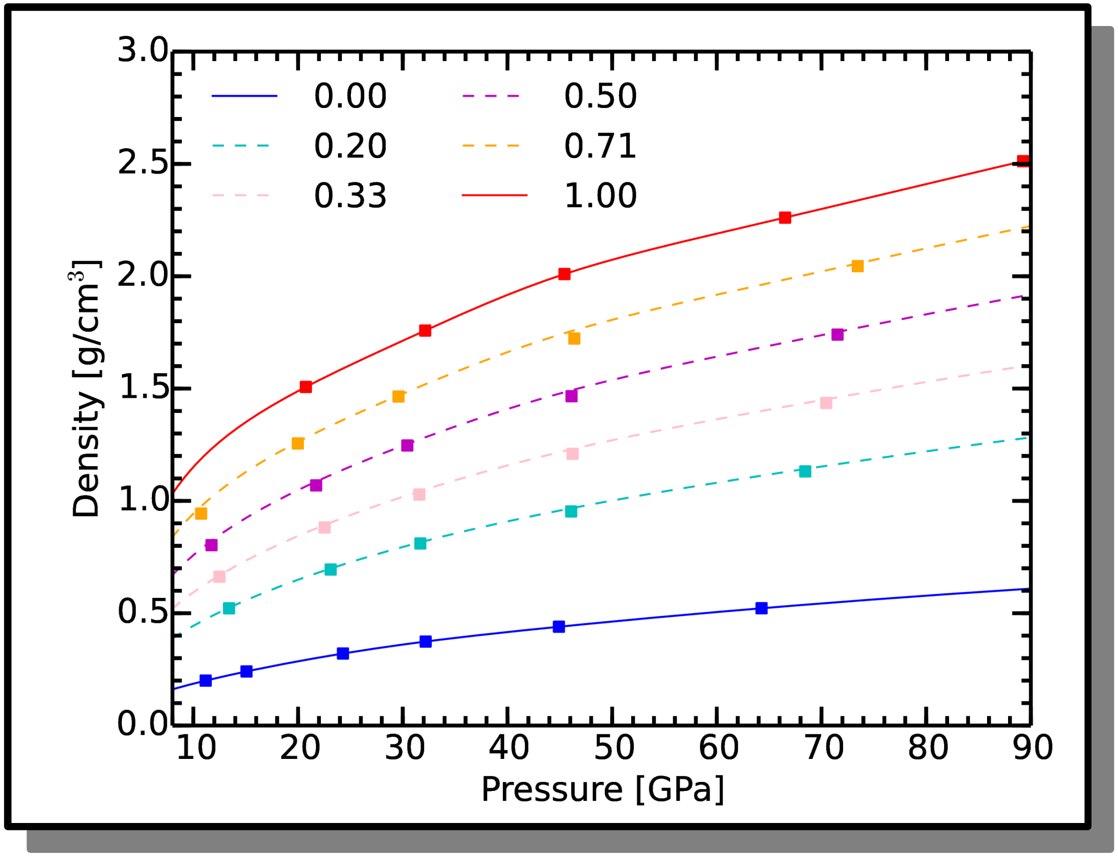
- Extraction of **thermodynamic** quantities from **molecular dynamics** based on **density functional theory** (MD-DFT)
- Highly **accurate** computations for the **Warm Dense Matter**
- Gives a data set on a wide range of parameters



- Simulations of water-hydrogen mixtures
- Different thermodynamic conditions
- Different concentrations

MD-DFT and EOS

6000 K



Soubiran & Militzer, ApJ 2015

- Comparison with the pure systems
- Very good agreement with an ideal mixing rule with an additive volume law
- Great help for the astrophysicists:
  → **only need EOS of pure systems**
- Composition?

Numerical Methods

- How do we compute the entropy?

Numerical Methods

- How do we compute the entropy?

- Thermodynamic integration using an alternate potential:

$$V_\lambda = \lambda V_{\mathrm{DFT}} + (1-\lambda)V_{\mathrm{cl}}$$

- Computation of the free-energy for given density, temperature and concentration

$$F_{\mathrm{DFT}} = F_{\mathrm{cl}} + \int_0^1 \left\langle V_{\mathrm{DFT}} - V_{\mathrm{cl}} \right\rangle_{V_\lambda} \mathrm{d}\lambda$$

Numerical Methods

- Phase transition at (P,T) → Gibbs free-energy

$$G = F + PV$$

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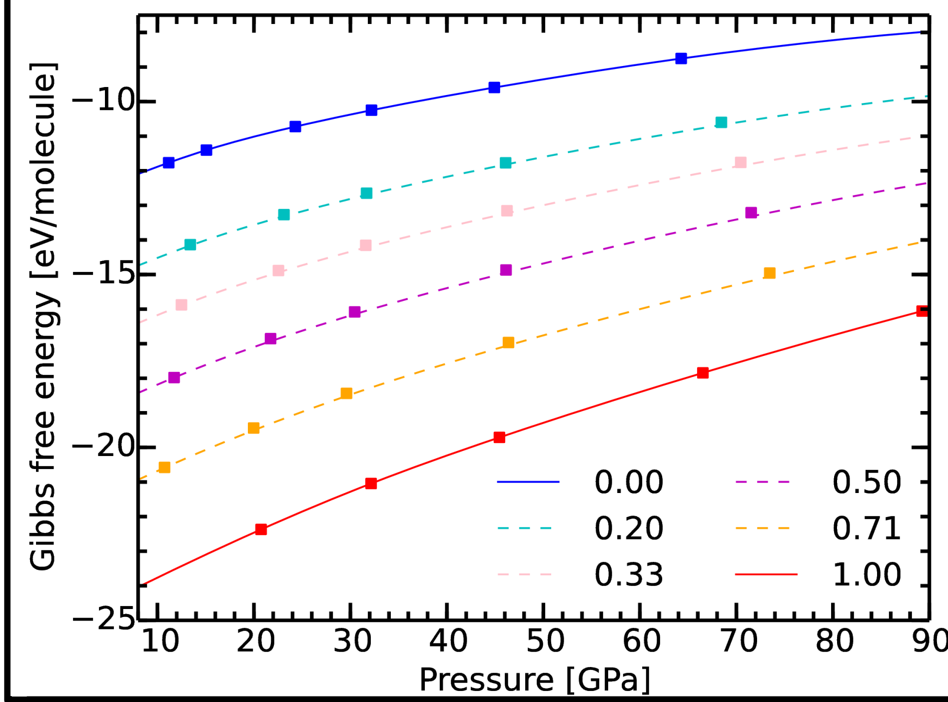
6000 K



Soubiran & Militzer, ApJ 2015

- **Complete EOS**
- Very good agreement with an ideal mixing rule with an additive volume law
- Can the small deviations lead to a phase separation?

Numerical Methods

- Phase transition at (P,T) → Gibbs free-energy

$$G = F + PV$$

- Computation of the Gibbs free-energy of mixing:

$$\Delta G(P,T,x_{H_2O}) = G(P,T,x_{H_2O}) - (1-x_{H_2O})G_{H_2}(P,T) - x_{H_2O}G_{H_2O}(P,T)$$

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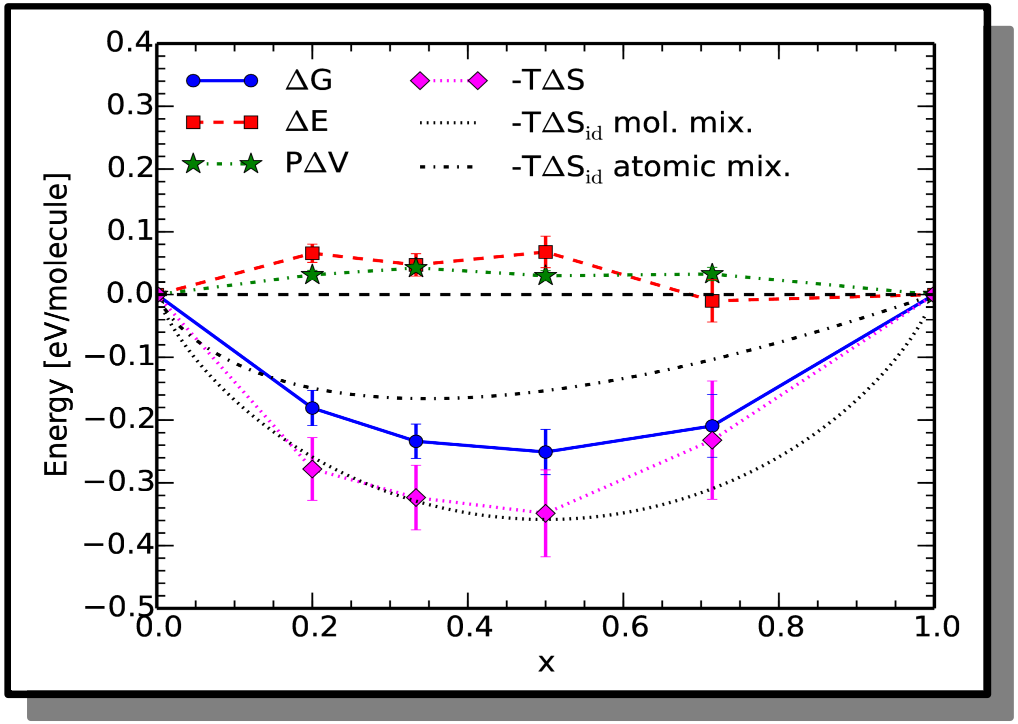
- Stabilty critarion:

$$\left. \frac{\partial^2 \Delta G}{\partial x_{H_2O}^2} \right|_{P,T} < 0$$ → **unstable**

Water - Hydrogen at intermediate temperature

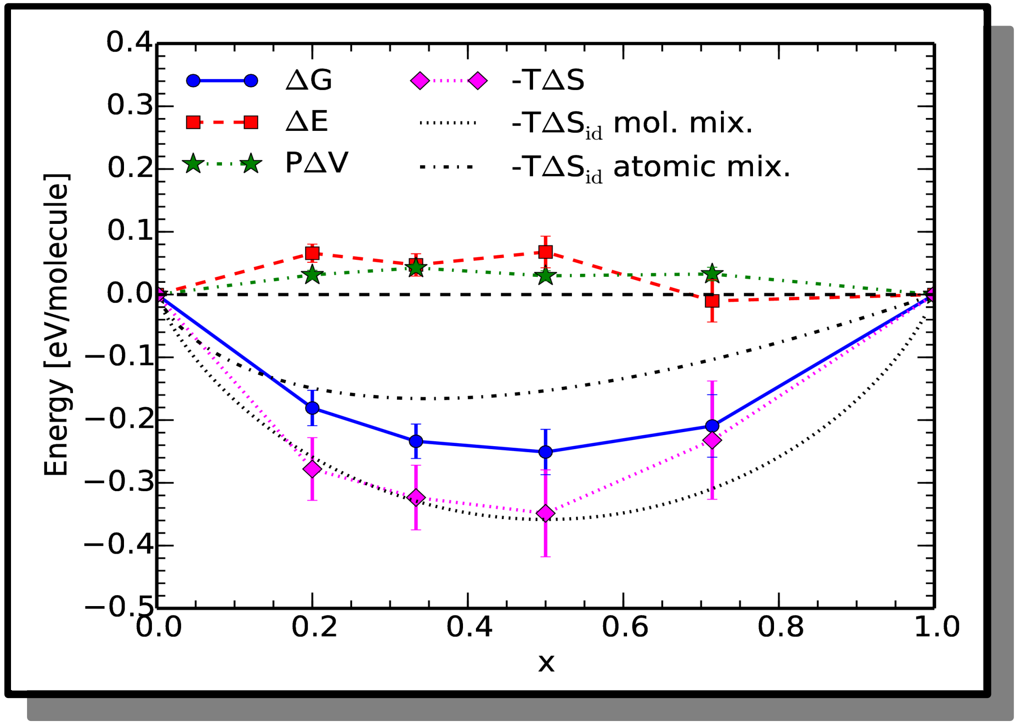


Soubiran & Militzer, ApJ 2015

- **Hull diagram**: ΔG as a function of the concentration for a given (P,T)

- At 6000K - 70 GPa, the diagram is convex (hull shape)
  → system is **stable**

Water - Hydrogen at intermediate temperature



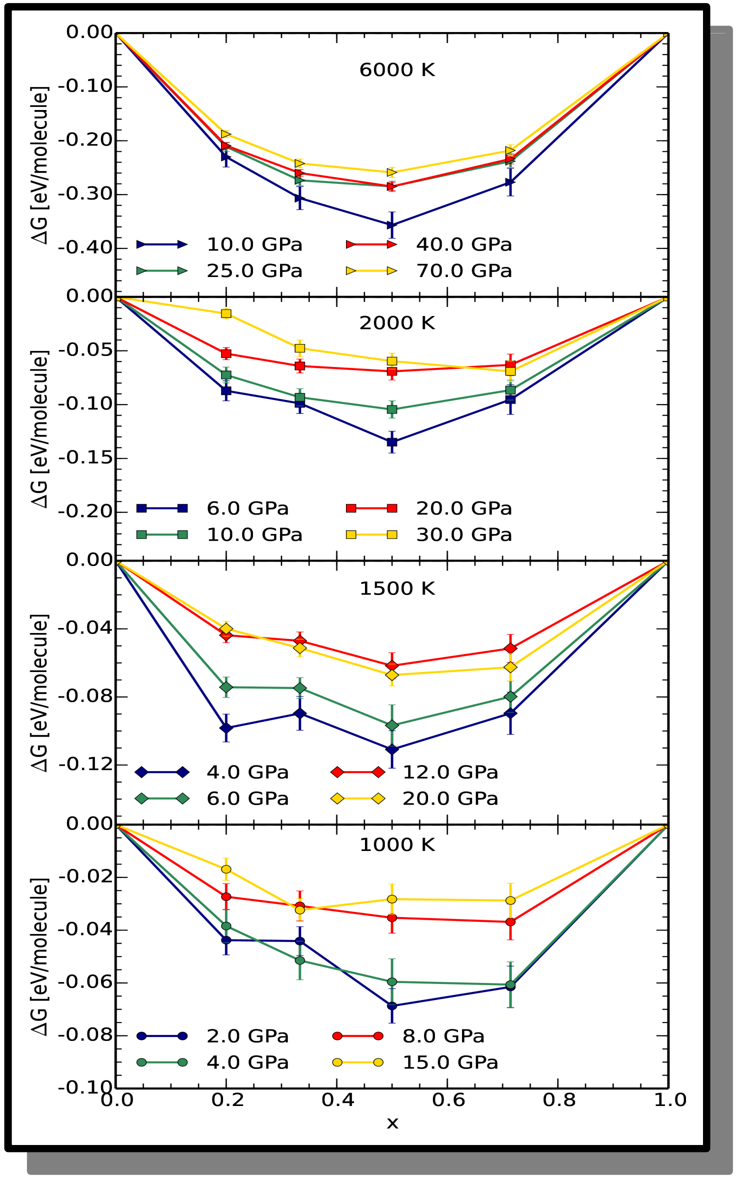
Soubiran & Militzer, ApJ 2015

- **Hull diagram**: ΔG as a function of the concentration for a given (P,T)

- At 6000K - 70 GPa, the diagram is convex (hull shape)
  → system is **stable**

- Decomposition of the different contributions
  → entropy has the main contribution
  → **ideal entropy of mixing of molecules**

Water - Hydrogen at other conditions

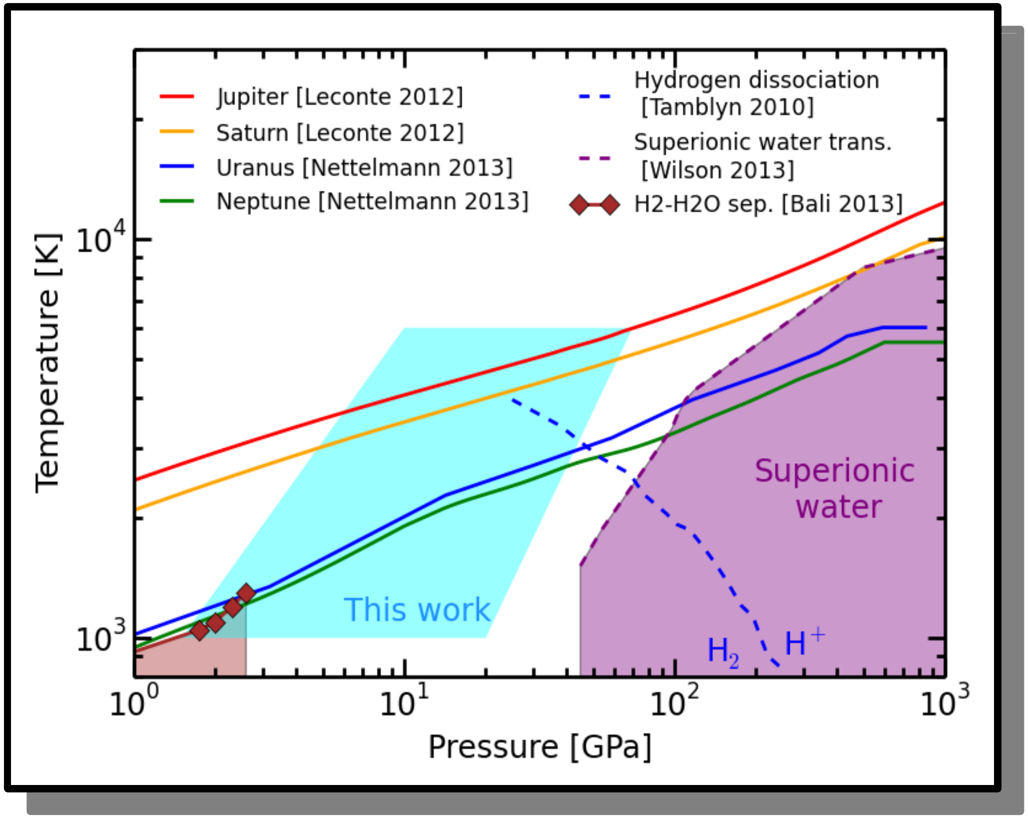


- From 1000K to 6000K, the diagram is convex (hull shape)
  → system is **stable**

→ **no phase separation in water-hydrogen mixture**

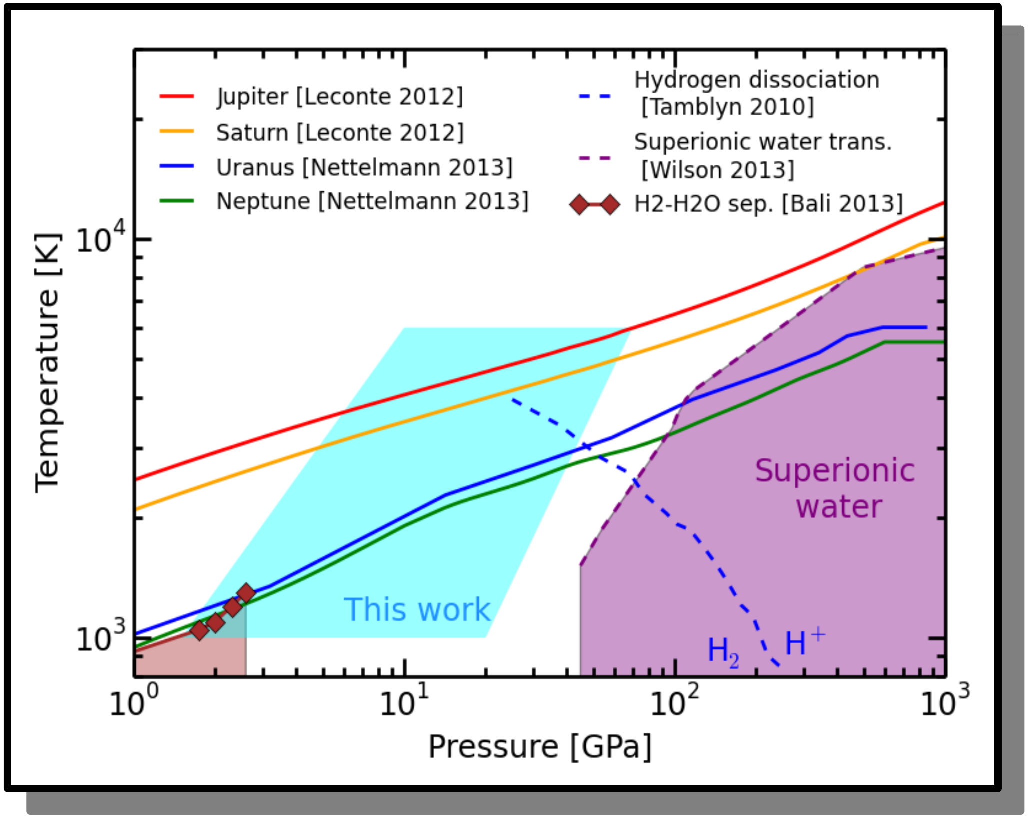
Soubiran & Militzer, ApJ 2015

Consequences for the icy giant planets



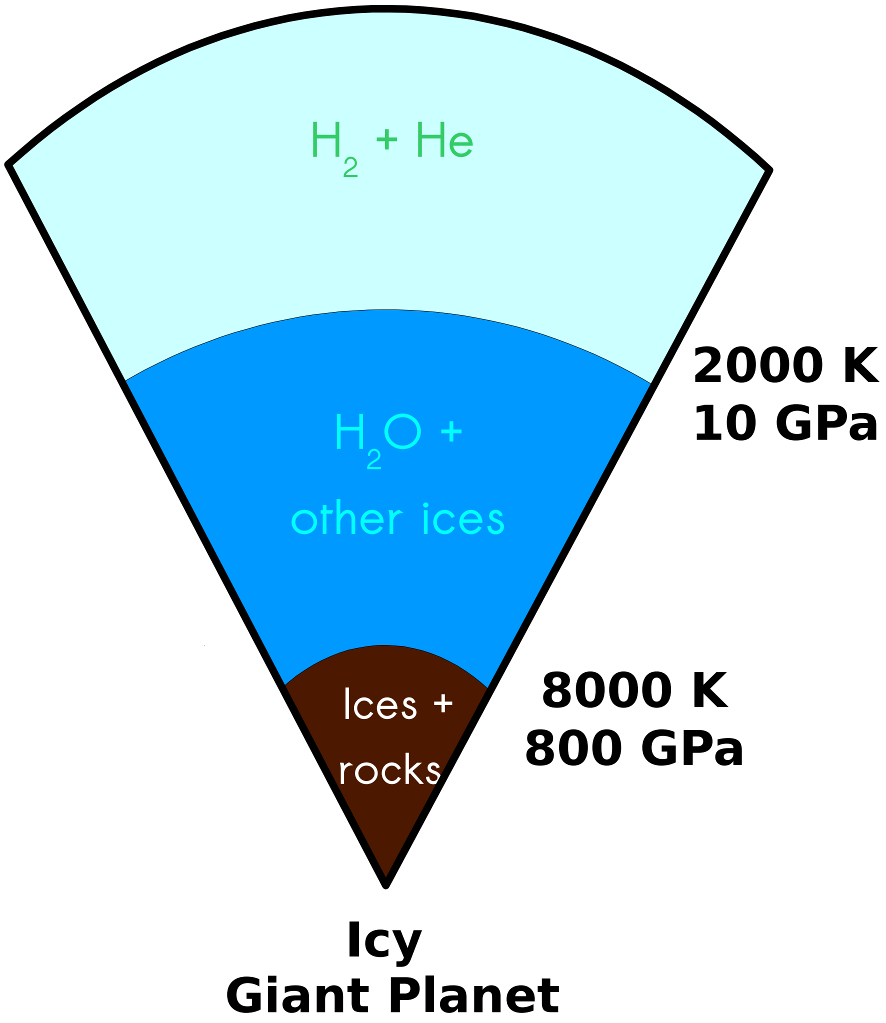
- Mixtures are stable above 1000K
- No phase separation in icy giant planets envelopes
- **Differentiated icy giant planets are thermodynamically unstable**

Consequences for the icy giant planets



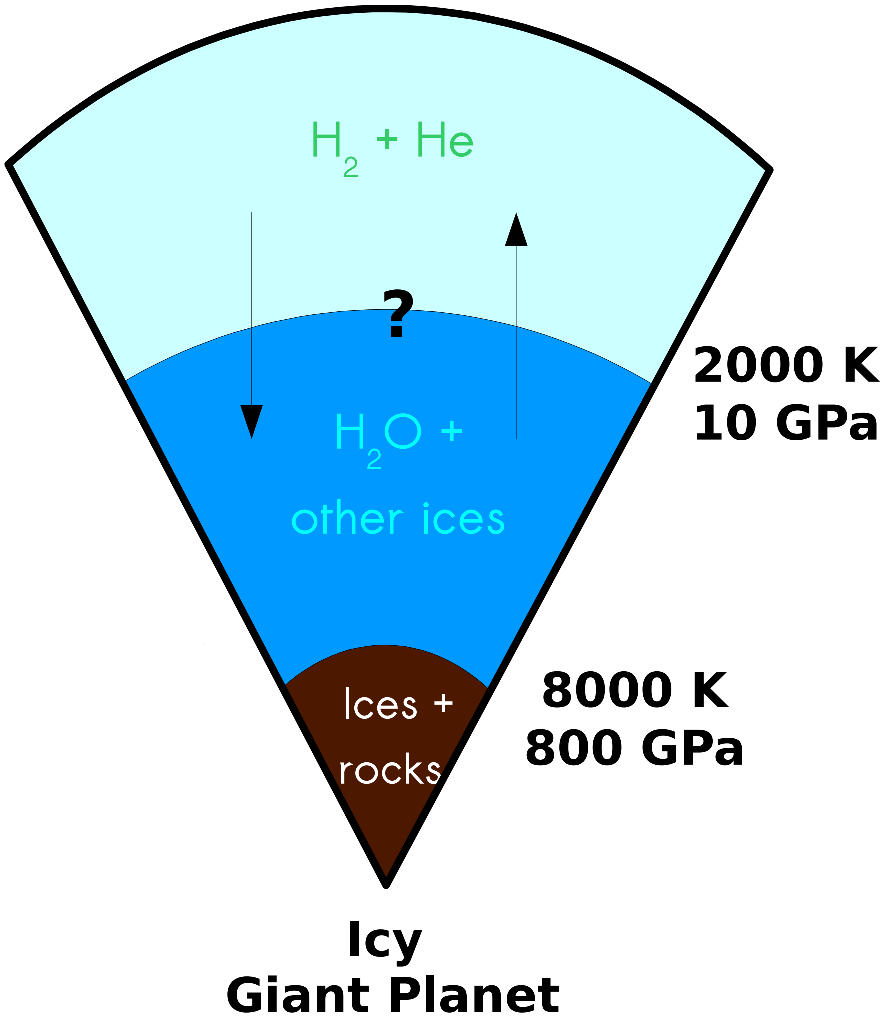
- Mixtures are stable above 1000K
- No phase separation in icy giant planets envelopes
- **Differentiated icy giant planets are thermodynamically unstable**
- What to expect for the structure?

Consequences for the icy giant planets



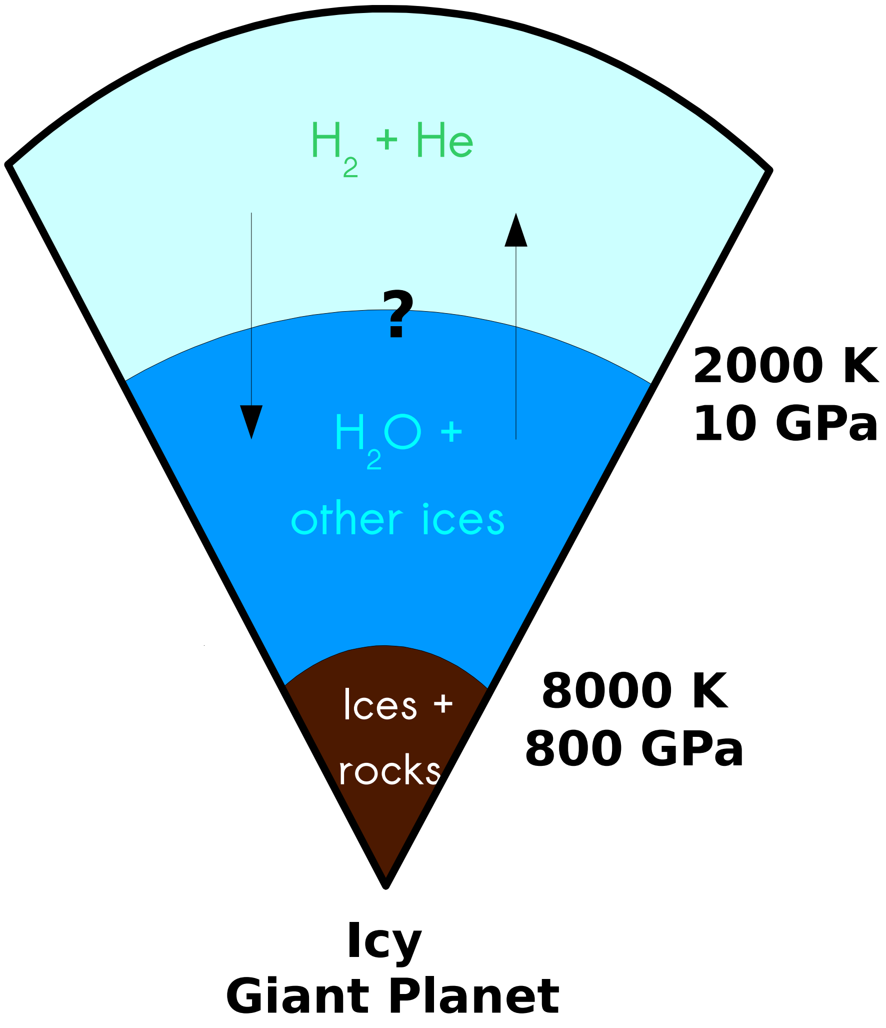
- Core accretion model: dense core surrounded by gaseous envelope

Consequences for the icy giant planets



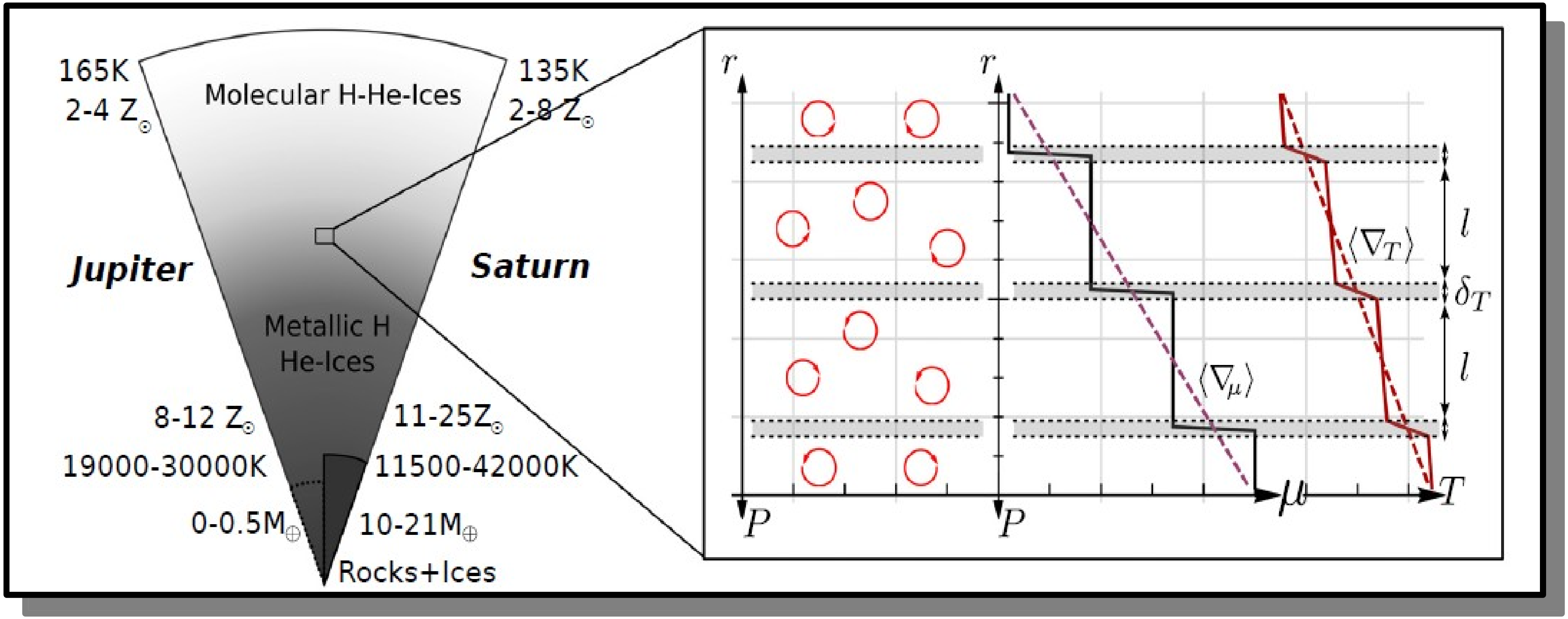
- Core accretion model: dense core surrounded by gaseous envelope
- How do water and hydrogen mix?

Consequences for the icy giant planets



- Core accretion model: dense core surrounded by gaseous envelope
- How do water and hydrogen mix?
- Diffusion? ~10^{12} years
- Convection? ~100 years
- Semi-convection?

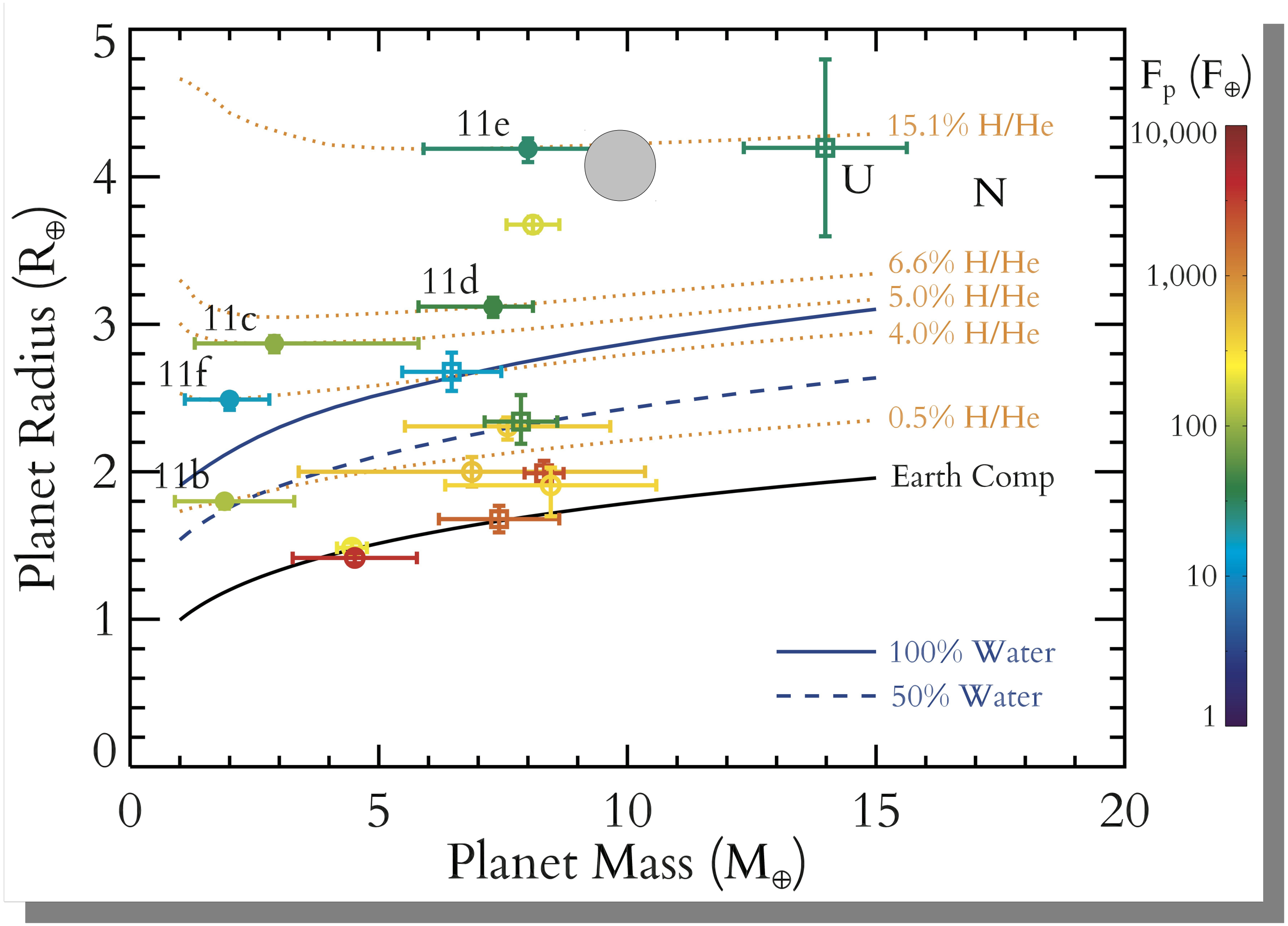
Semi-convection in planets



Leconte & Chabrier, A&A 2012

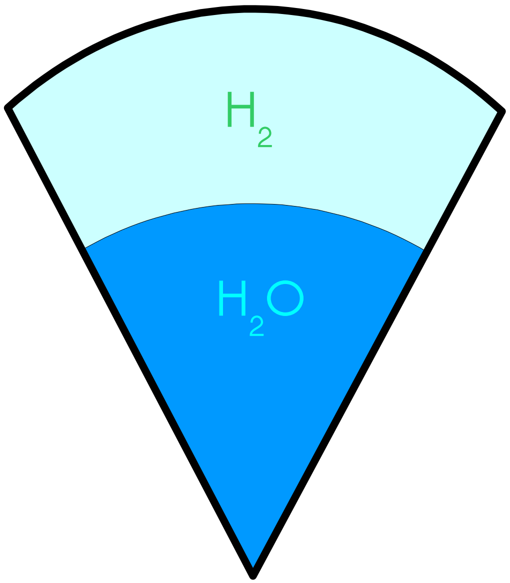
- Stabilizing gradient of composition
- Successive layers: diffusive/convective
- Characterization of the semi-convection
  → transport properties

Exoplanets composition

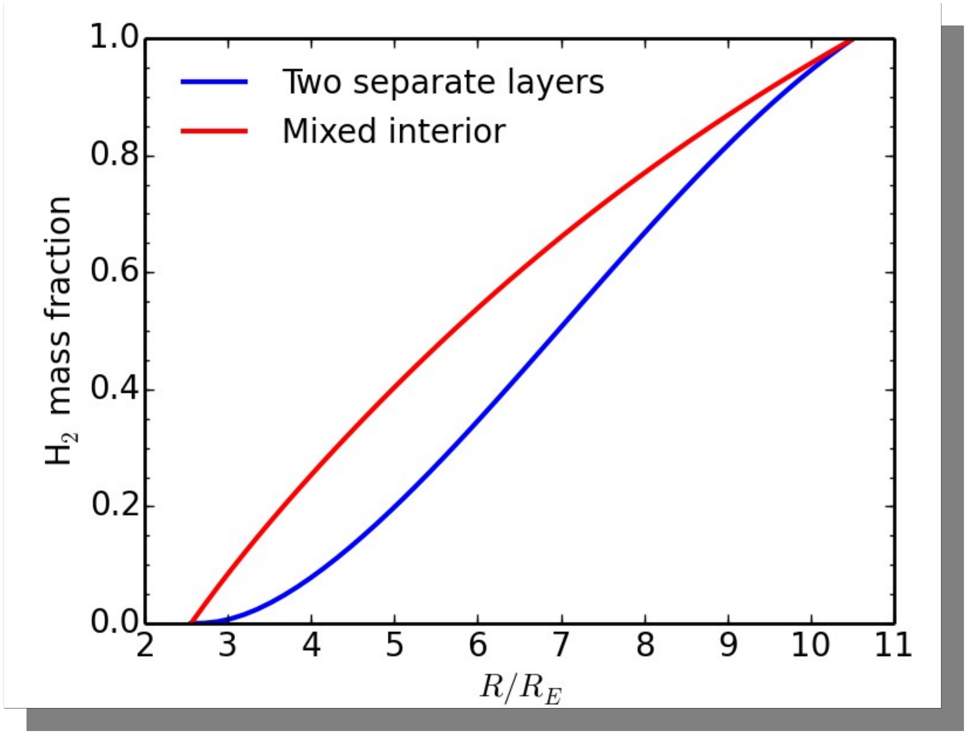


Lissauer et al. 2013

Exoplanets composition



**~ 8 %
hydrogen**



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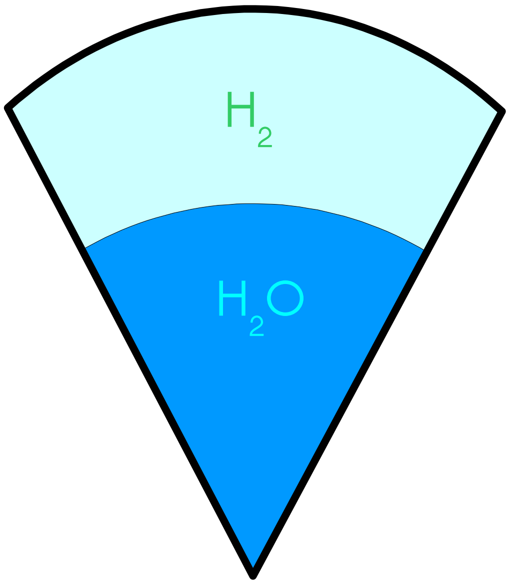
Exoplanets composition



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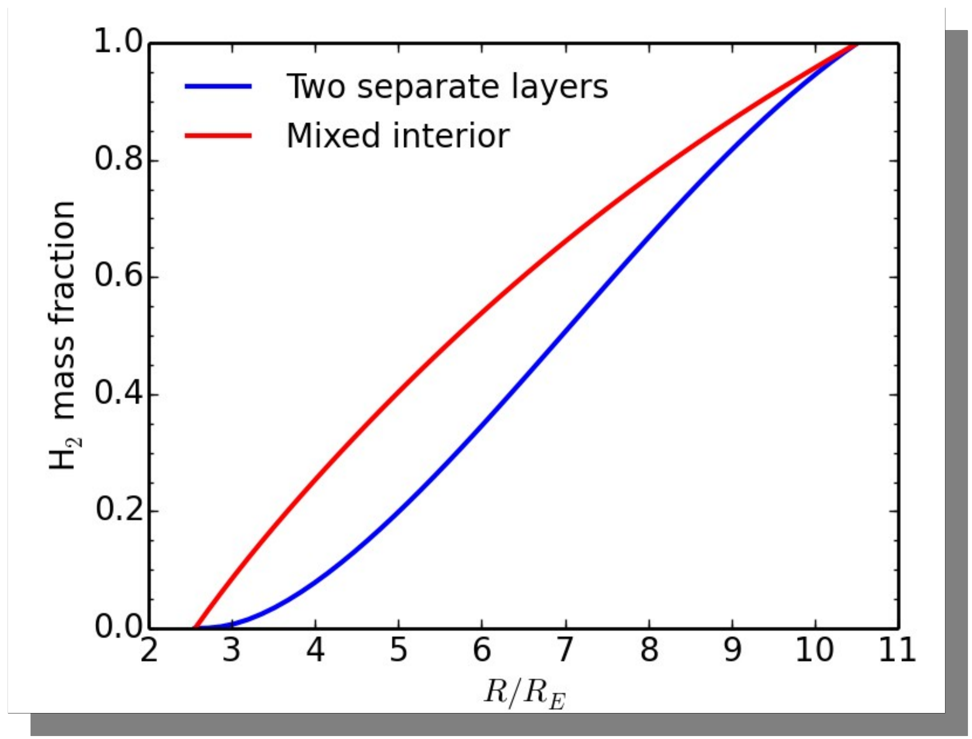

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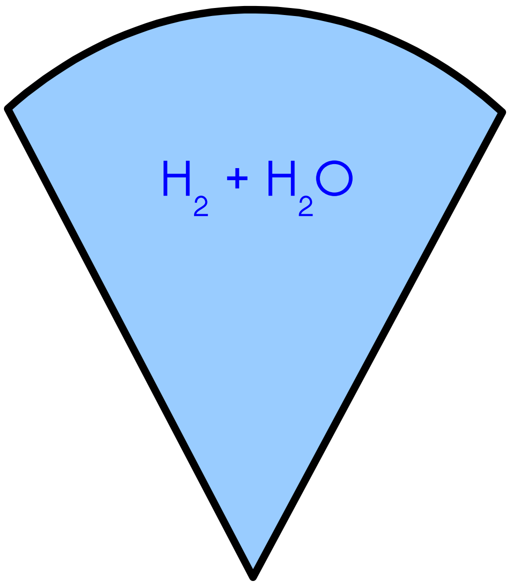
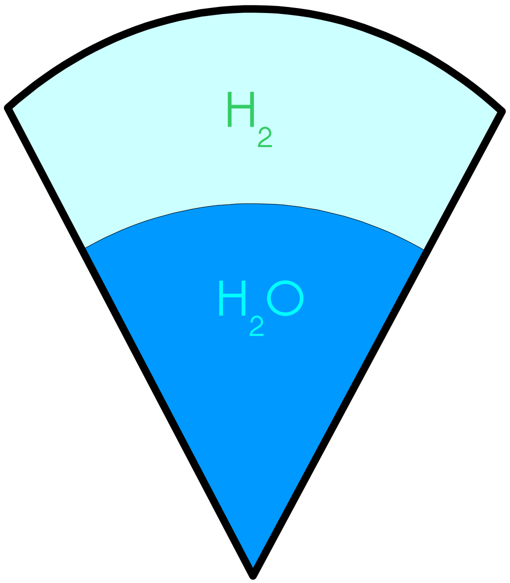


~ 25 %
hydrogen

Exoplanets composition



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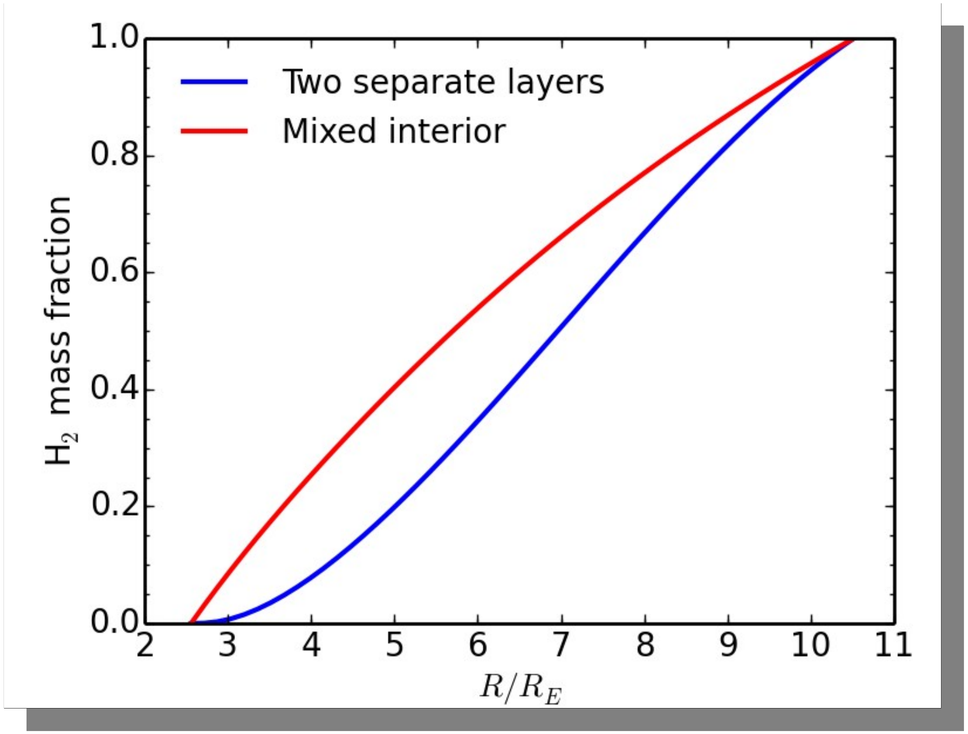

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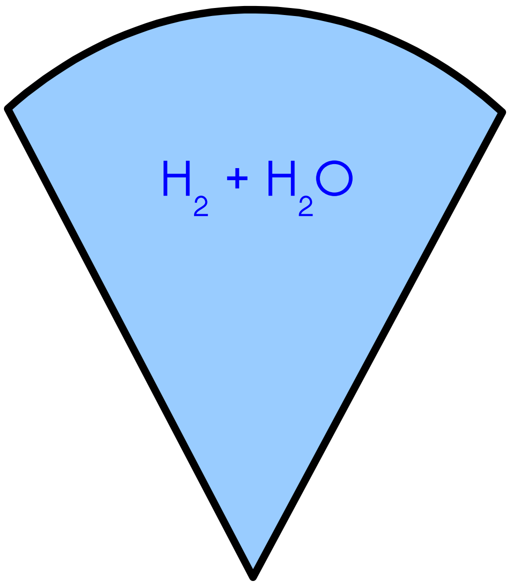

~ 25 %
hydrogen

More hydrogen can fit into a mixed planet

Conclusions

- Ab initio simulations predict **homogeneous H_2-H_2O mixtures** to be **thermodynamically stable** in all proportions on the 2-70 GPa and 1000-6000 K parameter range

- But a planet can be **differentiated** if it has been formed differentiated and the **mixing** process was very **inefficient**

- A better characterization of the **semi-convection** is needed as well as a better determination of the **transport properties**

- The **differentiation** of a planet changes the **composition** inferred from mass-radius relationships.

THANK YOU!