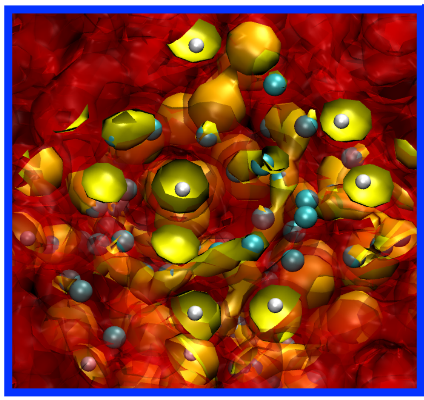
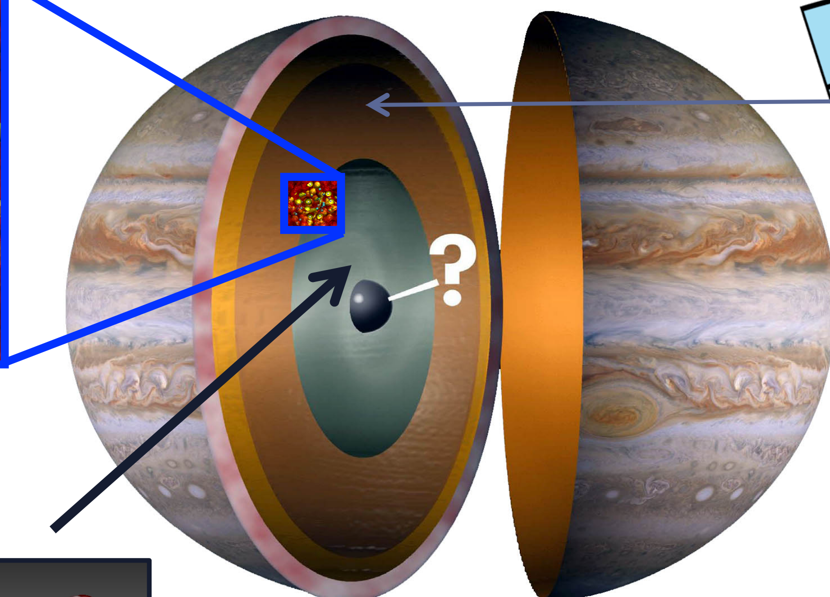
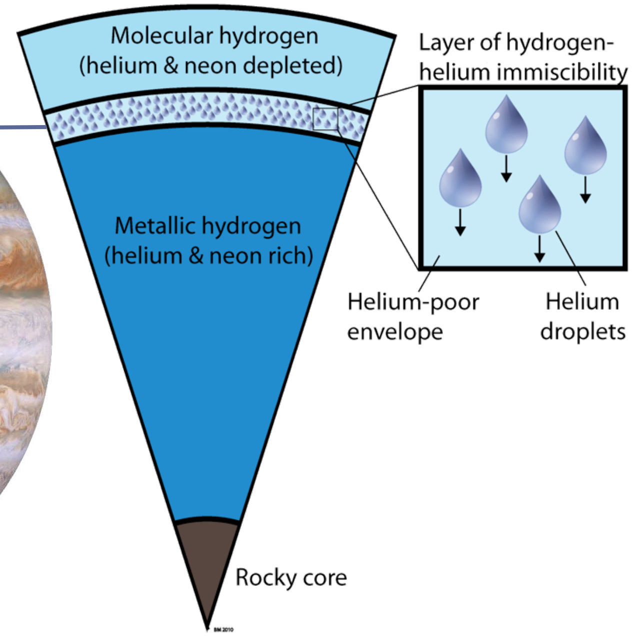
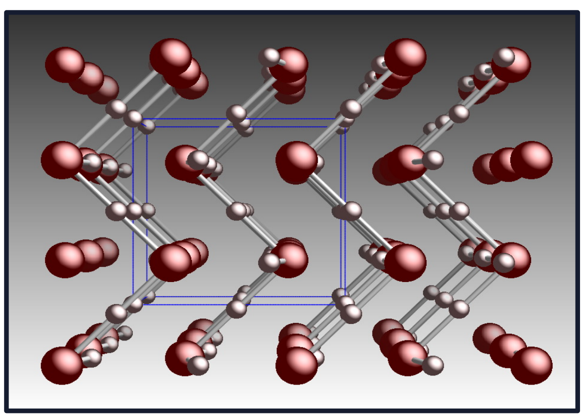
# Helium Rain and Core Erosion in Gas Giant Planets Predicted with Ab Initio Simulations







**Burkhard Militzer**

*University of California, Berkeley*

http://militzer.berkeley.edu

# Outline

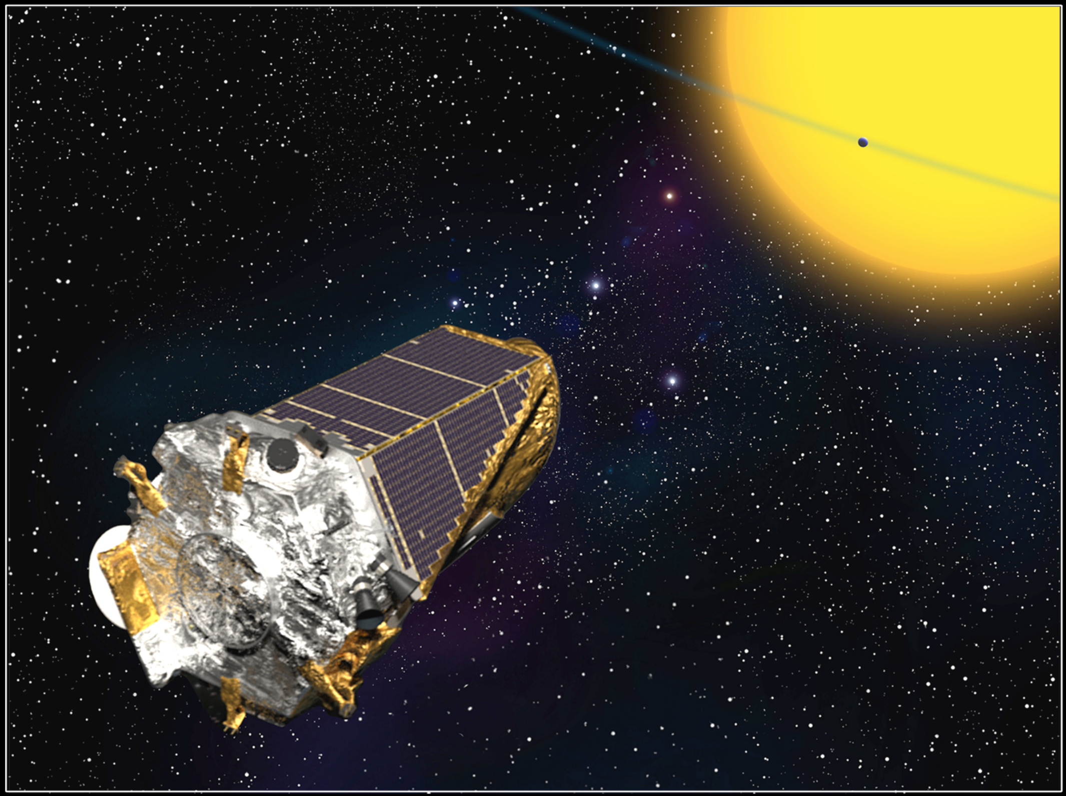
1. Introduction to Exoplanets and Simulations
2. Helium rain on Jupiter
3. Phase diagram of water ice
4. Erosion of icy and rocky materials in cores in giant planets

***Results by Hugh Wilson and Shuai Zhang***

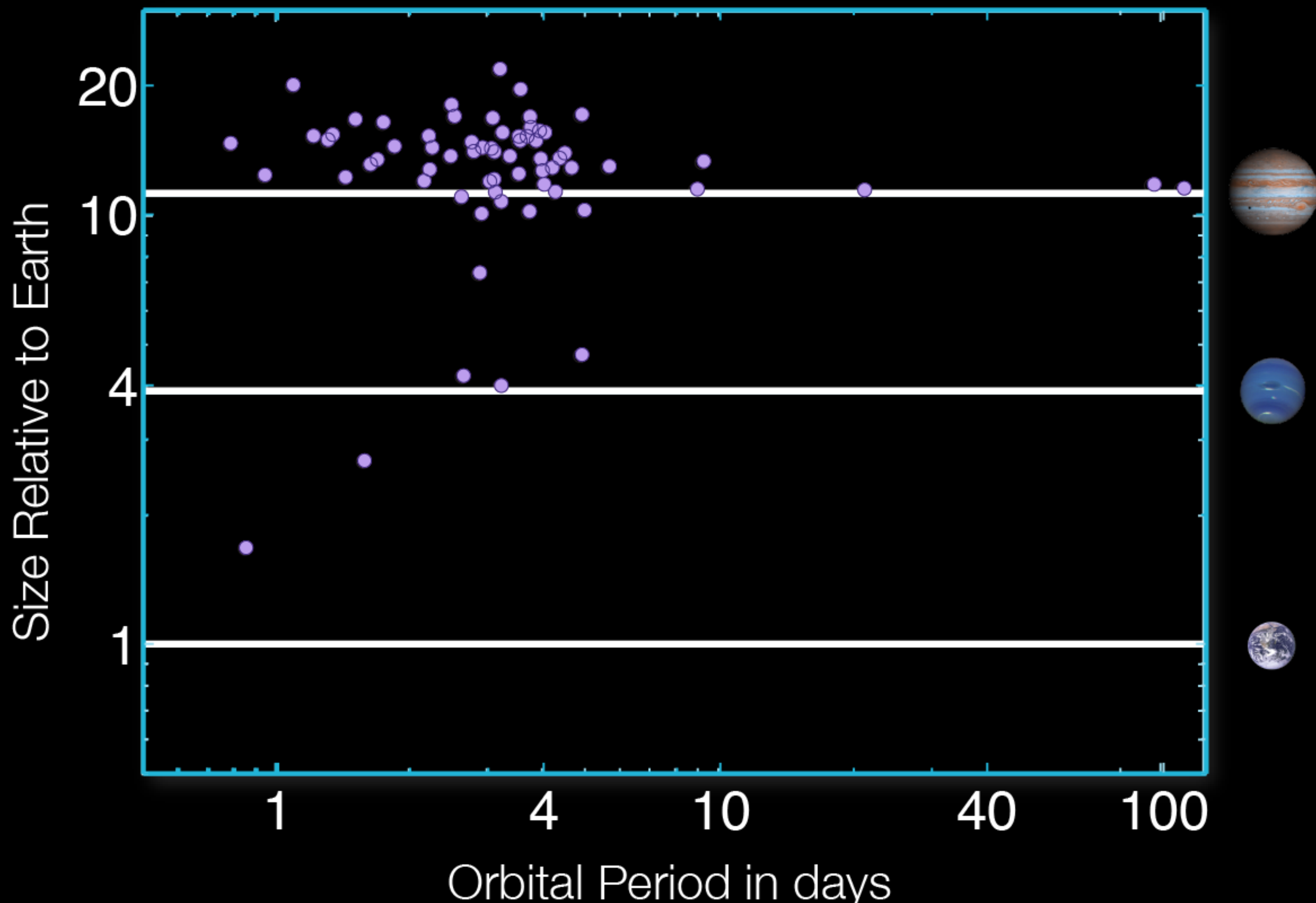
Supported by NASA and NSF.

# NASA’s Kepler Mission

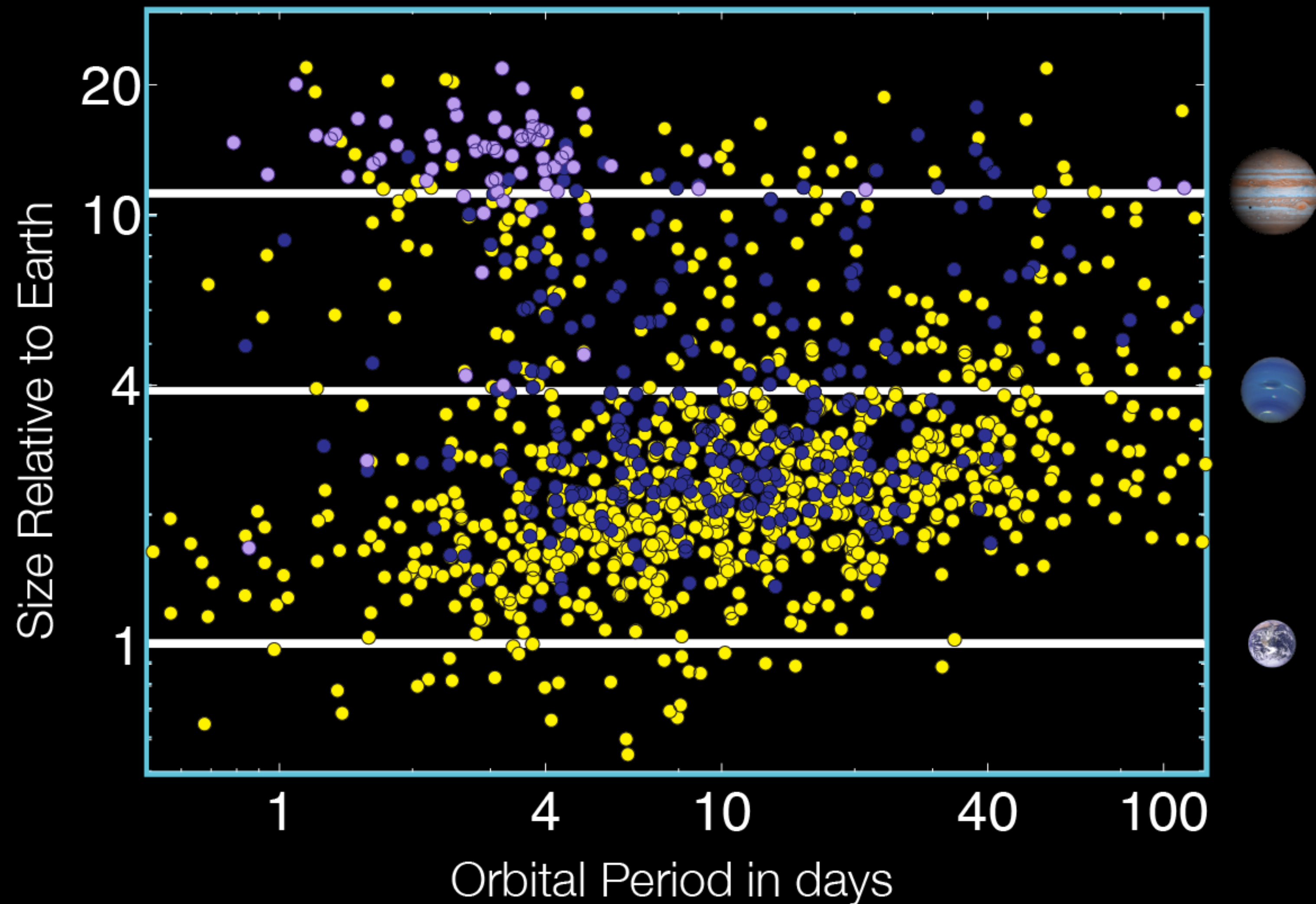
- Determine the frequency of Earth-size and larger planets in the habitable zone of sun-like stars
- Determine the size and orbital period distributions of planets

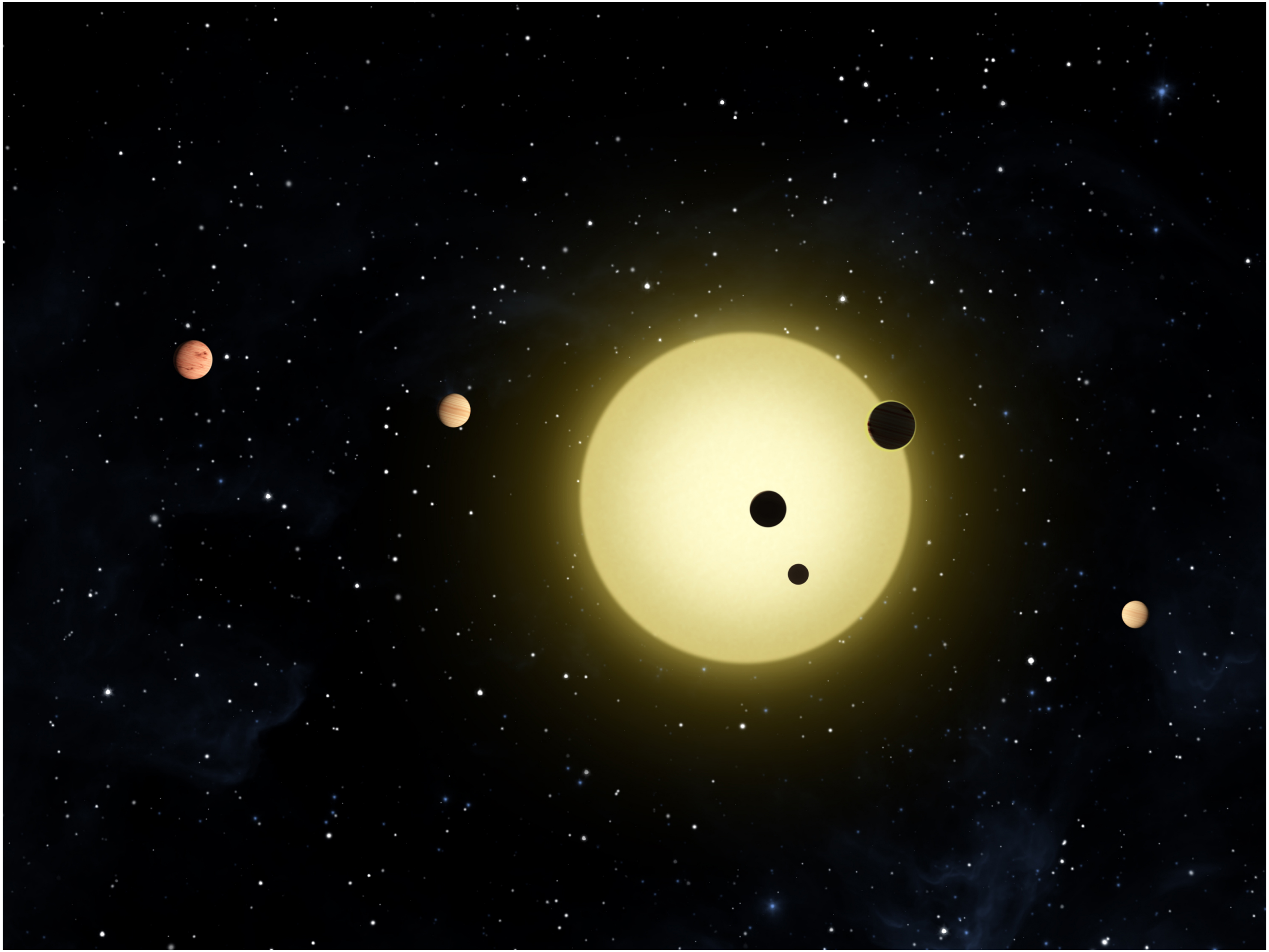



# Pre-Kepler Transiting Planets - 2009



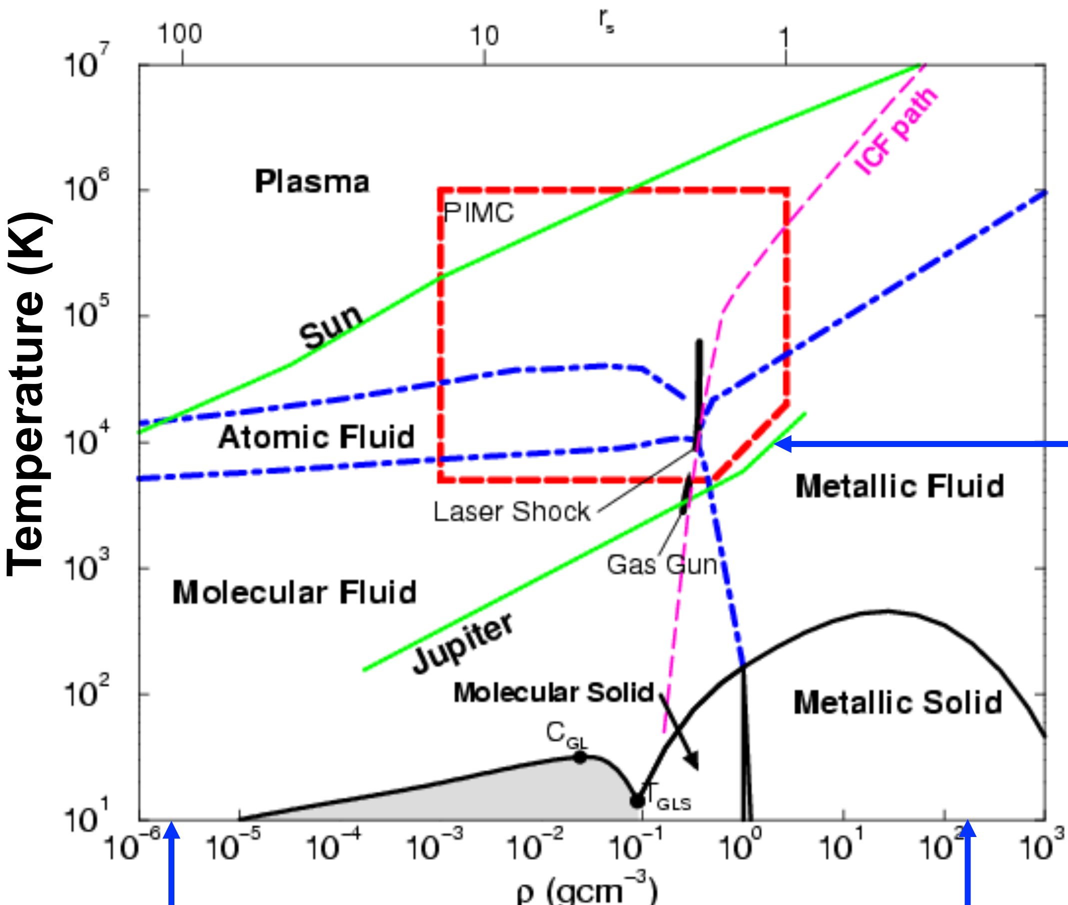
# Kepler Candidates as of February 1, 2011



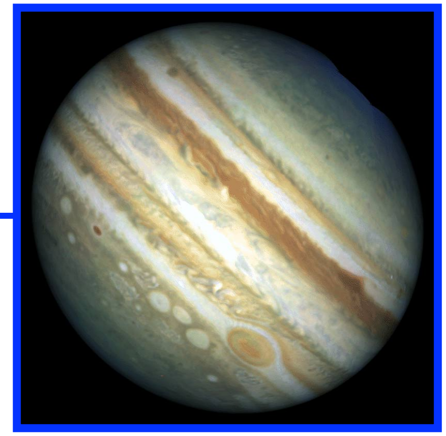


# I. Ab Initio Simulations of Materials at High Pressure

# <u>Focus:</u> Characterization of the Interior of Solar and Extrasolar Giant Planets




**Solar GP: Jupiter, Saturn**



n=$10^{18}$ cm$^{-3}$

**Density**

n=$10^{26}$ cm$^{-3}$

# Paul Dirac (1929):

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too ***complex to be solved***.

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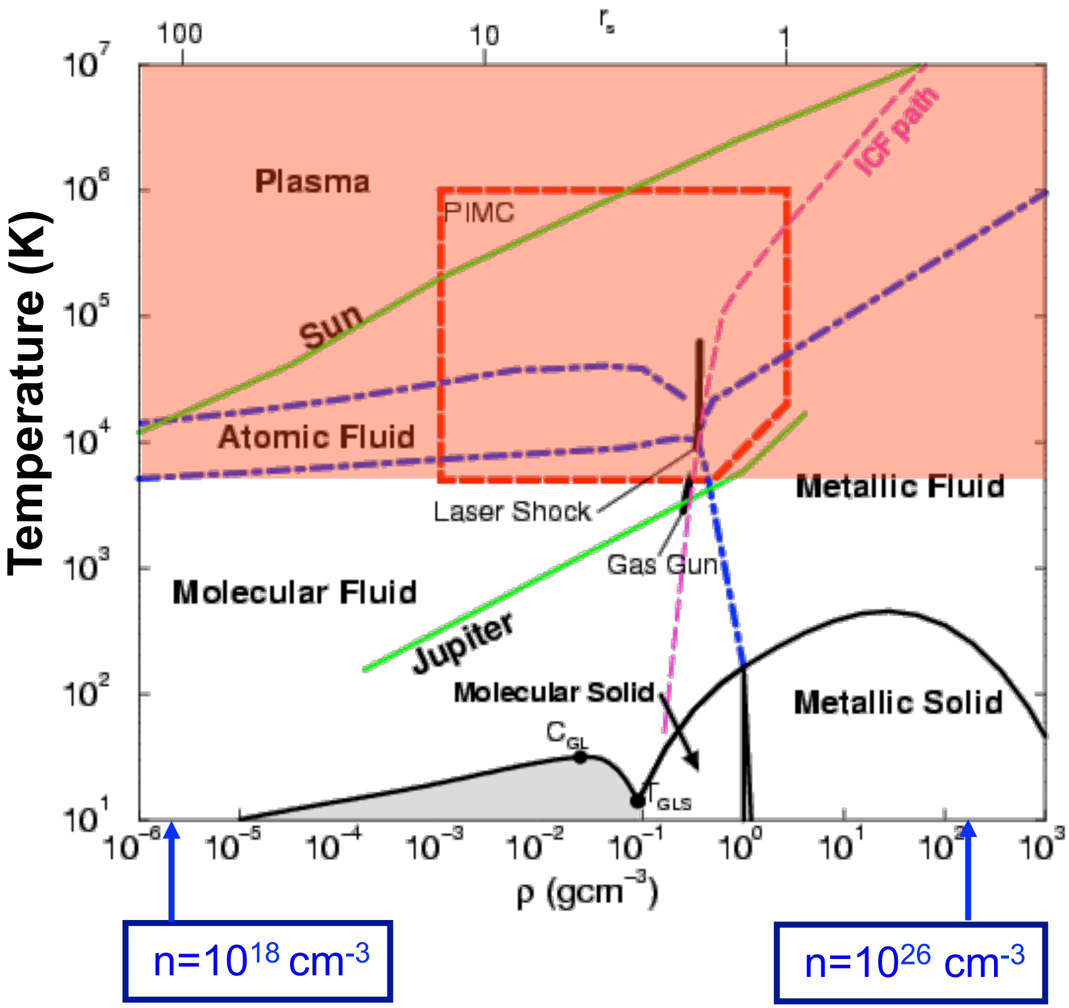
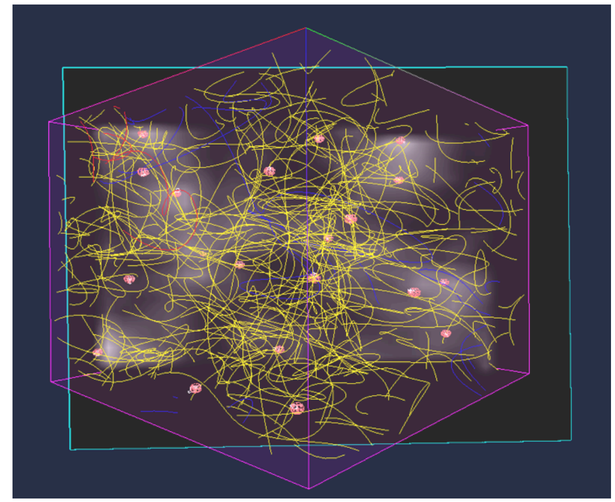
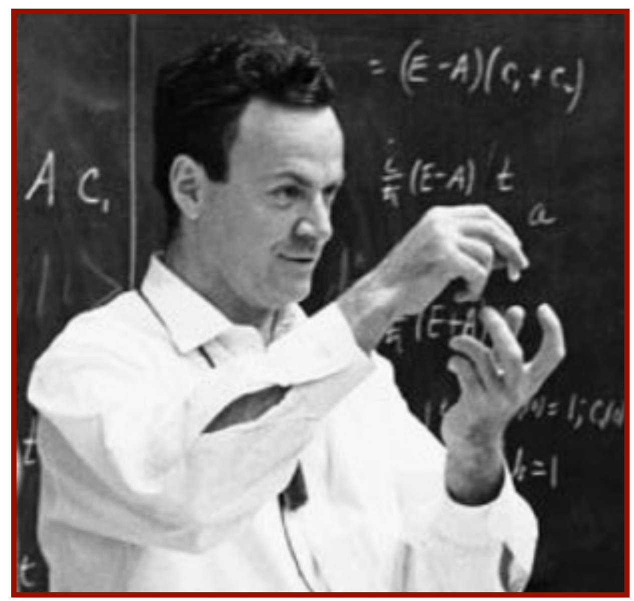
The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too ***complex to be solved*** ***EXACTLY***.

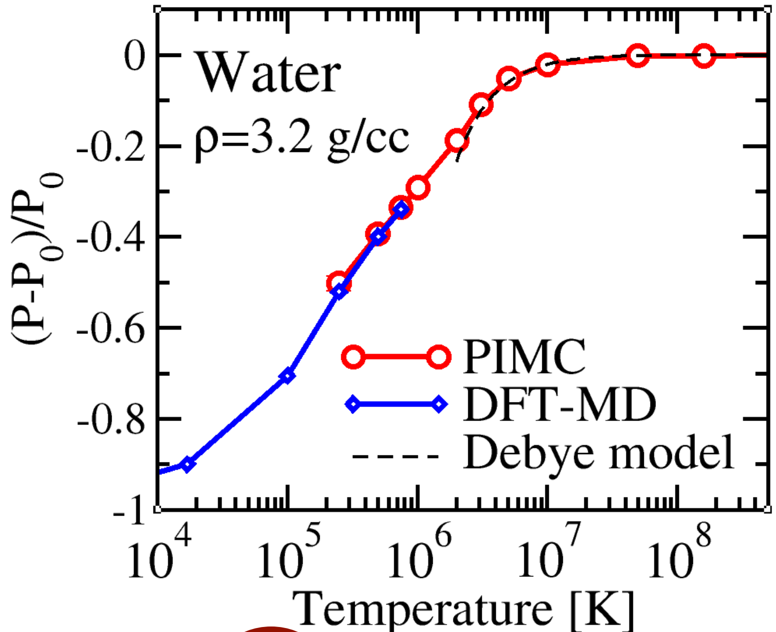
# 1) Path integral Monte Carlo for T>5000K



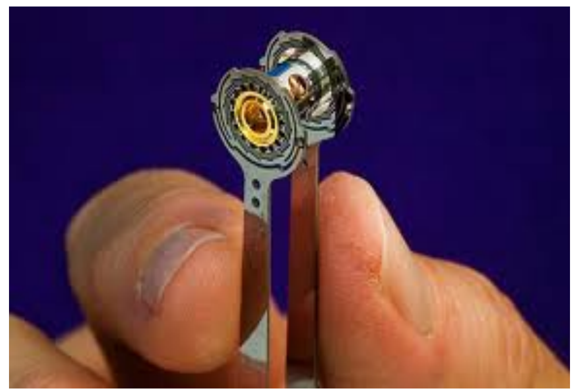





# New Path Integral Monte Carlo Simulations of Heavier Elements Aid Fusion Capsule Design

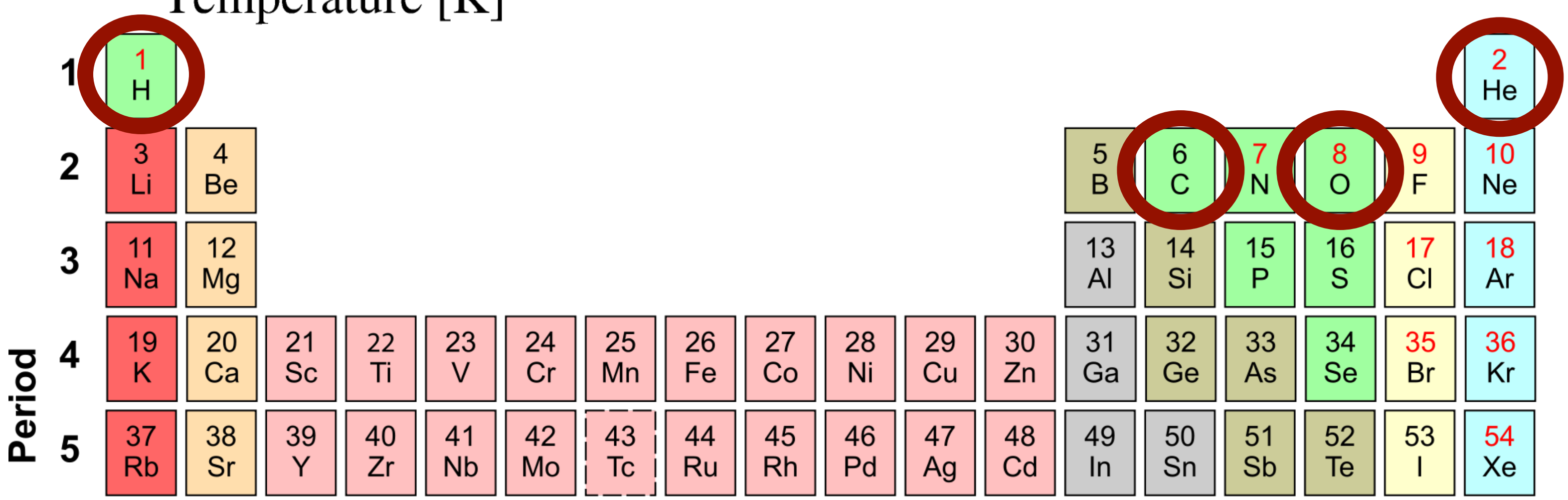



ICF Hohlraum

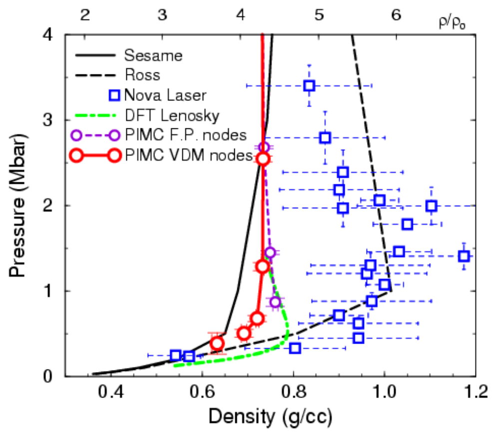


ICF Capsule

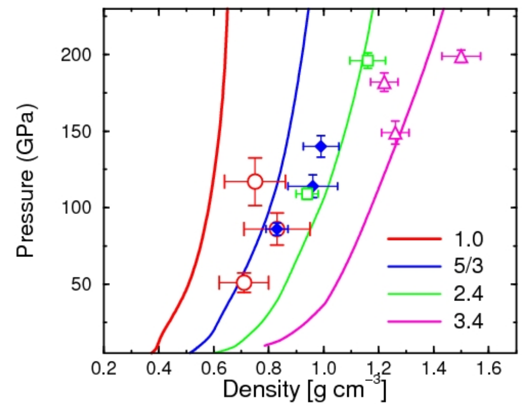
Driver, Militzer, Phys. Rev. Lett. (2012).



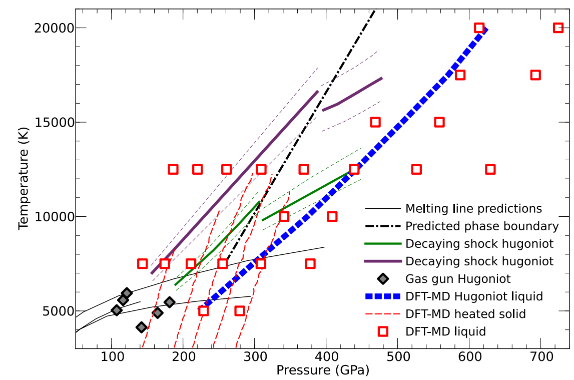
# Comparison of Ab initio Simulations with Shock Wave Experiments




**Hydrogen**
Militzer et al., Phys. Rev. Lett. (2000, 2001, 2011)

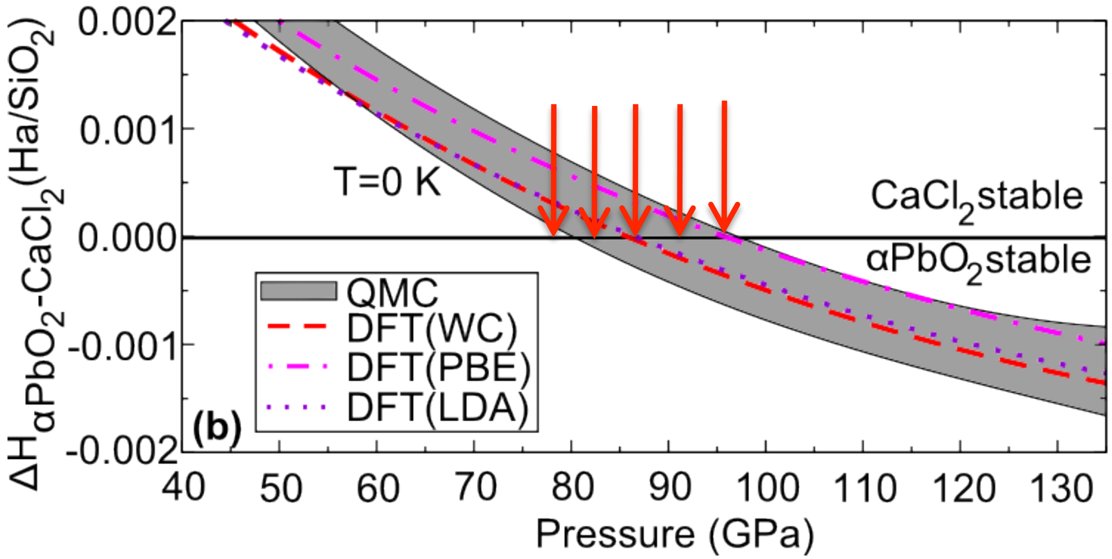



**Helium**
Militzer
PRL (2006), PRB (2009)




**Liquid $MgSiO_3$**
Militzer
Submitted (2012)

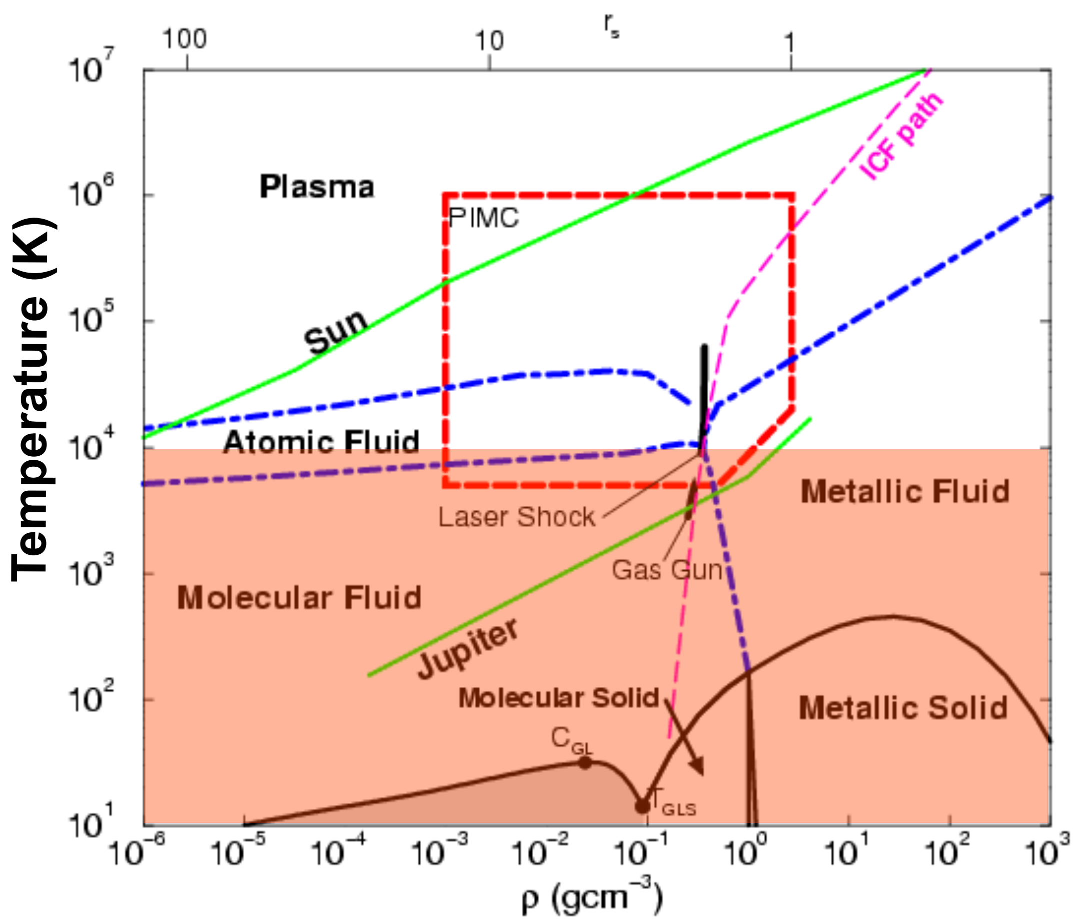
# Quantum Monte Carlo Calculations of $SiO_2$ Phases at Mantle Pressures

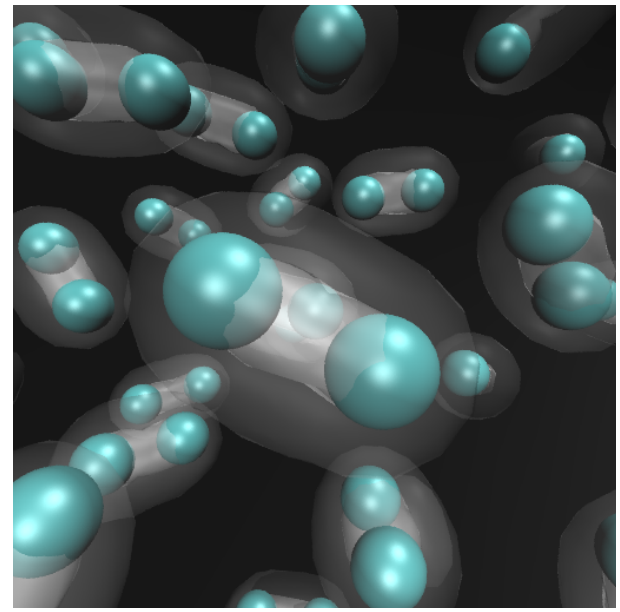



Not associated with global seismic discontinuity

**K. Driver *et al. Proc. Nat. Acad. Sci. 107 (2010) 9519***

# 1) Path integral Monte Carlo for T>5000K
# 2) Density functional molecular dynamics below



Born-Oppenheimer approx. MD with classical nuclei:

**$F = m\,a$**

Forces derived DFT with electrons in the instantaneous ground state.

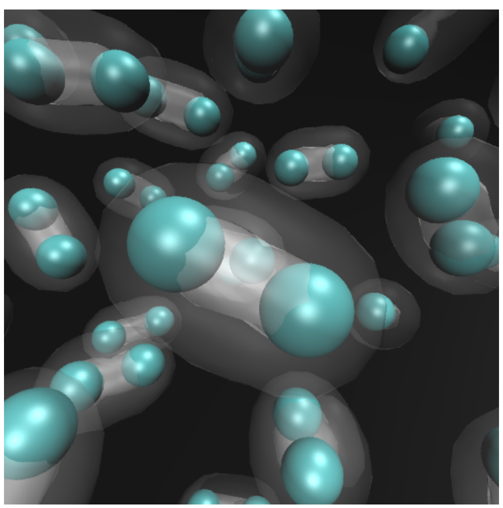
# What is meant by first-principles simulations?

Schrödinger equation:

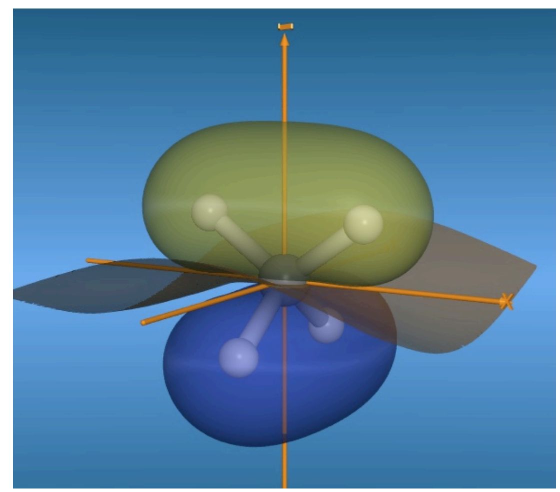
$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\,\psi(\vec{r}) + V(\vec{r})\,\psi(\vec{r}) = E\,\psi(\vec{r})$$

Look for an antisymmetric solution (Pauli exclusion):

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \chi_1(\mathbf{x}_1) & \chi_2(\mathbf{x}_1) & \cdots & \chi_N(\mathbf{x}_1) \\ \chi_1(\mathbf{x}_2) & \chi_2(\mathbf{x}_2) & \cdots & \chi_N(\mathbf{x}_2) \\ \vdots & \vdots & & \vdots \\ \chi_1(\mathbf{x}_N) & \chi_2(\mathbf{x}_N) & \cdots & \chi_N(\mathbf{x}_N) \end{vmatrix}$$

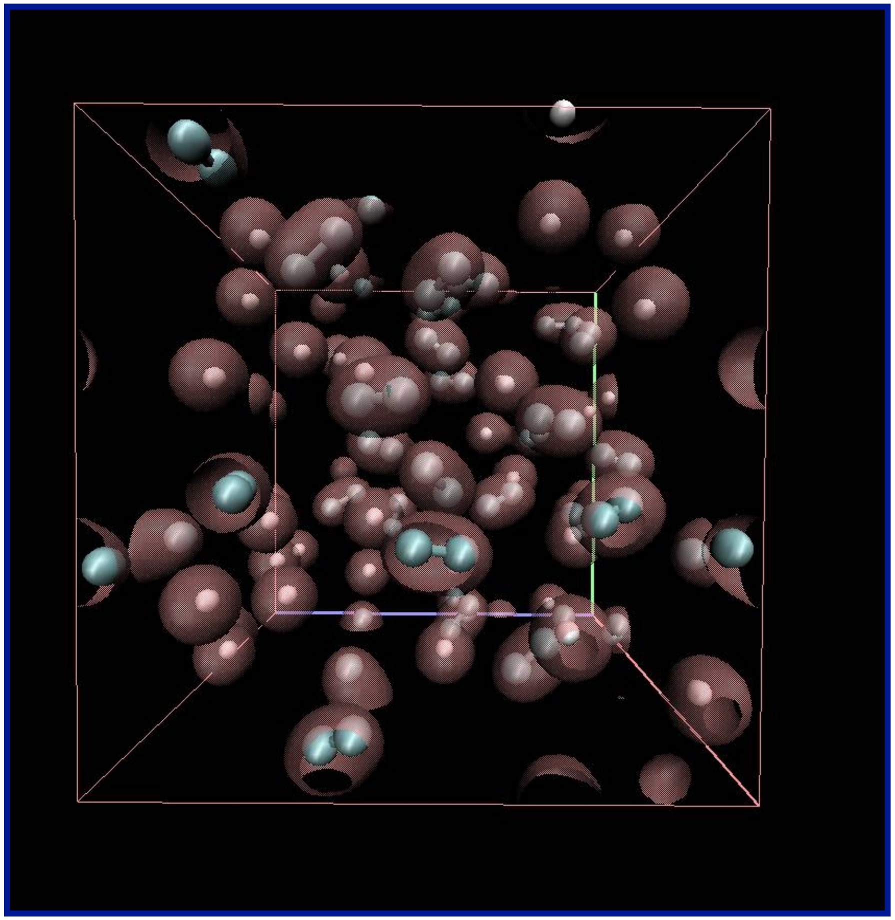


Simulation of molecular hydrogen

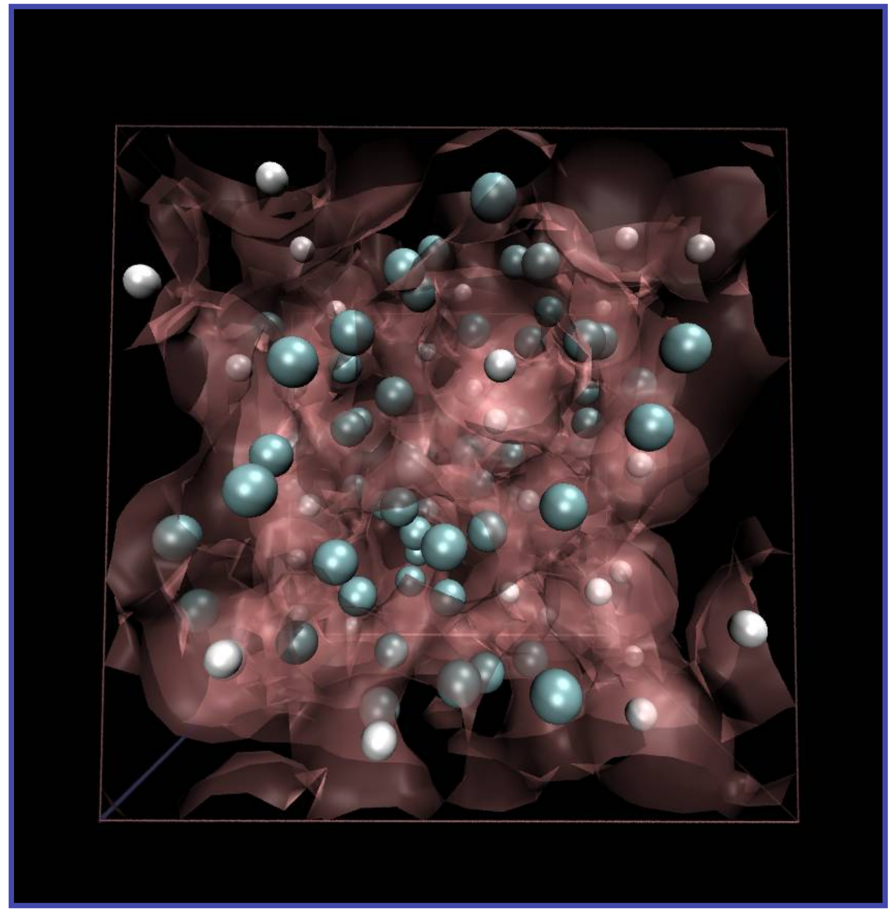


Methane - molecular orbitals

# Comparison of molecular and metallic hydrogen

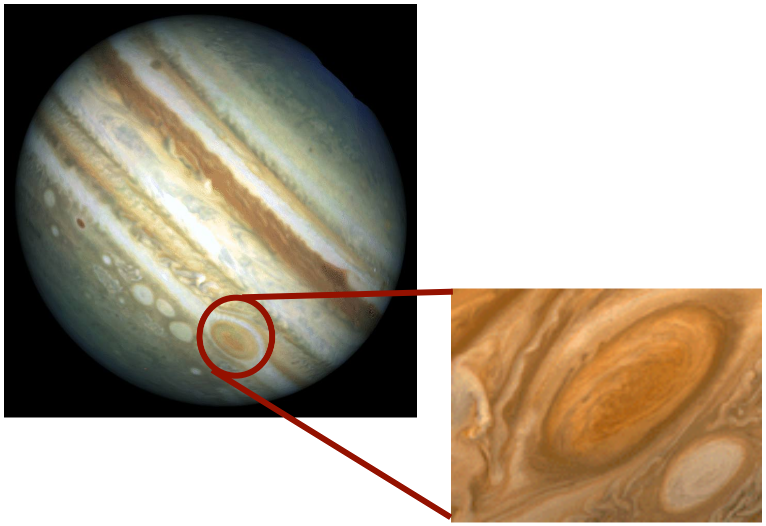


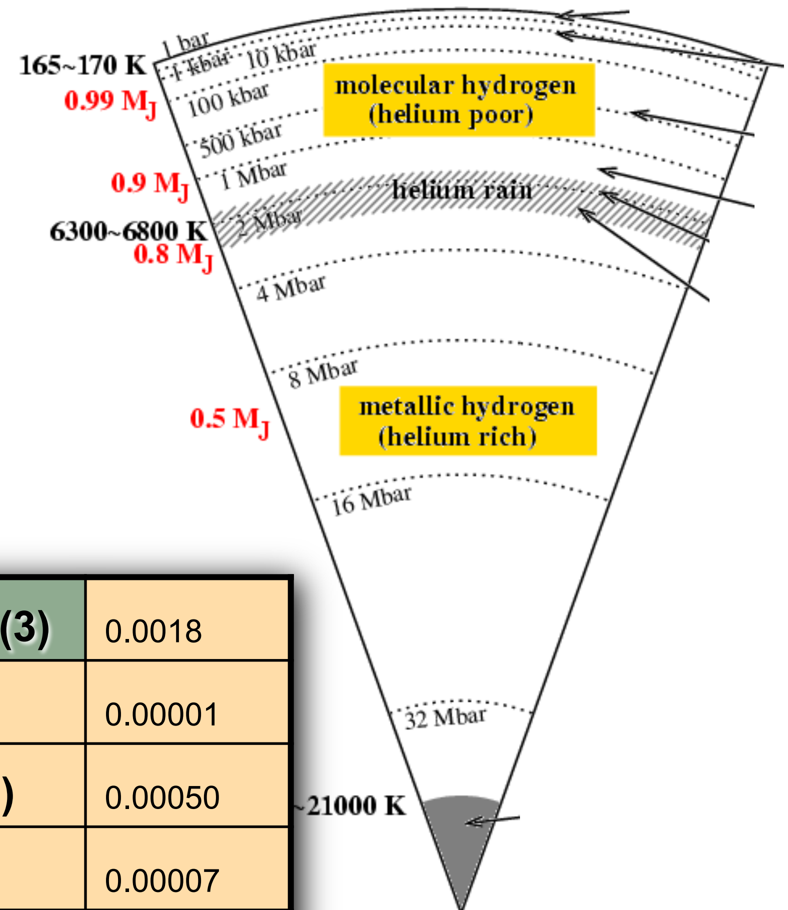
Molecular hydrogen



Metallic hydrogen

# Jupiter's Composition



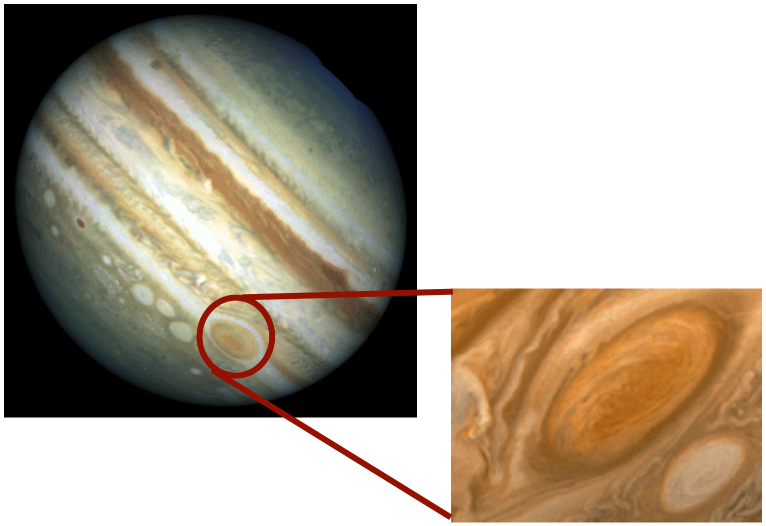


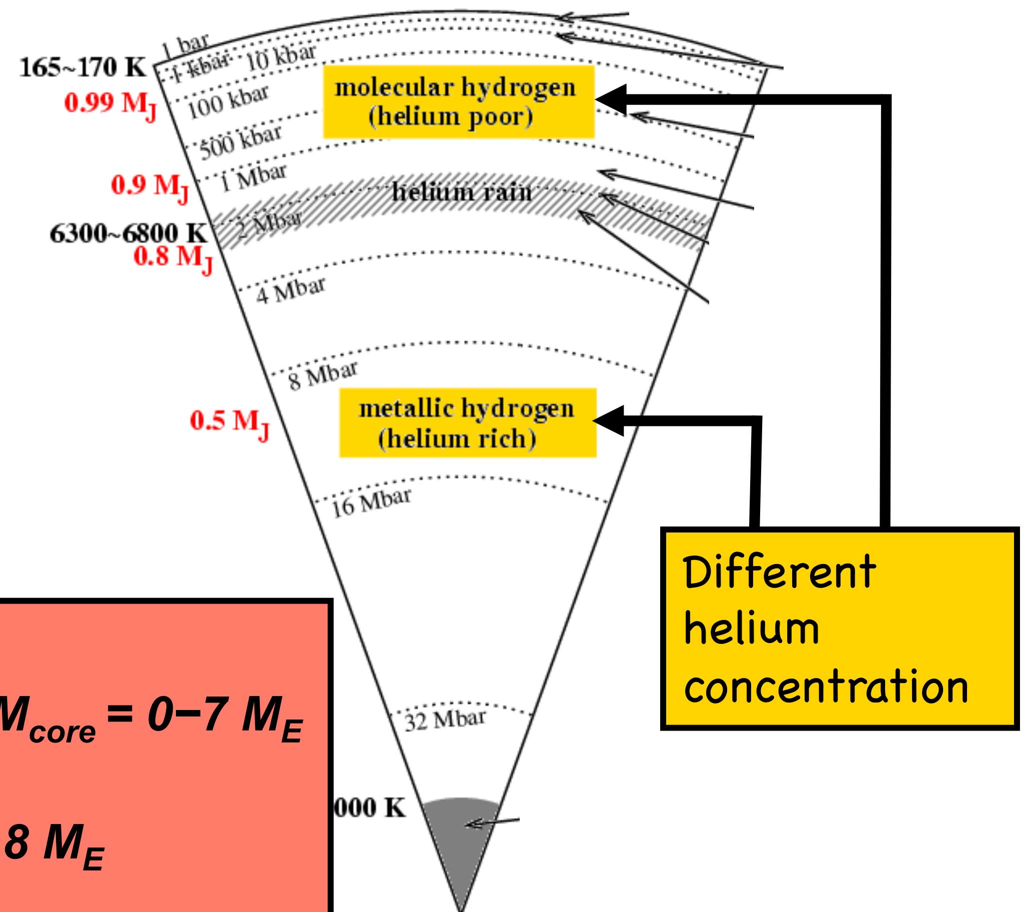

**<u>Composition on the surface</u>** <u>(solar):</u>

| | | | | | |
|---|---|---|---|---|---|
| **H** | **0.742** | 0.736 | **Ne** | **0.00023(3)** | 0.0018 |
| **He** | **0.231(4)** | 0.249 | **P** | **< 0.00007** | 0.00001 |
| **C** | **0.009(2)** | 0.0029 | **S** | **0.00091(6)** | 0.00050 |
| **N** | **< 0.012** | 0.00085 | **Ar** | **< 0.00015** | 0.00007 |
| **O** | **< 0.0035** | 0.0057 | **"Z"** | **0.027** | 0.015 |

Guillot et al. (Jupiter book, 2002, chap.3 )

# The Size of Jupiter's Core is uncertain



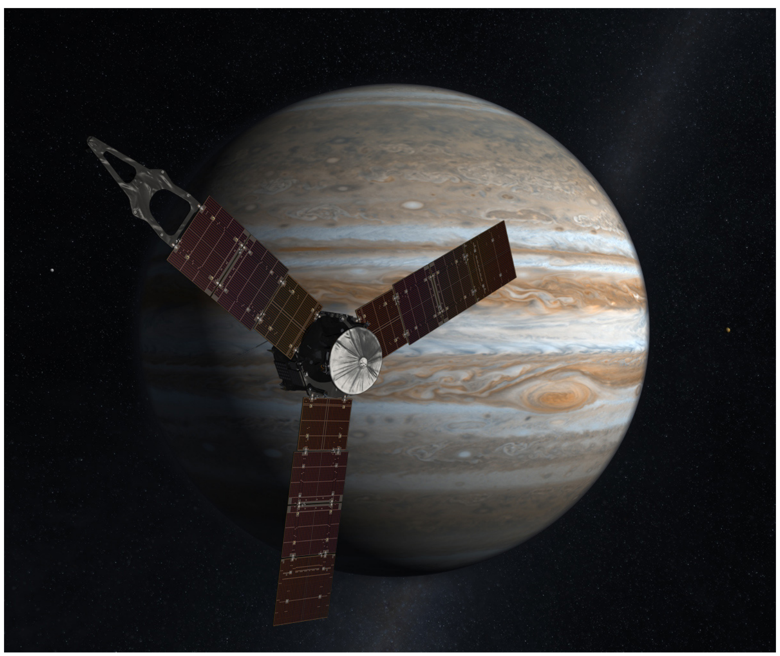



**A) Typical models by Guillot *et al.*: $M_{core} = 0–7\ M_E$**

**B) We derived a model: $M_{core} = 14–18\ M_E$**

Guillot et al. (Jupiter book, 2002, chap.3 )

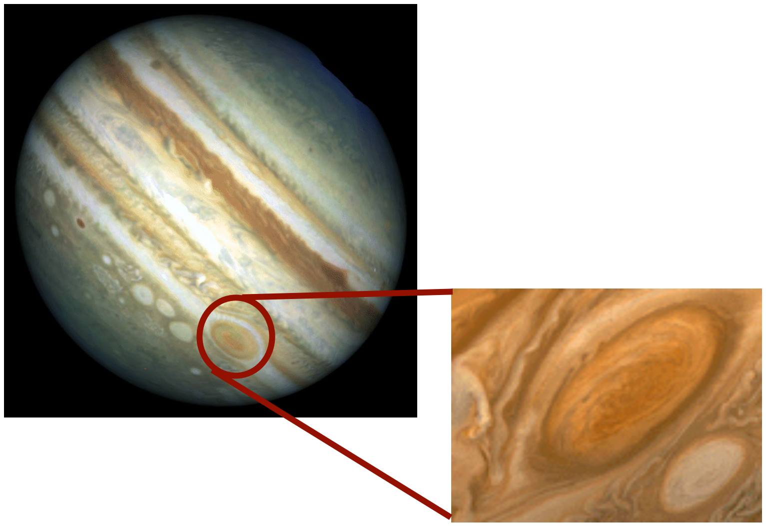
# Juno Mission
## launched successfully August 2011

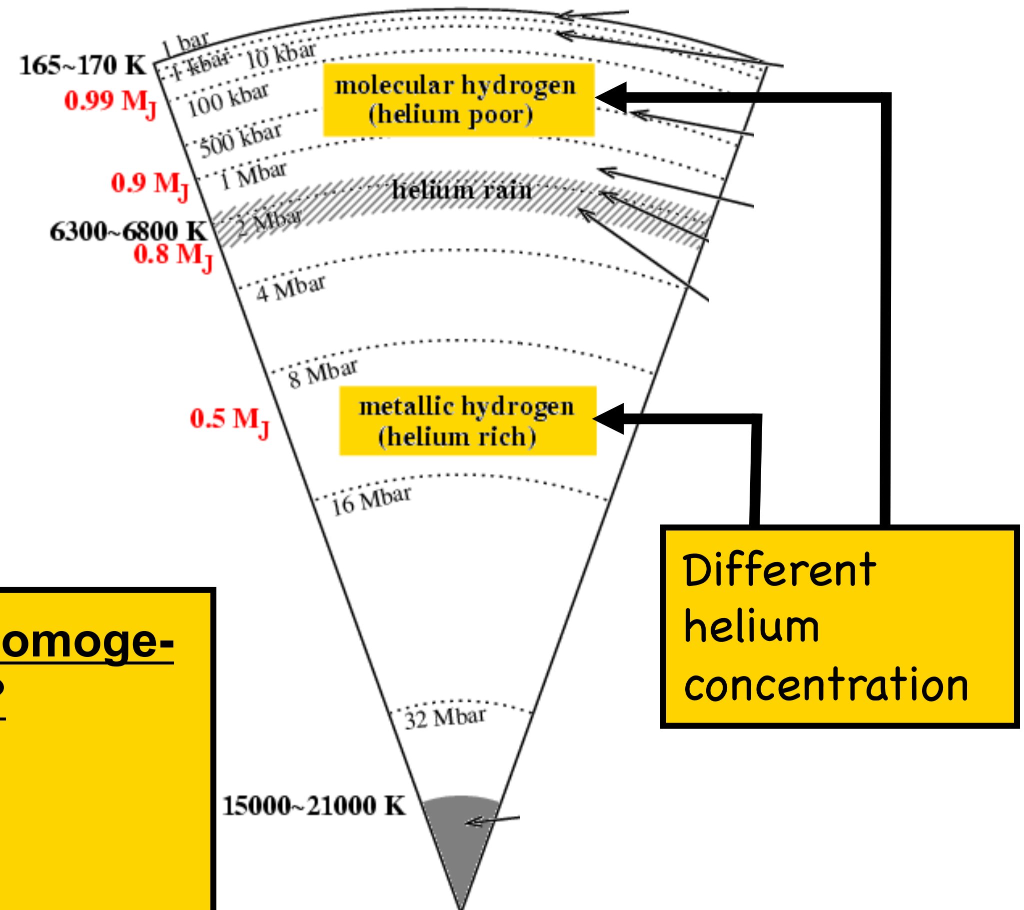


**Mission Timeline:**

- **Launch - August 2011**
- **Earth flyby gravity assist - October 2013**
- **Jupiter arrival - July 2016**
- **End of mission (deorbit) - October 2017**

# Jupiter's Interiors

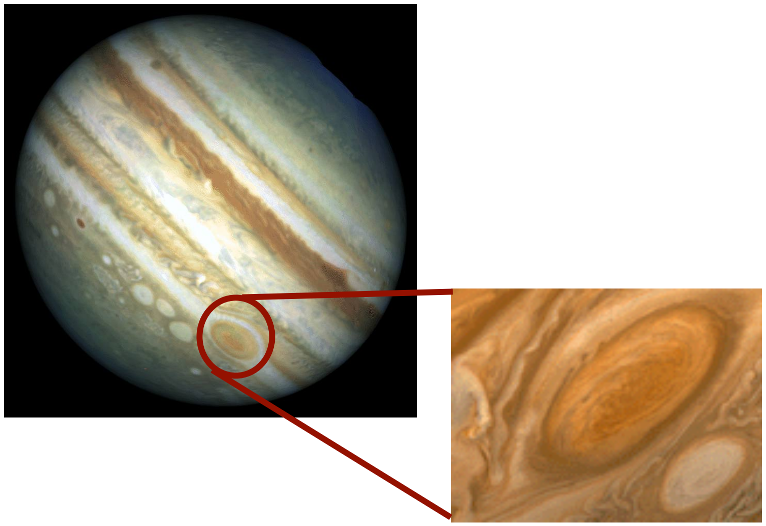


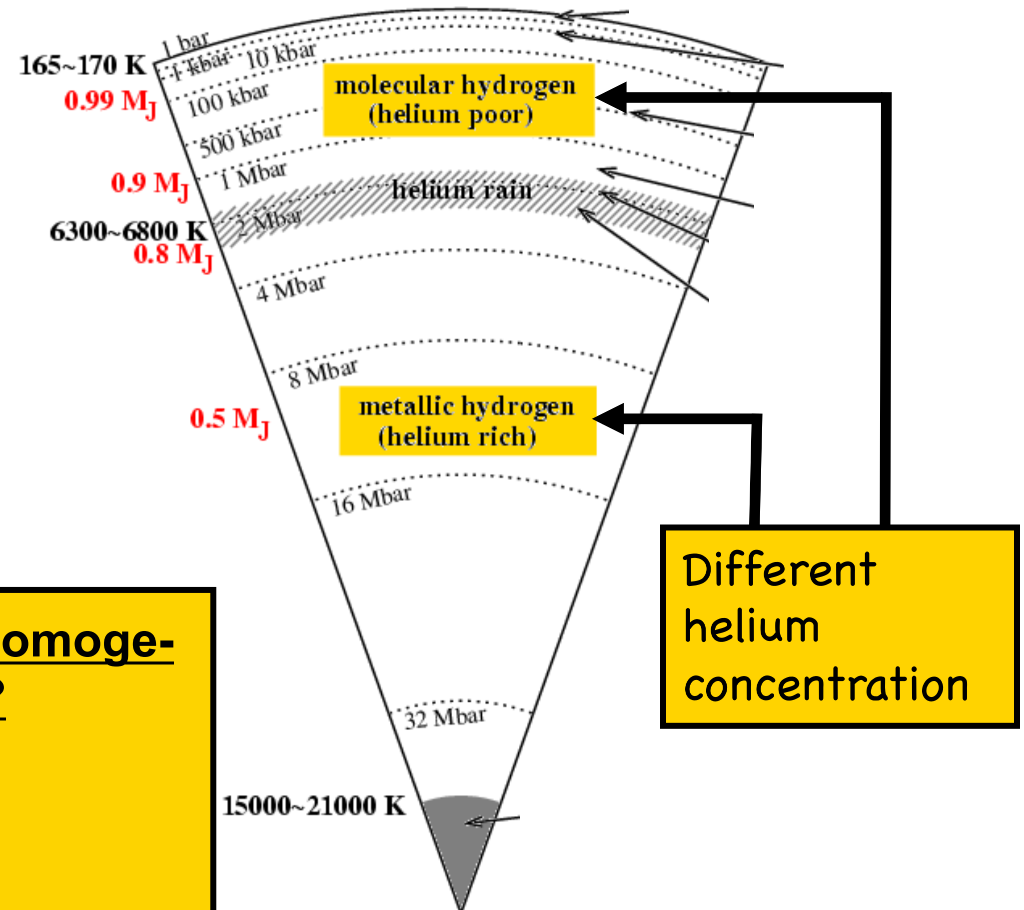



**<u>Which processes can introduce inhomogeneities into Jupiter's gas envelope?</u>**

Guillot et al. (Jupiter book, 2002, chap.3 )

# Jupiter's Interiors



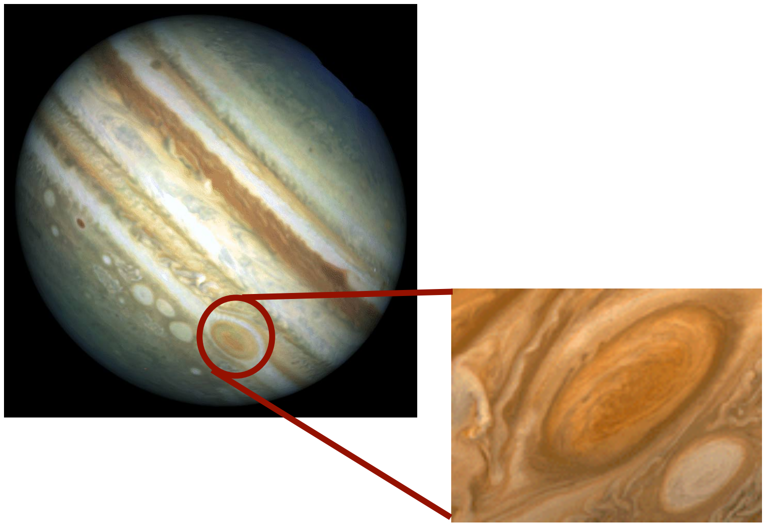


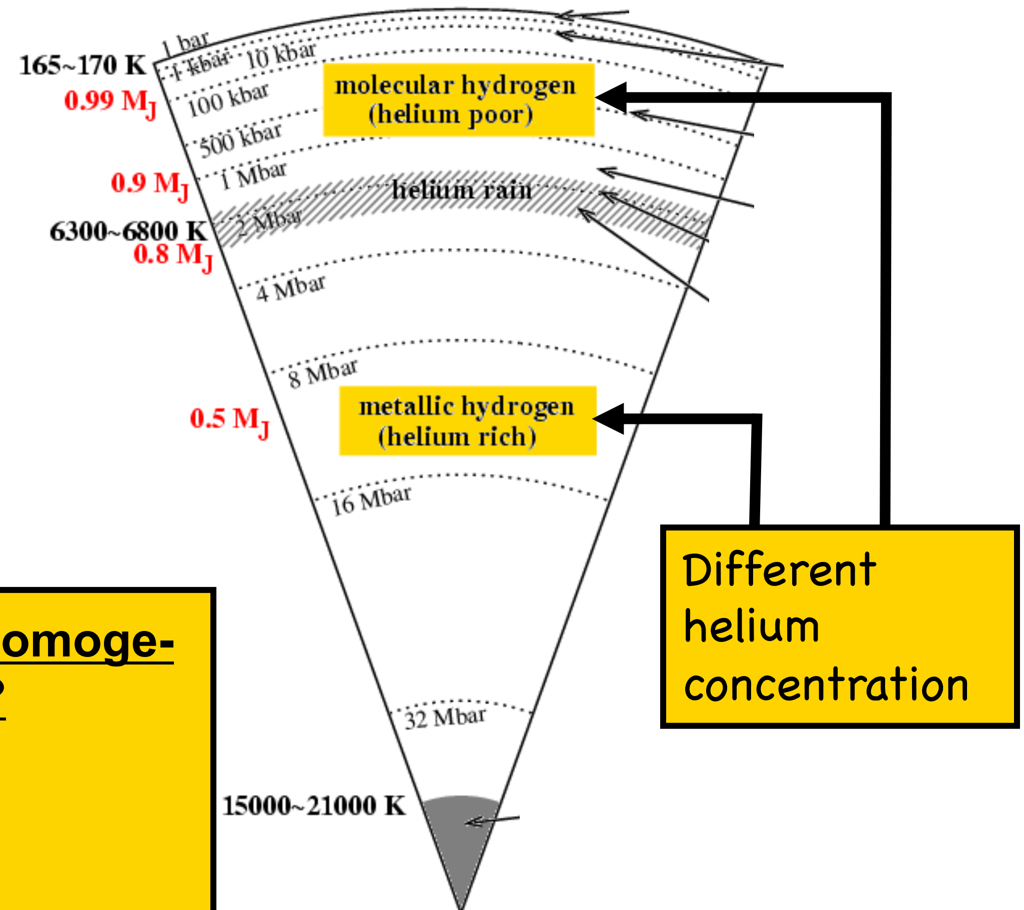

**<u>Which processes can introduce inhomogeneities into Jupiter's gas envelope?</u>**

- **first order phase transition from molecular to metallic hydrogen**

Guillot et al. (Jupiter book, 2002, chap.3 )

# Jupiter's Interiors



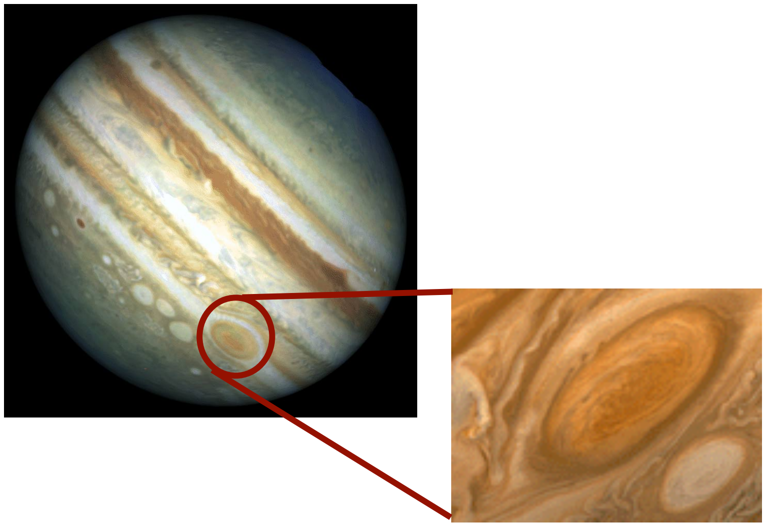


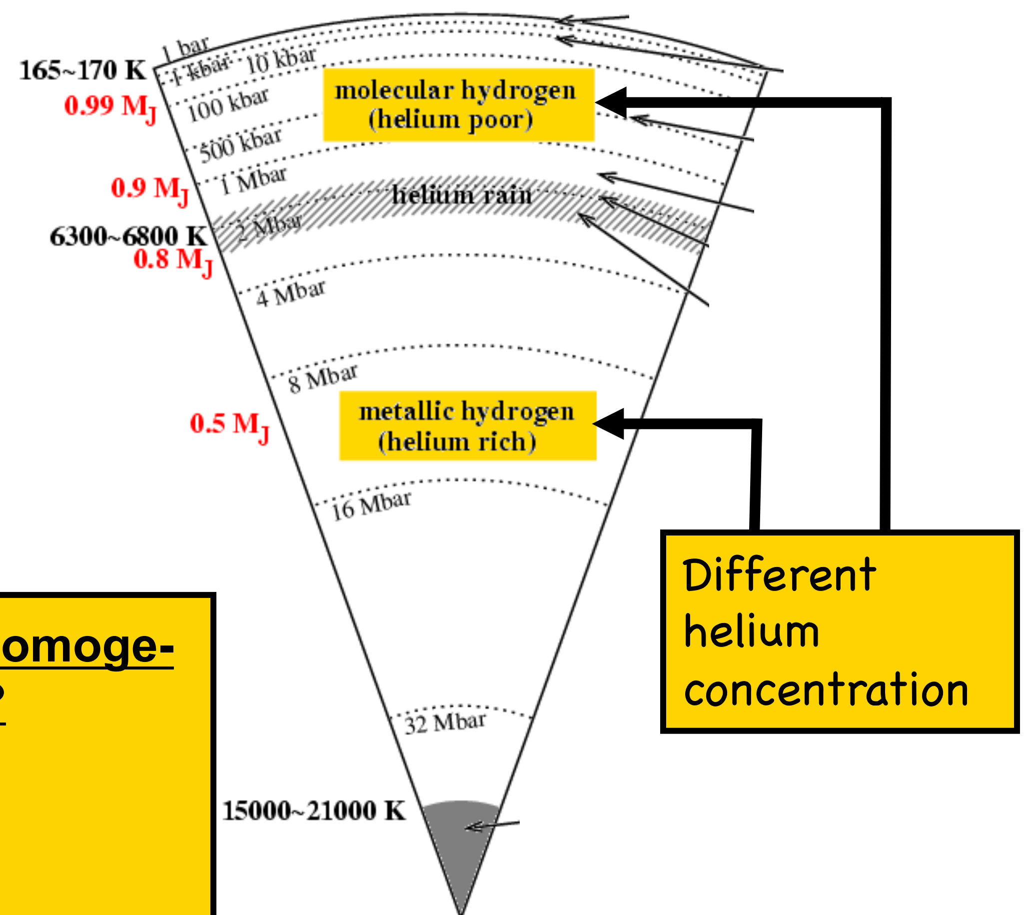

**<u>Which processes can introduce inhomogeneities into Jupiter's gas envelope?</u>**

- **first order phase transition from molecular to metallic hydrogen**
- **helium rain**

Guillot et al. (Jupiter book, 2002, chap.3 )

# Jupiter's Interiors





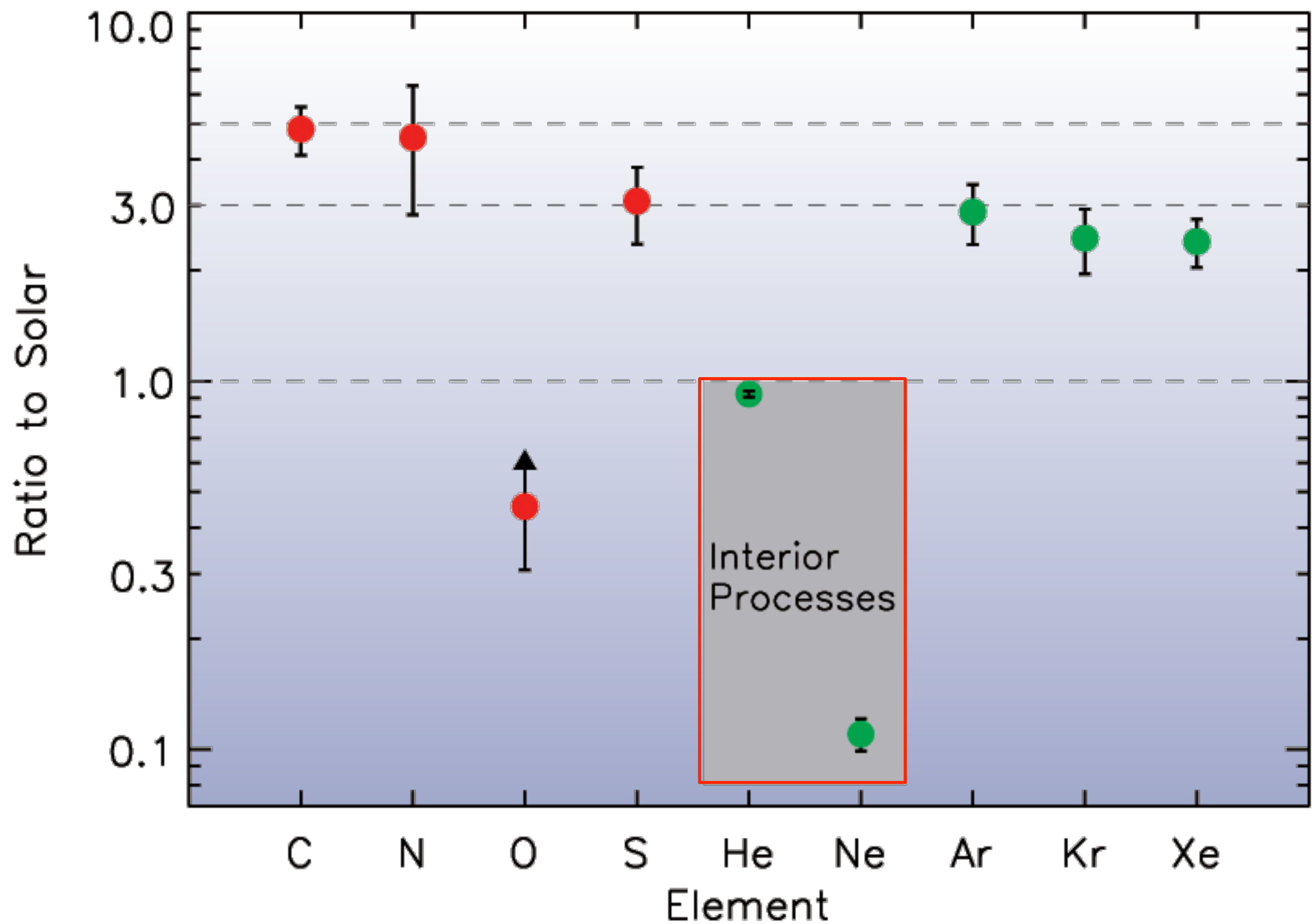

**<u>Which processes can introduce inhomogeneities into Jupiter's gas envelope?</u>**

- **first order phase transition from molecular to metallic hydrogen**
- **helium rain**
- **core erosion**

Guillot et al. (Jupiter book, 2002, chap.3 )

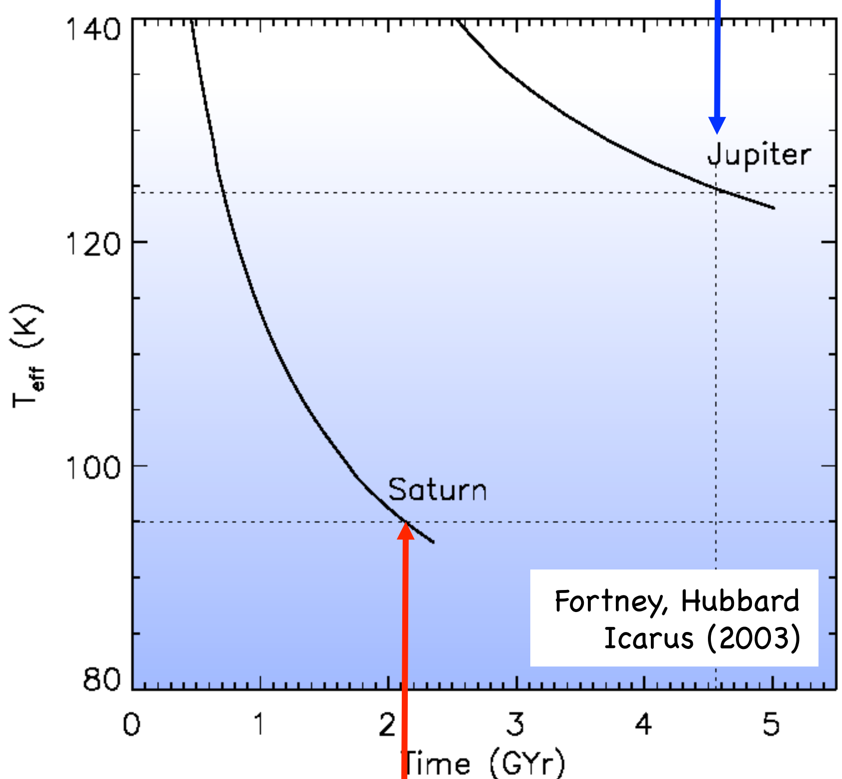
# II. Helium Rain on Jupiter

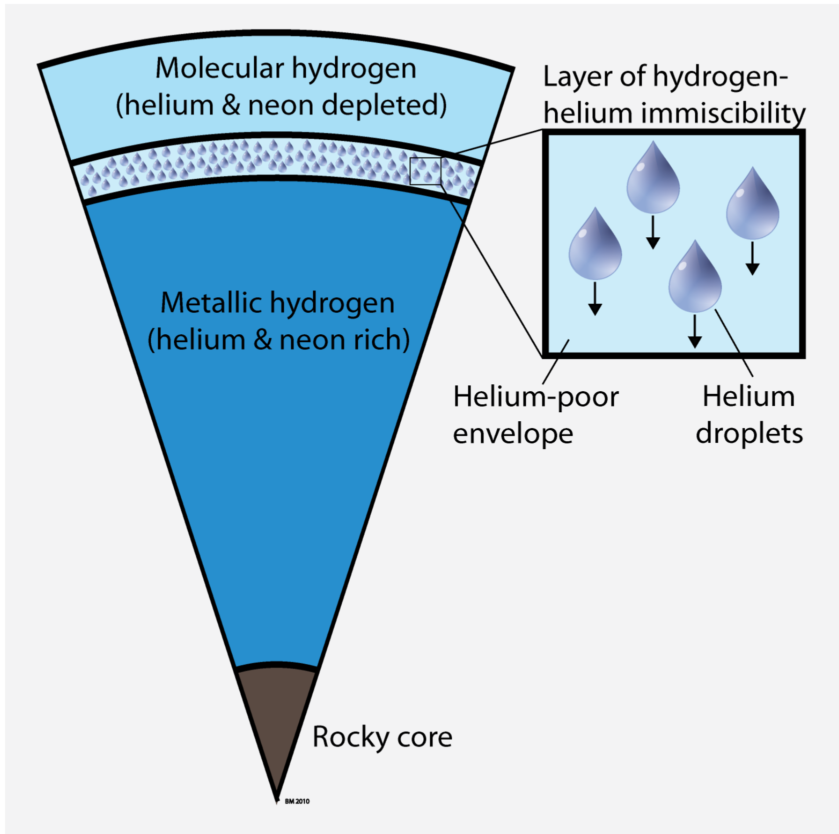
# Galileo Entry Probe found: Helium and Neon depleted in Jupiter's Atmosphere



# Why does Saturn cool so slowly? Observed Excess in Luminosity

Jupiter's cooling rate is in agreement with model predictions



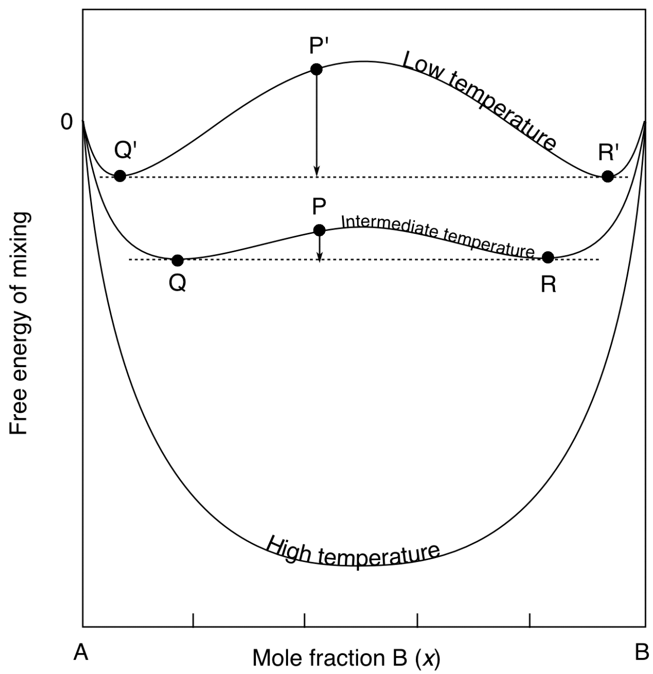



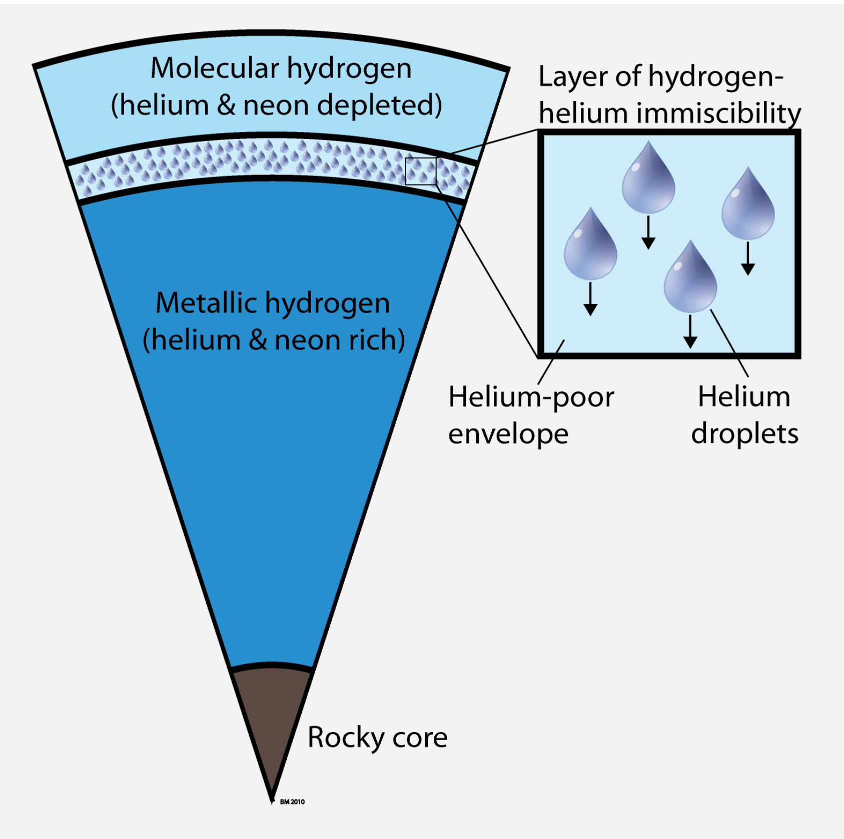

Model for Saturn consistently predict too fast cooling rates (by ~2 Gyrs)

# Can hydrogen and helium become immiscible? Helium rain inside Saturn?

Mixing free energy $\Delta G_{mix}(P,T)$:

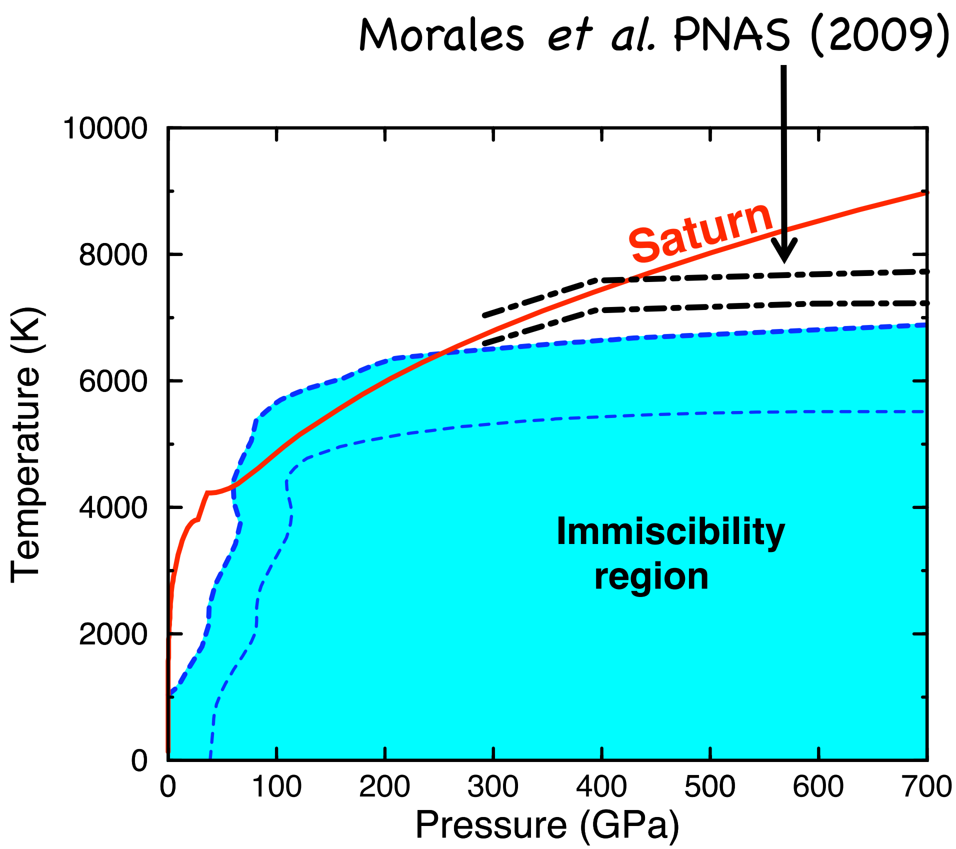
$$\Delta G_{mix}(x) = G(x) - x\, G_{He} - (1-x)\, G_H$$

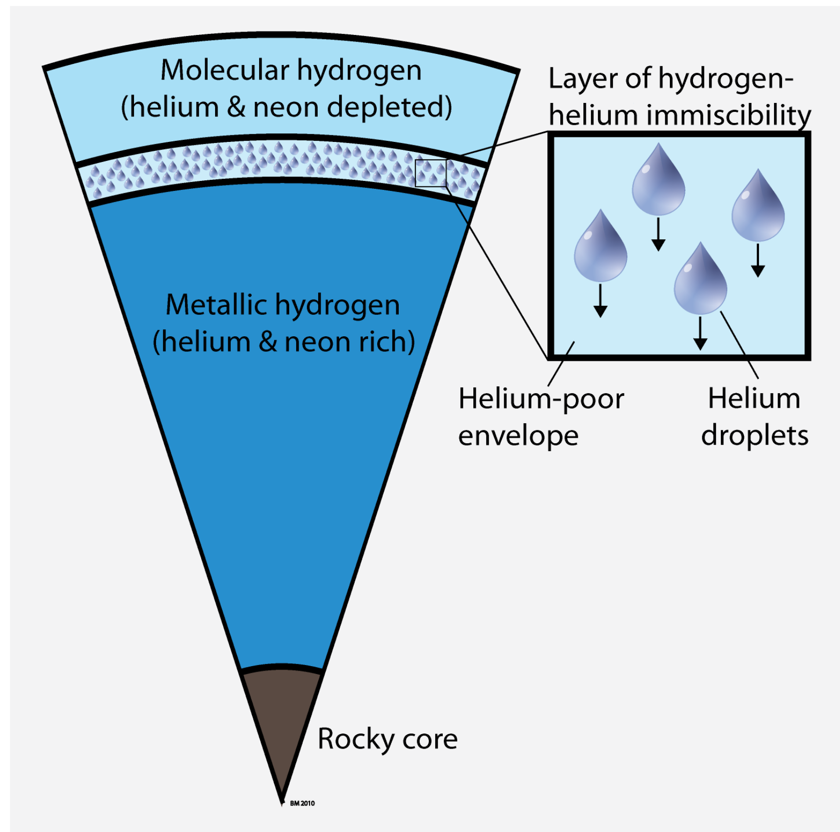



$G(P,T) = E + PV - TS$ Main difficulty is to calculate the mixing entropy!

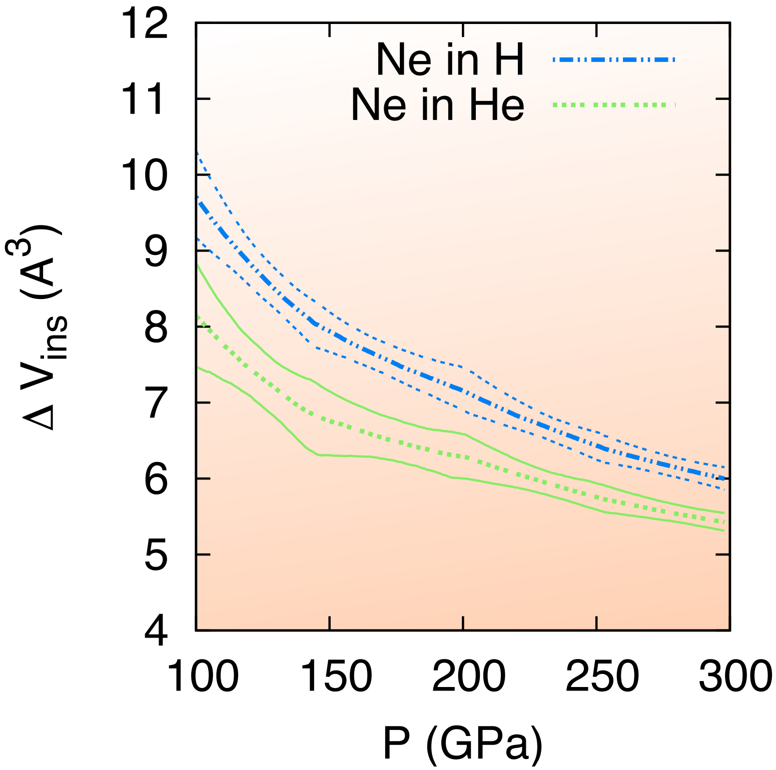
# Now we have good theoretical evidence for hydrogen-helium immiscibility in Saturn




*G*(P,T)=E+PV-TS Main difficulty is to calculate the mixing entropy!

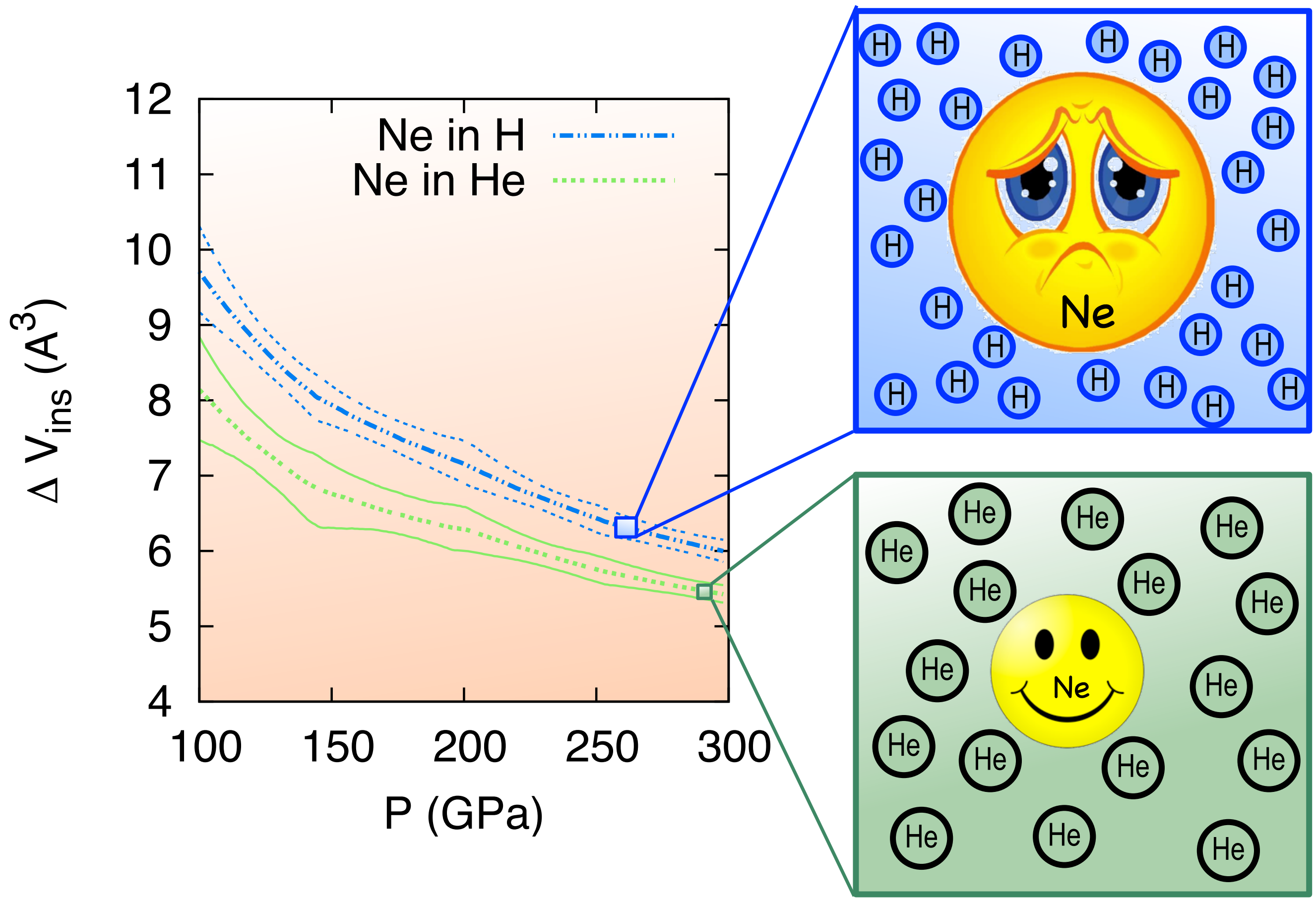
# Gibbs Free Energy Calculations with Thermodynamic Integration




1. Determine density for given and P and T

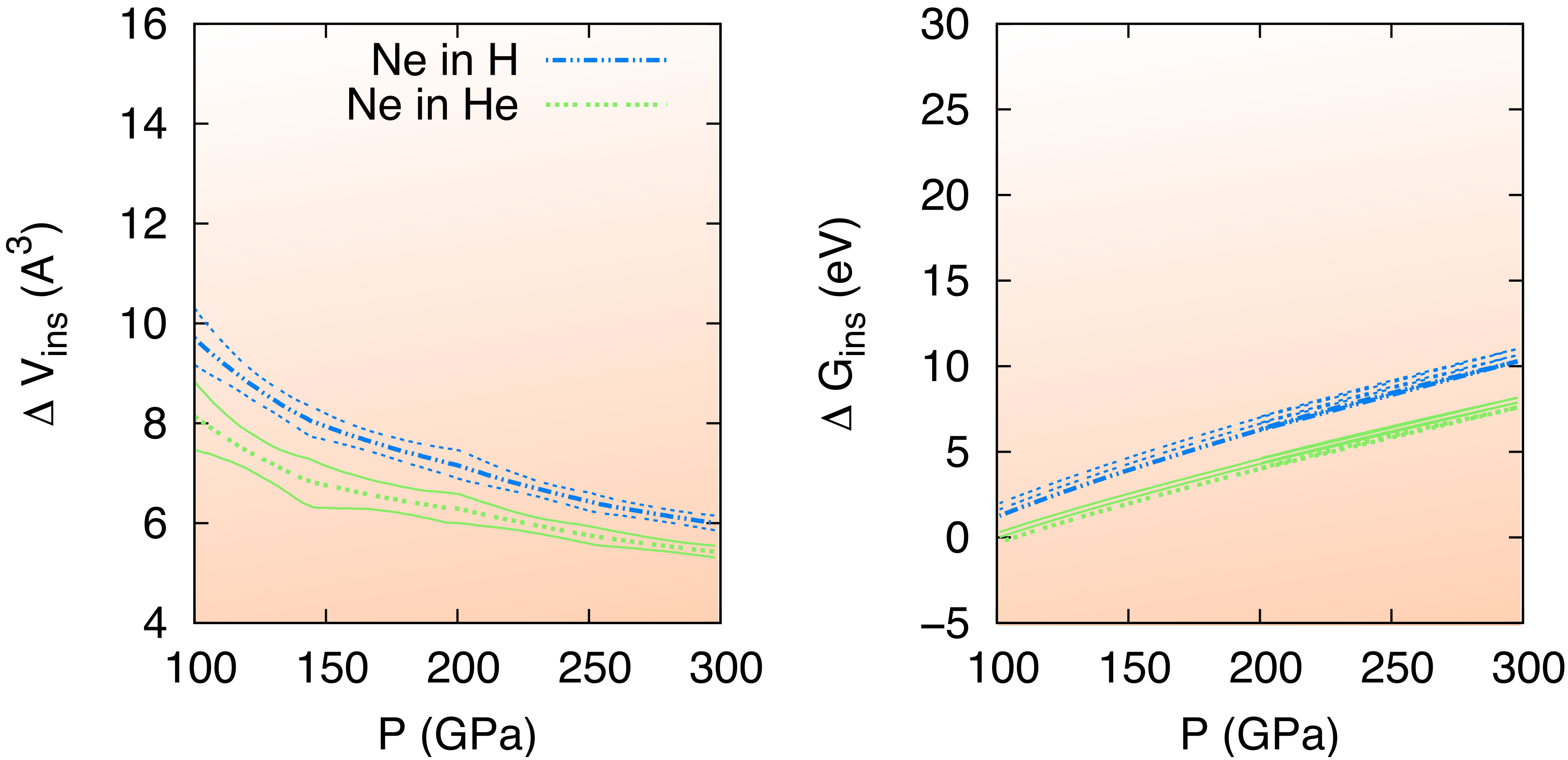
Where does neon given the choice between a hydrogen and helium rich phase? $G(P,T)=E+PV-TS$

# Neon prefers a helium droplet over the hydrogen-rich fluid




Where does neon given the choice between a hydrogen and helium rich phase? $G(P,T)=E+PV-TS$

# Gibbs free energy calculation for neon insertion in hydrogen and helium

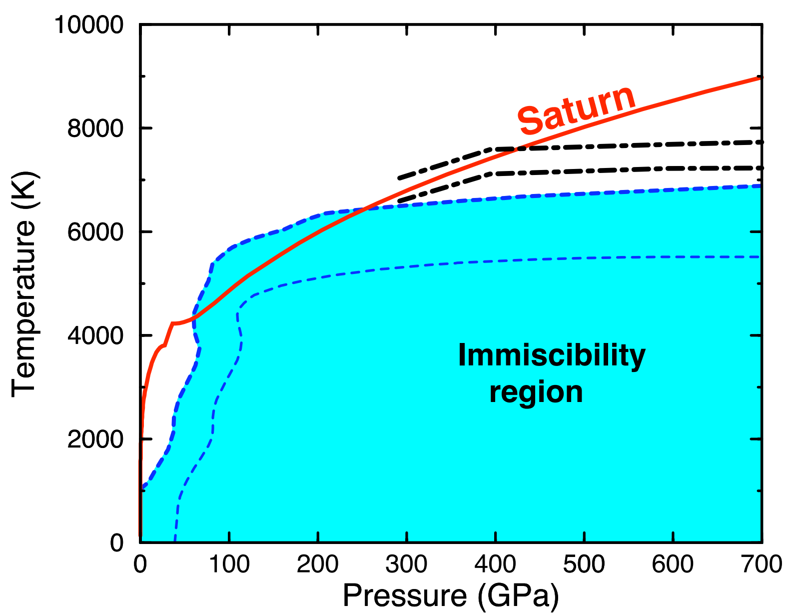


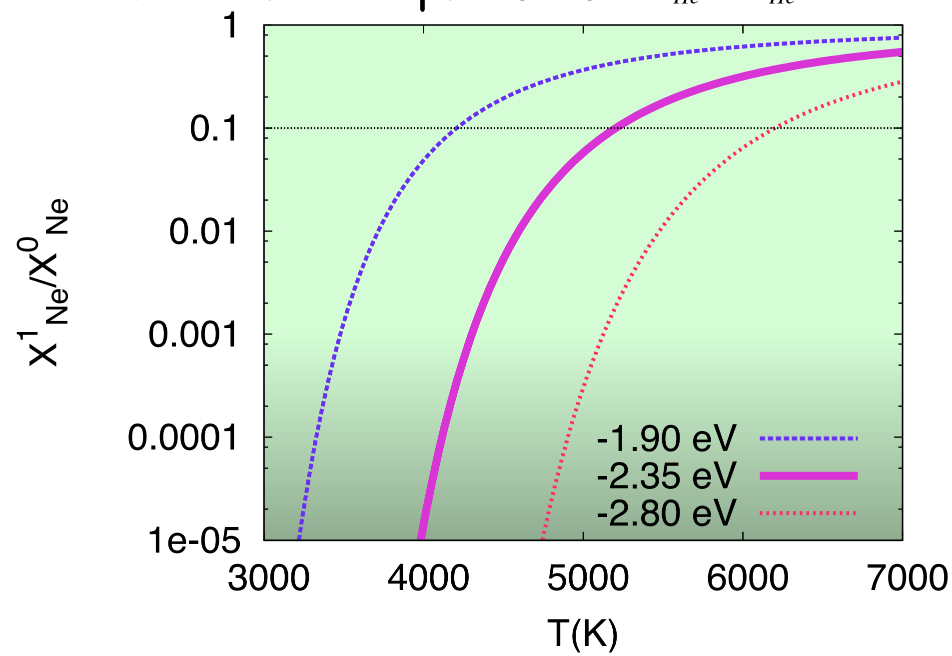
# Neon depletion is consistent with helium depletion in Jupiter

Roulston and Stevenson (1995)

$$\frac{dX_{Ne}}{dt} = X_{He} \exp\left(\frac{\Delta G}{k_B T}\right) \frac{dX_{He}}{dt}$$

Neon depletion vs temperature at fixed helium depletion of $X^0_{He} - X^1_{He} = 1.2\%$




Quantitative agreement between:

- 1.2% reduction in helium from solar.
- 9-fold reduction in neon from solar.
- ΔG=−2.35eV at 5000K

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SONNENSYSTEM

## Helium wäscht Edelgas aus den Jupiterwolken

Die Jupitersonde Galileo hat Planetologen vor rund 15 Jahren viele Erkenntnisse geliefert und ein paar neue Rätsel aufgegeben. Eines glauben sie nun gelöst zu haben: Die Frage, warum in der Atmosphäre des Gasriesen nur ein Zehntel der Menge des Edelgases Neon zu finden ist, die im Baumaterial des Sonnensystems ursprünglich enthalten war. Laut Hugh Wilson und Burkhard Militzer von der University of California in Berkely belegen Modellrechnungen, dass eine Art Edelgasregen auf Jupiter verantwortlich ist.

universo a la vista

SOBRE LAS ACTIVIDADES, LA INVESTIGACION Y LOS DESCUBRIMIENTOS EN ASTRONOMIA

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MARTES 23 DE MARZO DE 2010

## La lluvia de helio en Júpiter explica la falta de neón en la atmósfera

En la Tierra, el helio es un gas utilizado para mantener a flote los globos. En el interior de Júpiter, sin embargo, las condiciones son tan extrañas que, según las predicciones de los científicos de la Universidad de California Berkeley, el helio se condensa en gotas y cae como lluvia.

SELECCION DE NOTAS

Informe especial: Alquimia cósmica en el laboratorio

El experimento de Rutherford en el siglo 21

Maxwell y el arte de

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Tuesday 23rd March, 2010

## Helium rain explains scarcity of neon in Jupiter's atmosphere

ANI Tuesday 23rd March, 2010

In a new research, scientists at the UC (University of California) Berkeley, US, have suggested that helium rain is the best way to explain the scarcity of neon in the outer layers of Jupiter.

Former British cabinet ministers Stephen Byers, Patricia Hewitt, and Geoff Hoon have been suspended amid claims the trio have been trying to sell their influence for profit through lobbying arrangements.

Neon dissolves in the helium raindrops and falls towards the deeper interior where it re-dissolves, depleting the upper layers of both elements, consistent with observations.

"Helium condenses initially as a mist in the upper layer, like a cloud, and as the droplets get larger, they fall toward the deeper interior," said UC Berkeley post-doctoral fellow Hugh Wilson, co-author of the research paper.

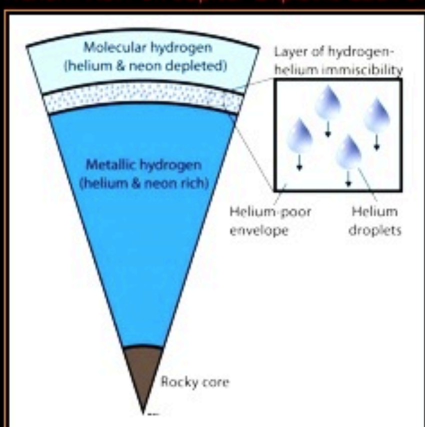
# THE MYSTERIES FROM ANCIENT CIVILIZATIONS TO THE UFO

WELCOME TO THE BLOG WHERE YOU CAN FIND NEWS FROM THE WEB ABOUT EVERYTHING THERE IS TO KNOW ABOUT THE MYSTERIES FROM ANCIENT CIVILIZATIONS TO THE UFO,THROUGH NIBIRU-PLANETX, SPACE,TO 2012 AND OTHER,WITH THE MYSTERIES ASSOCIATED TO THEY,TILL NOW NOT KNOW."WHAT UNTIL YESTERDAY WAS UNKNOWN , WILL BE THE KNOWLEDGE OF TODAY"!



WEDNESDAY, MARCH 24, 2010

## Helium Rain on Jupiter Explains Lack of Neon in Atmosphere




A slice through the interior of Jupiter shows the top layers that are depleted of helium and neon, the thin layer where helium drops condense and fall, and the deep interior where helium and neon again mix with metallic hydrogen. (Credit: Burkhard Militzer/UC Berkeley)

#sustainability

## Bill Gates building nuclear reactor (but it's only a little one)

EMMA WOOLLACOTT | Tue 23rd Mar 2010, 08:48 am

Bill Gates (yes, really) and Toshiba are reported to be building a next-generation nuclear reactor.

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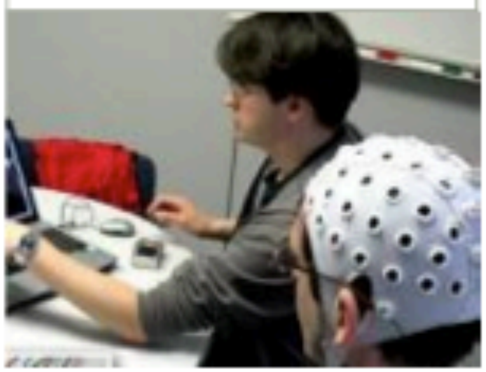
#communication



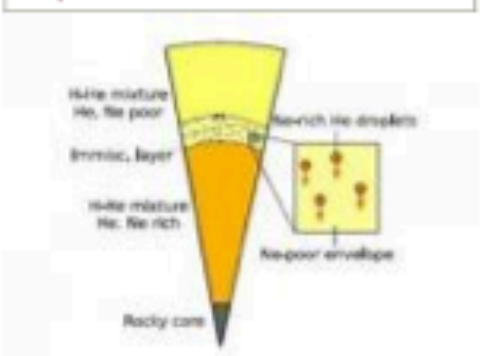
## Portable mind-reader lets users write with their thoughts

EMMA WOOLLACOTT | Tue 23rd Mar 2010, 07:28 am

European scientists have developed the first portable device that allows users to type merely by thinking.

---

#space

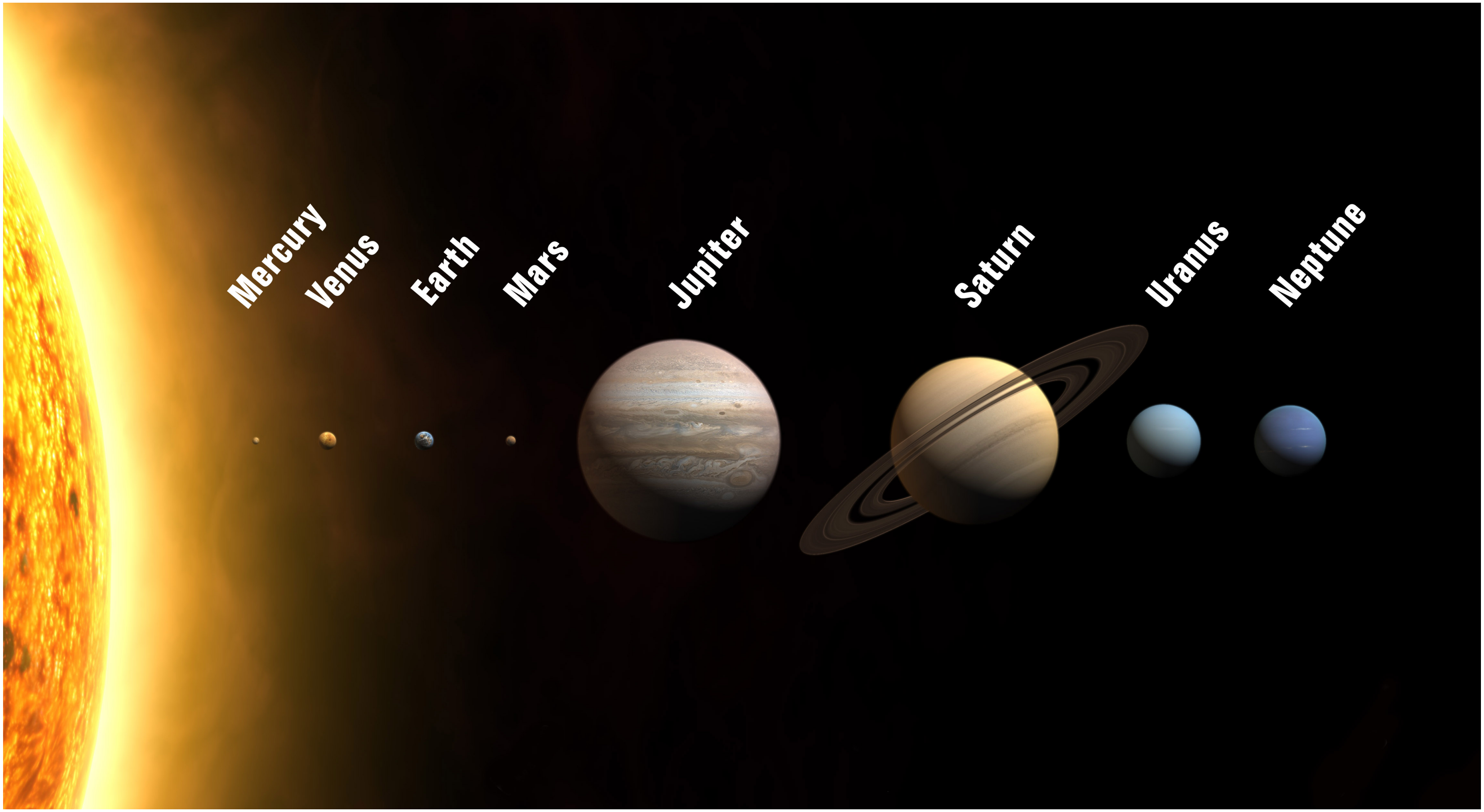



## Helium falls like rain on Jupiter

EMMA WOOLLACOTT | Tue 23rd Mar 2010, 05:38 am

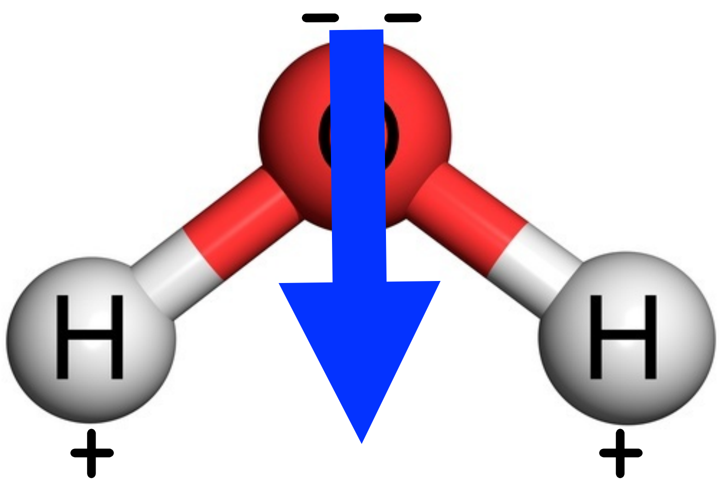
New research suggests that it's raining helium in the interior of Jupiter. UC Berkeley scientists reckon this is the best way to explain why there's so much less neon in the outer layers of the planet than predicted.

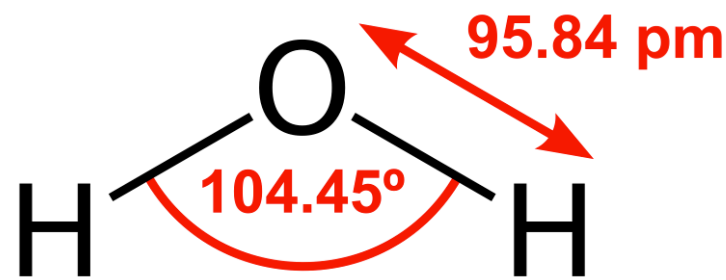
# Why grew the giant plants so large while all terrestrial planets stayed small? Because they form beyond the ice line.

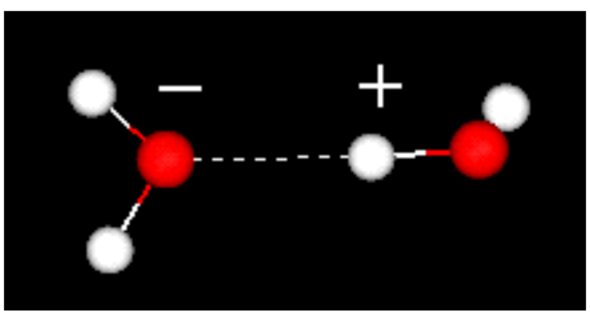


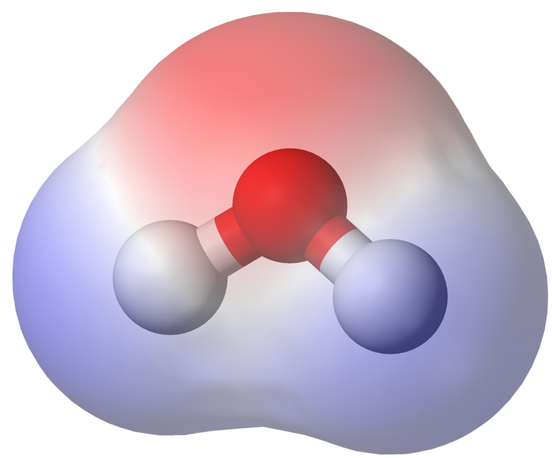
# III. New Phases of Water Ice

# Properties of the Water Molecule

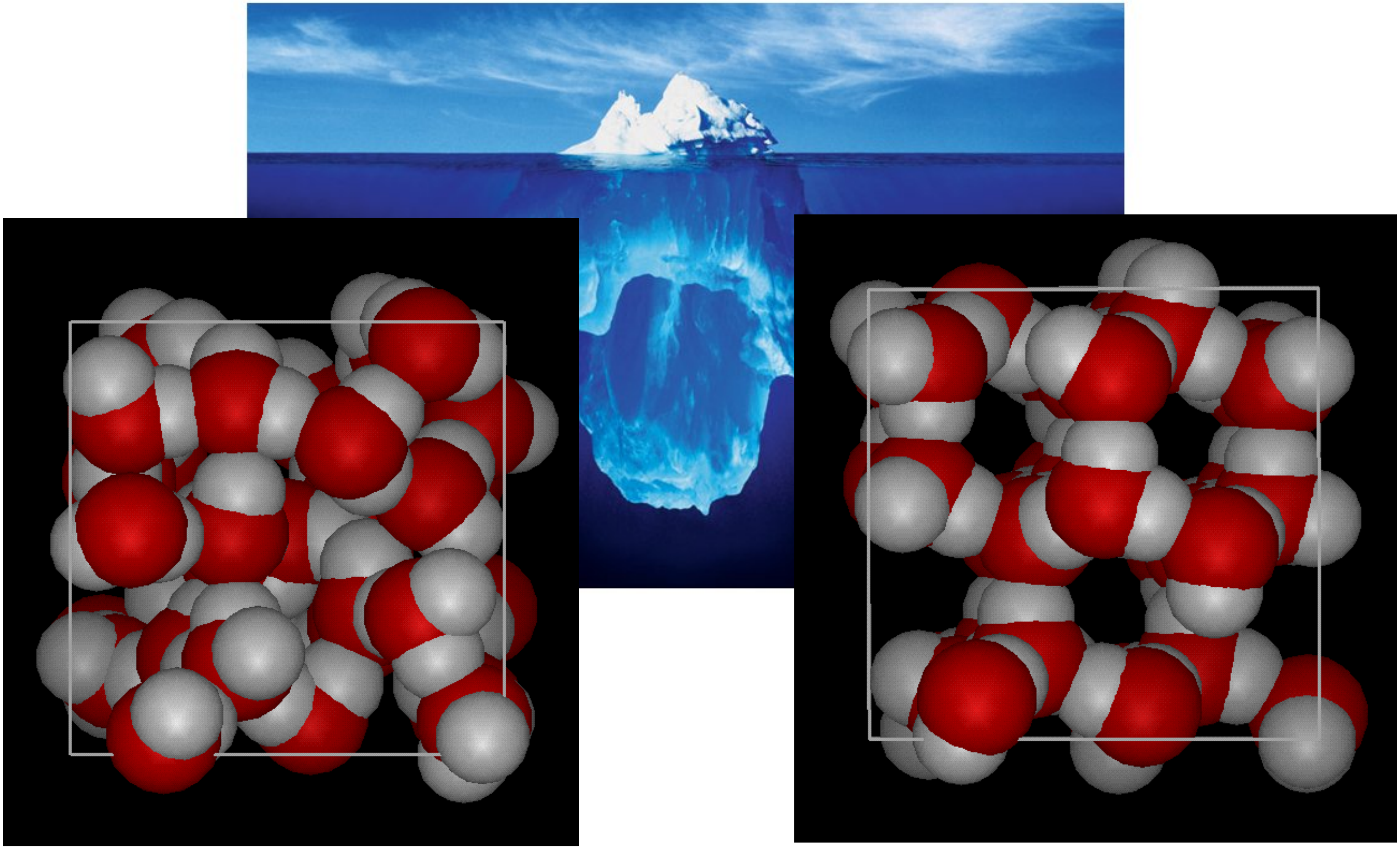


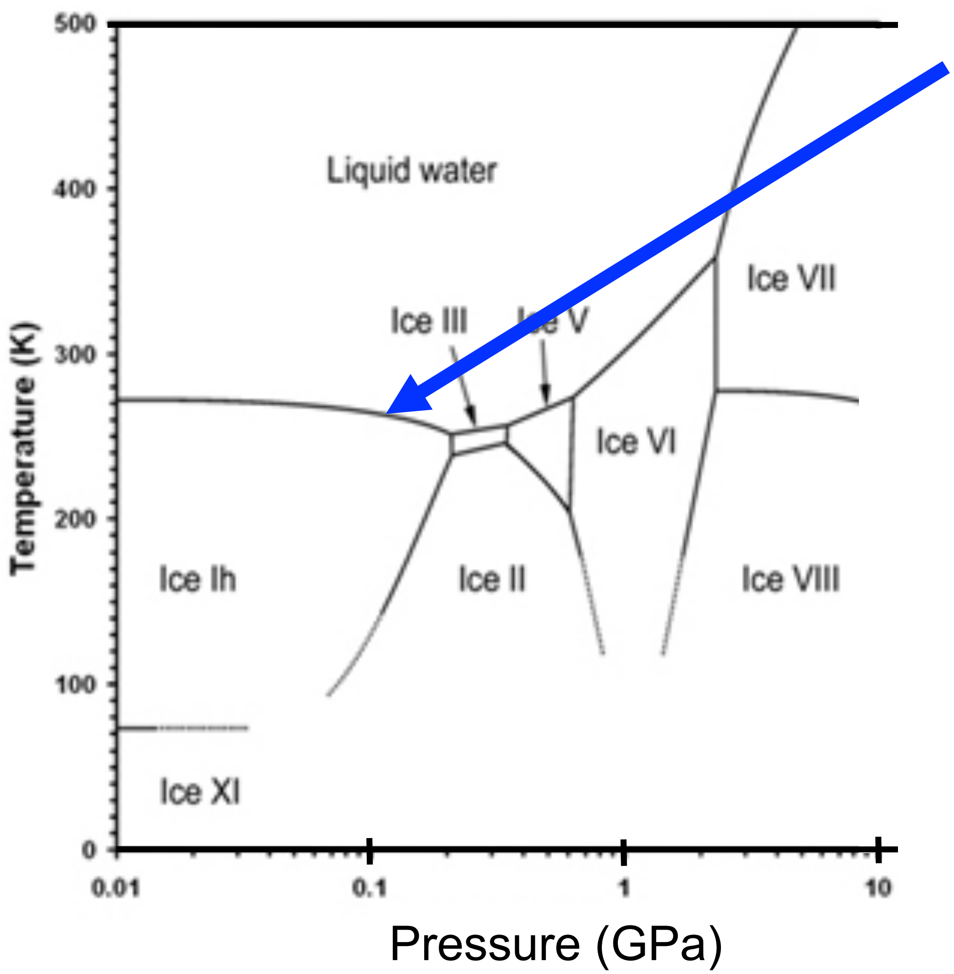



# Why is Water Denser Than Ice?



Other examples where liquid is denser than the solid:
silicon, gallium, germanium, antimony, bismuth, plutonium

# Phase Diagram of water ice

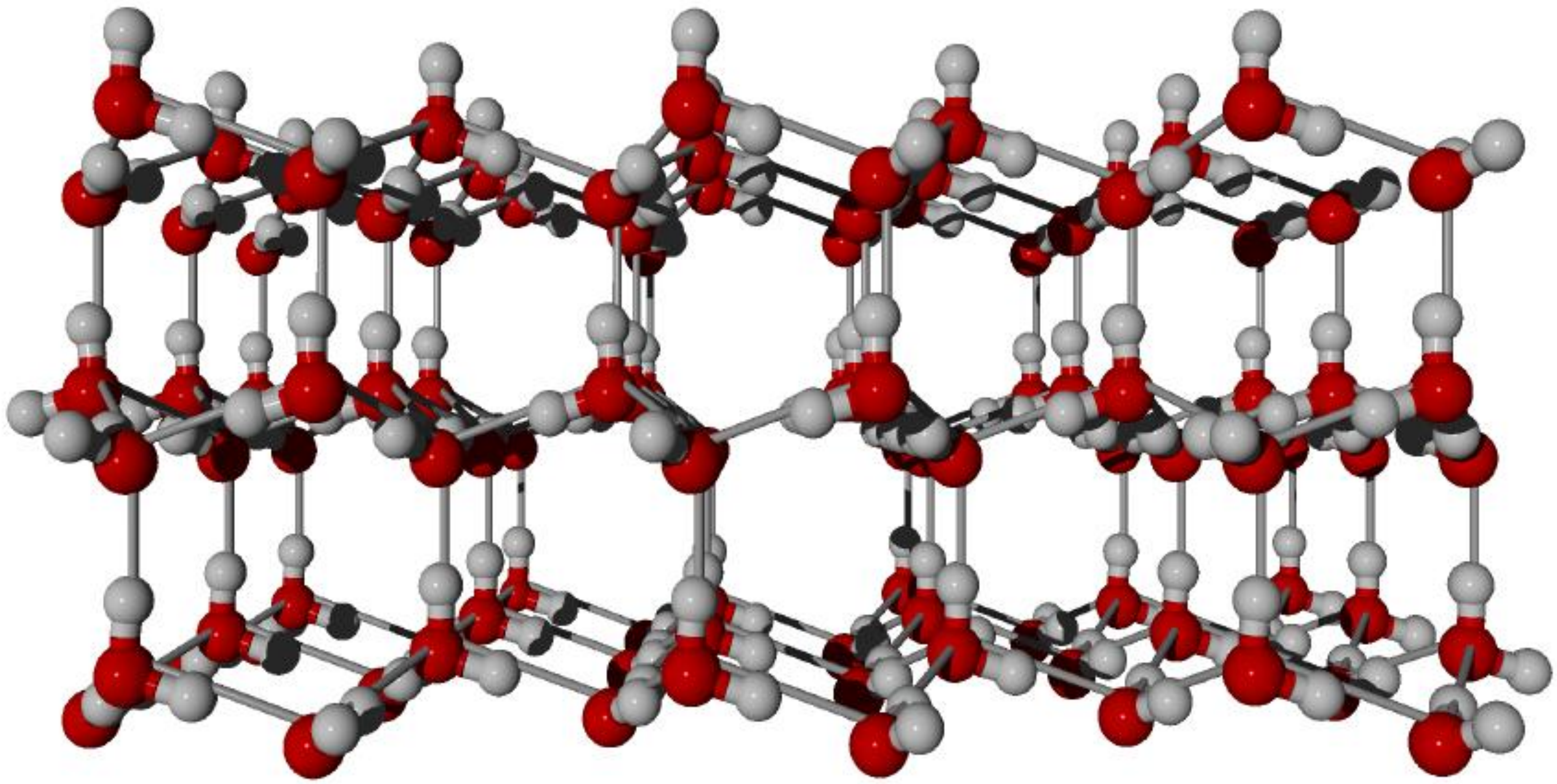



Ice 1h has negative Clapeyron slope:

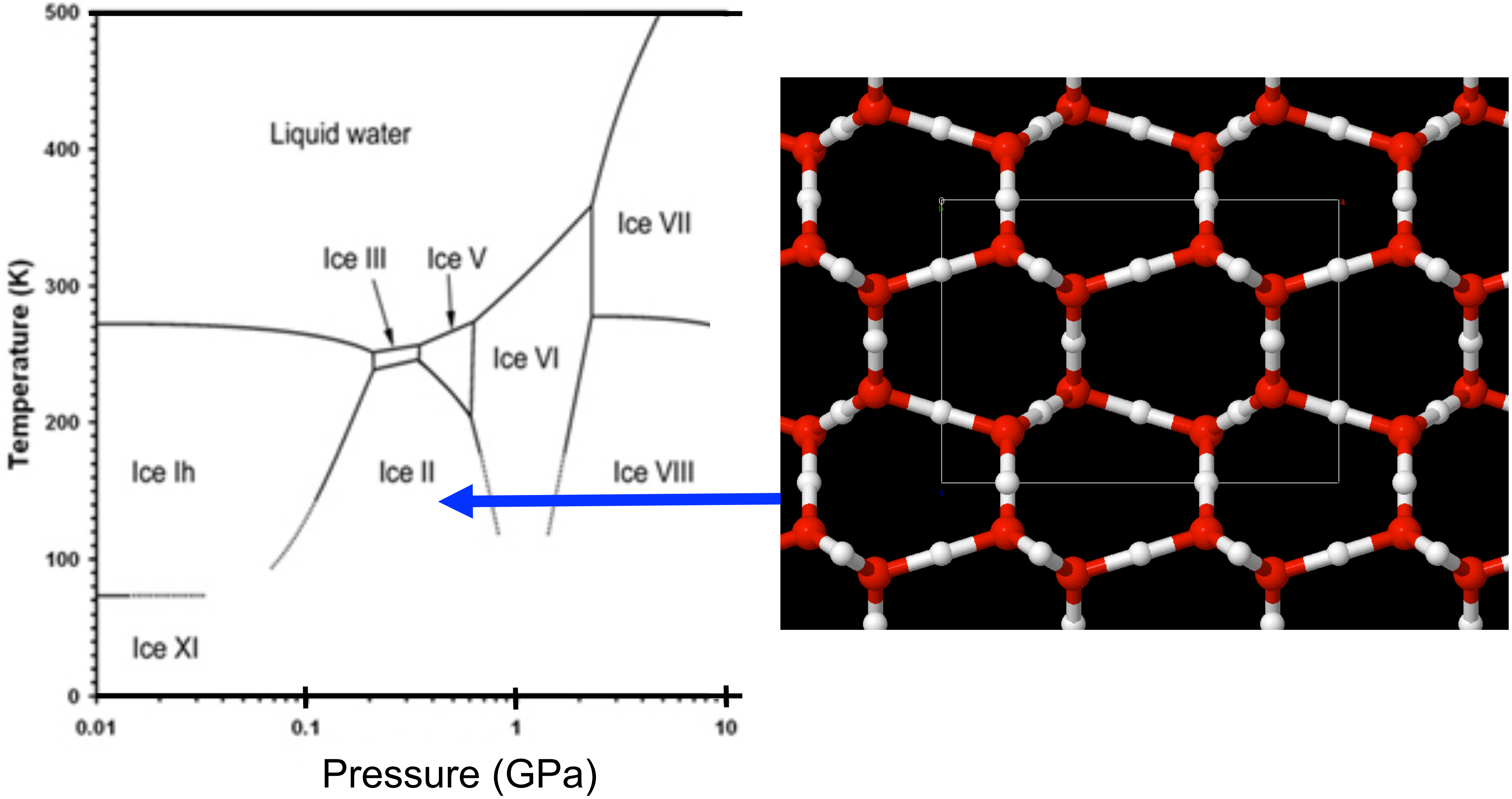
$$\frac{dT_{melt}}{dP} = \frac{V_{liquid} - V_{solid}}{S_{liquid} - S_{solid}} = \frac{\Delta V < 0}{\Delta S > 0} < 0$$

$G(\mathrm{P,T}) = \mathrm{E+PV-TS}$

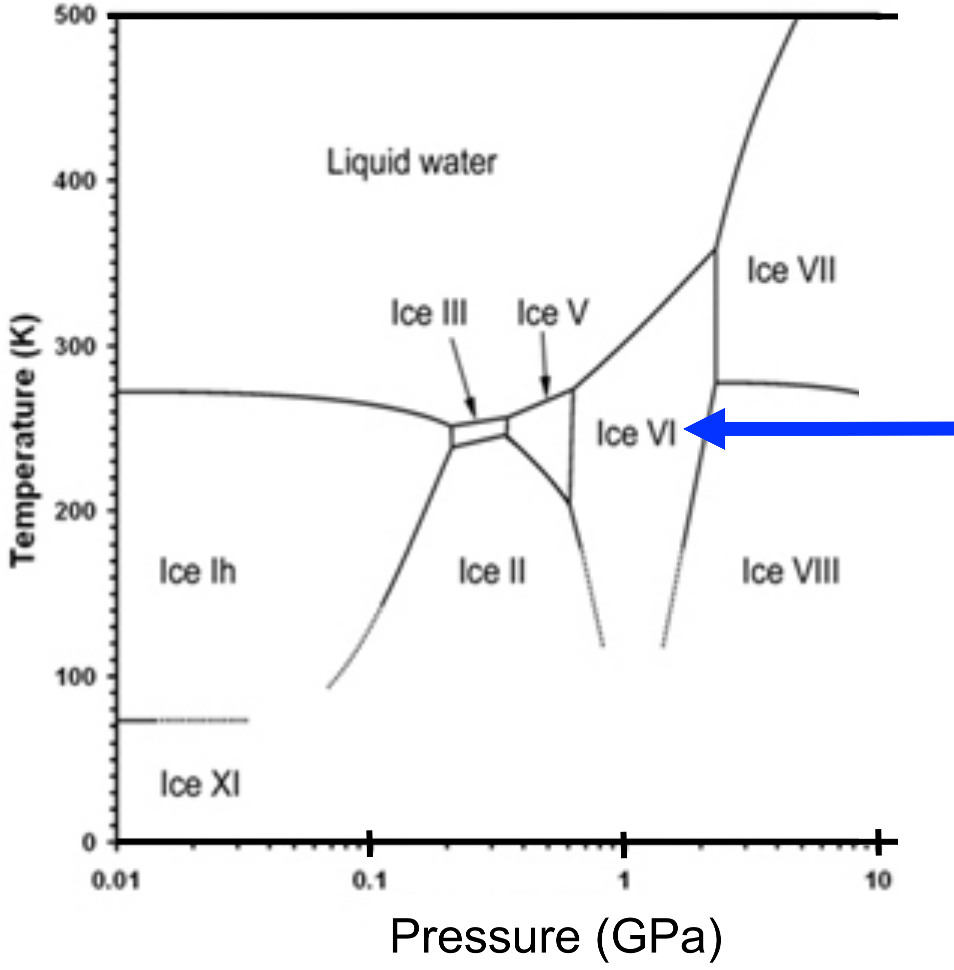
# The Ice in Your Freezer is Hexagonal: Ice 1h

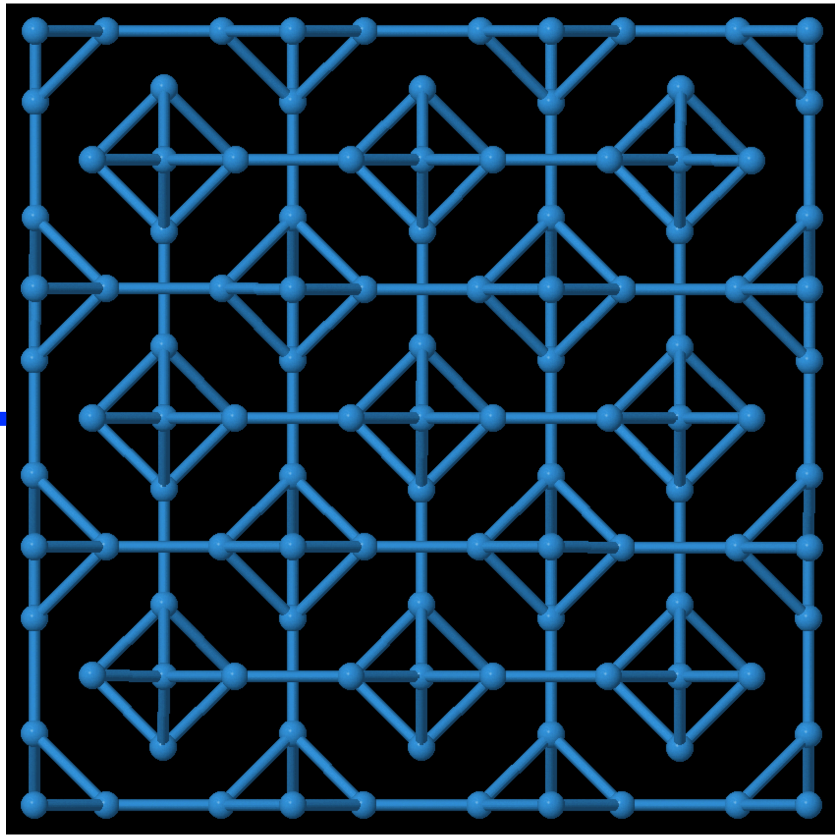


# Ice II is rhombohedral (Unit cell angles α=β=γ=90°)



# Ice VI is a self-clathrate

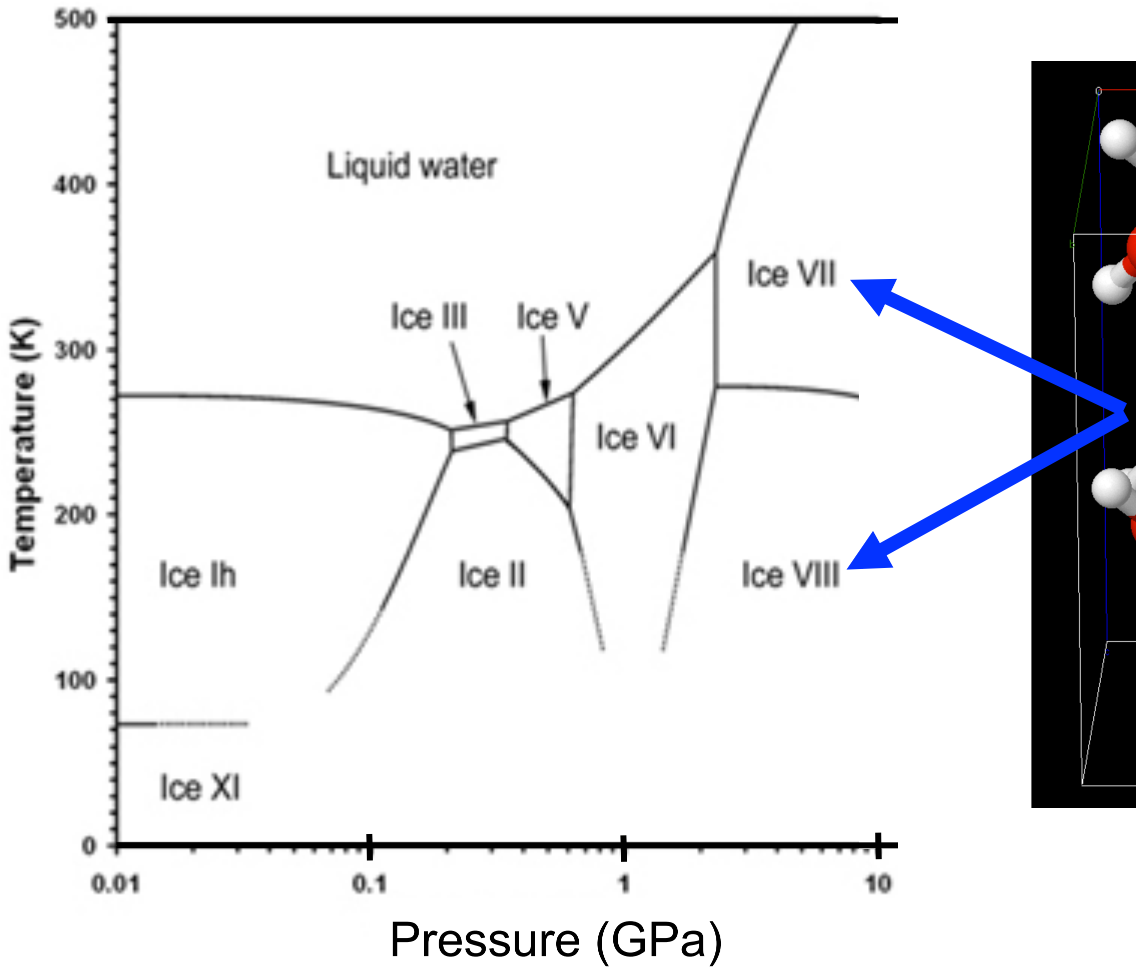


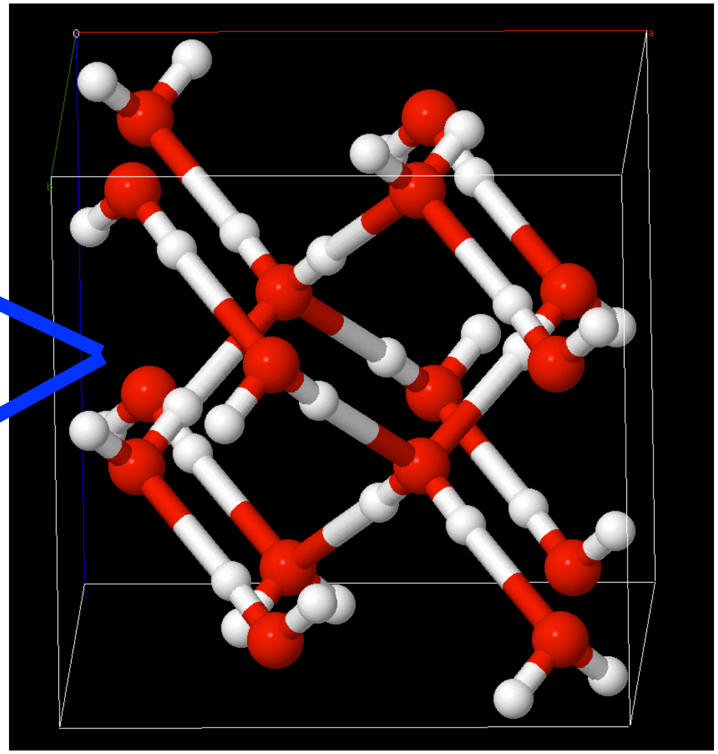



# Pauling's Ice Rules

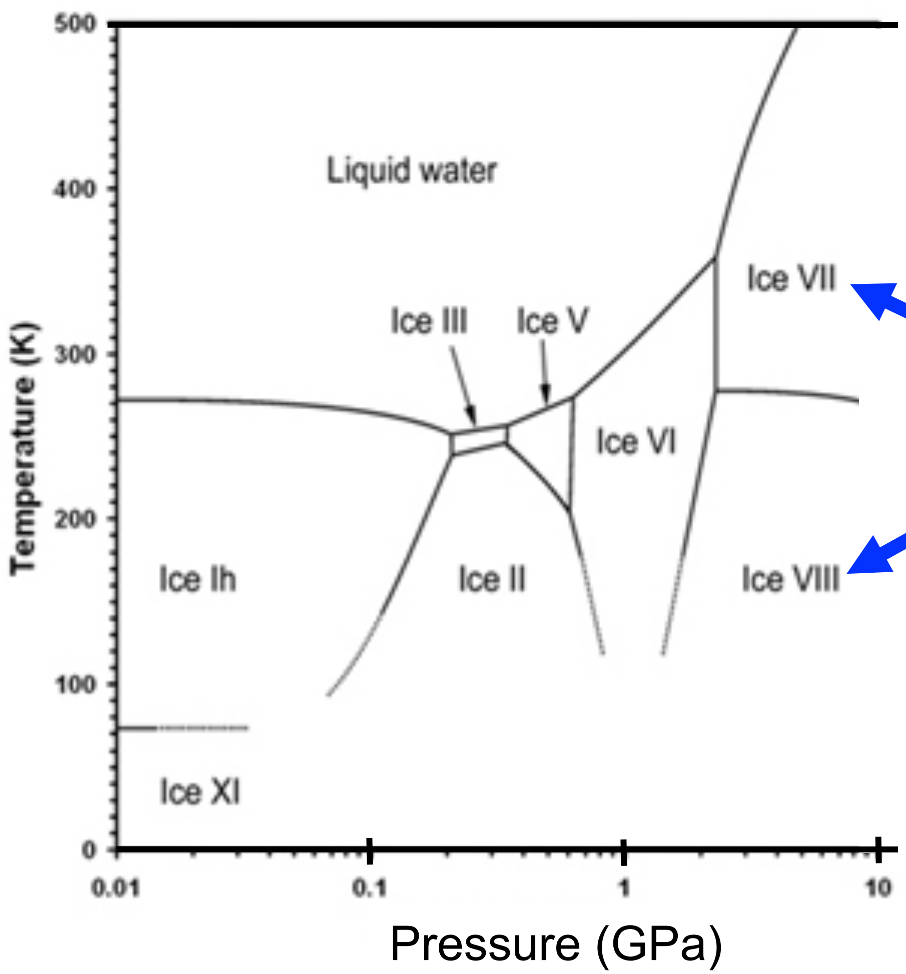
1) Every oxygen atom has two covalent bonds
2) Every oxygen atom has two hydrogen bonds (tetrahedral coordination)
3) In between two oxygen atoms, there can only be one H atom.
4) Dipole moment of the unit cell should be zero.

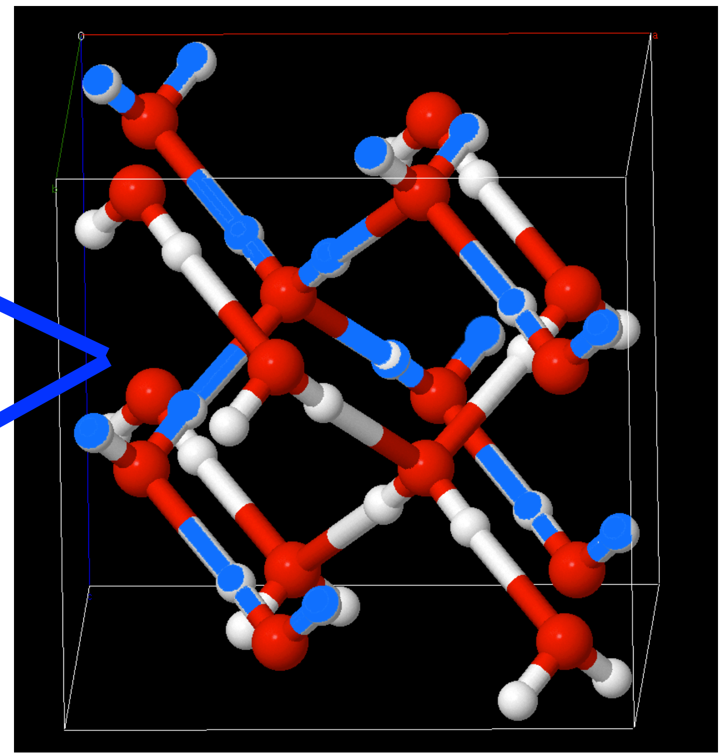
# Ice VII (proton-disordered) and Ice VIII (proton-ordered)



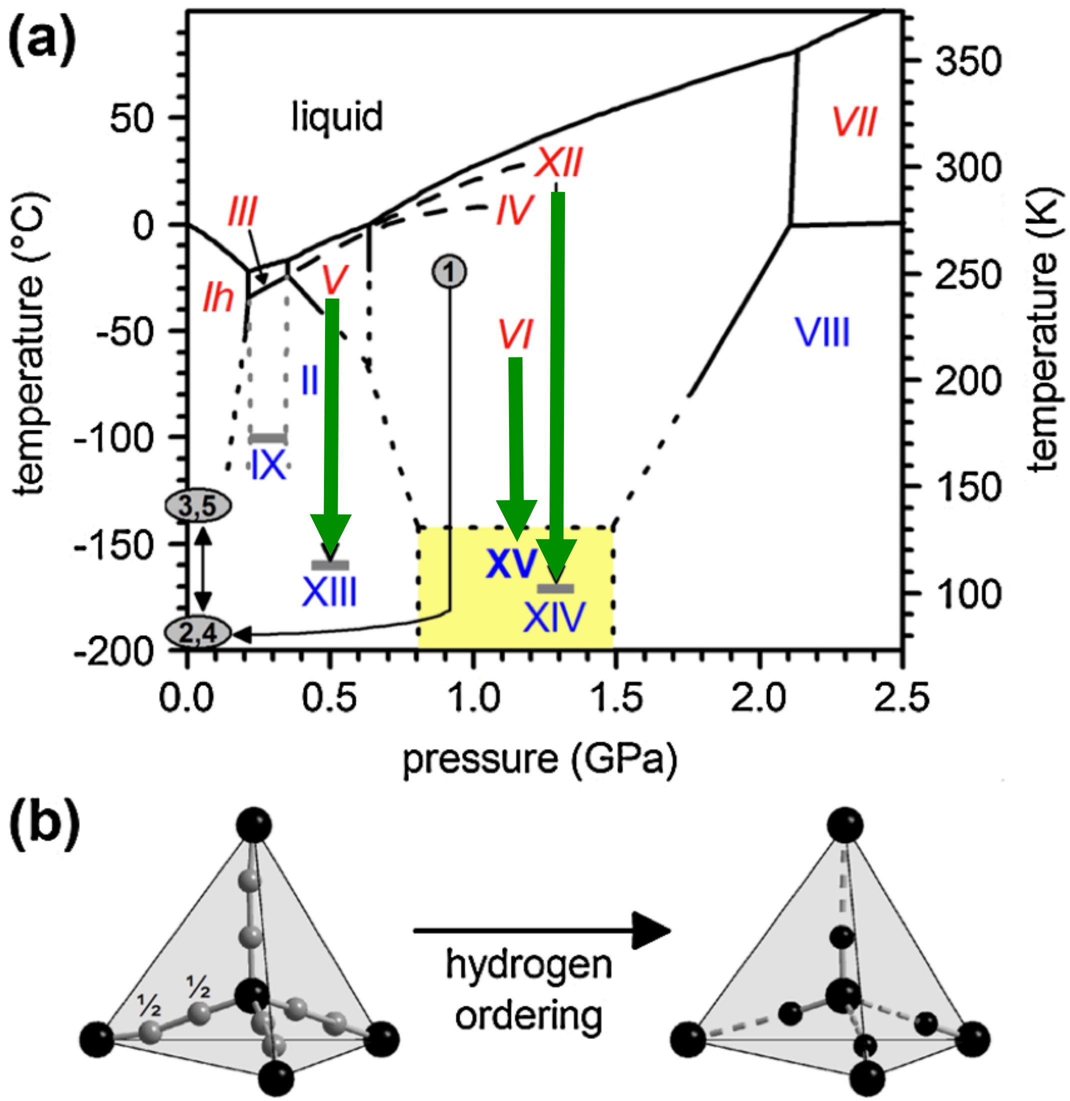



# Ice VII (proton-disordered) and Ice VIII (proton-ordered)

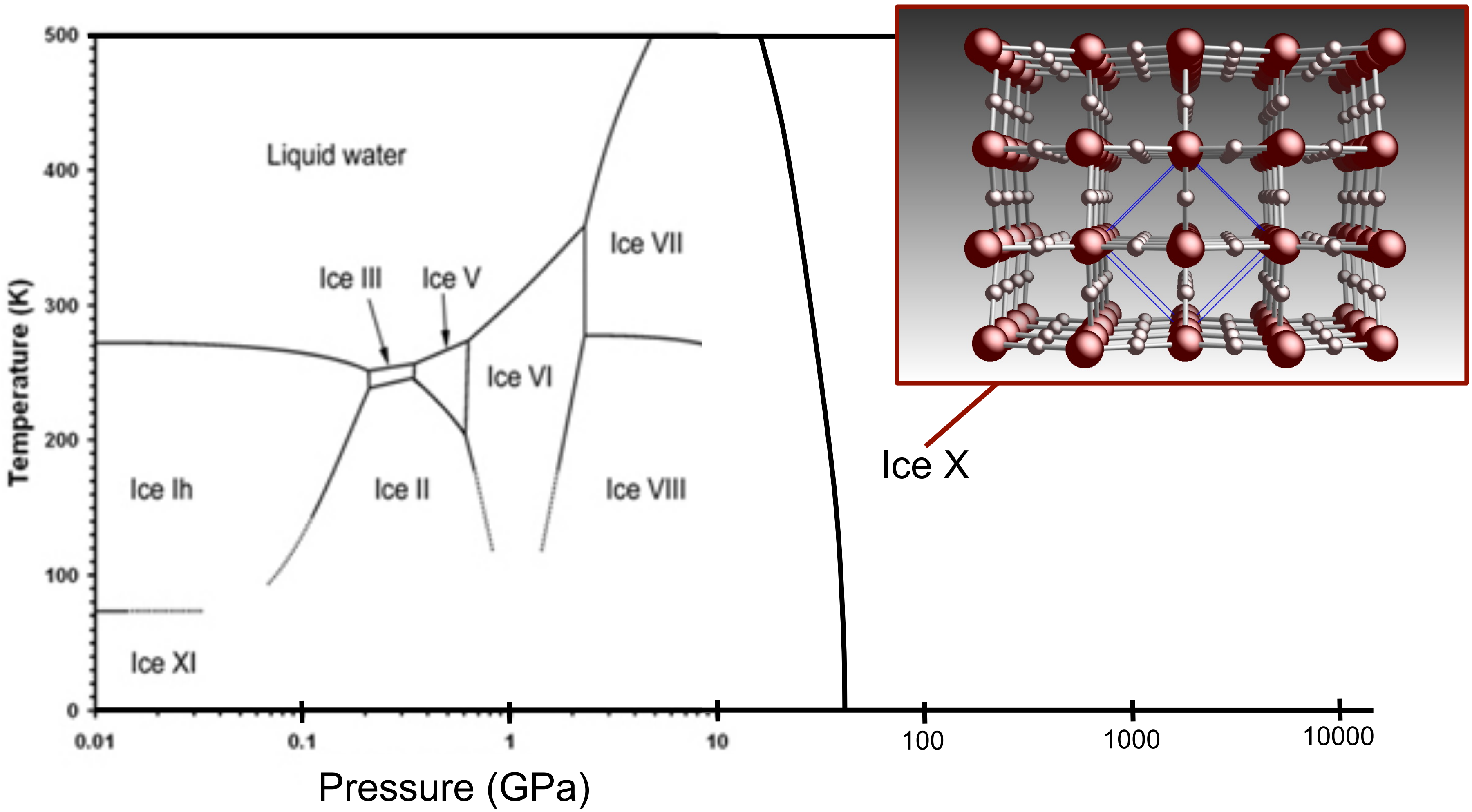


# Ice XIII, XIV, and XV all discovered by proton ordering (by adding KOH)

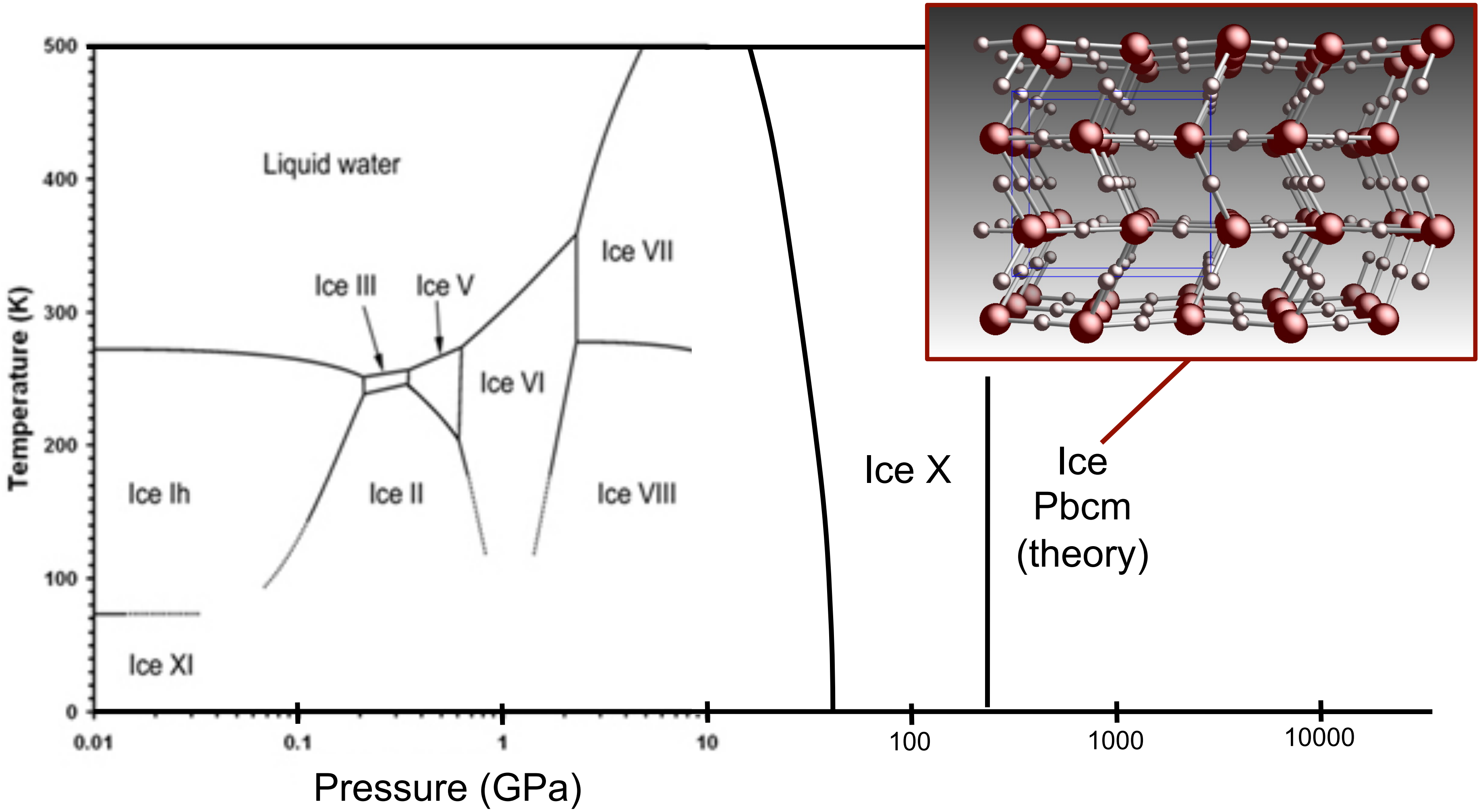


# Phase Diagram of water ice



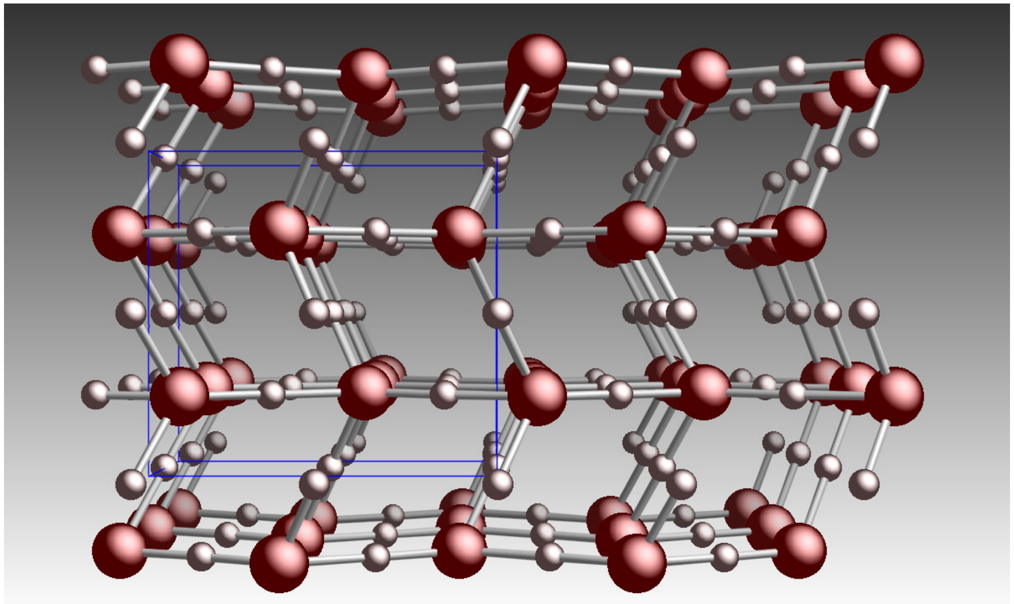

Ice X: the highest pressure phase seen in experiments.

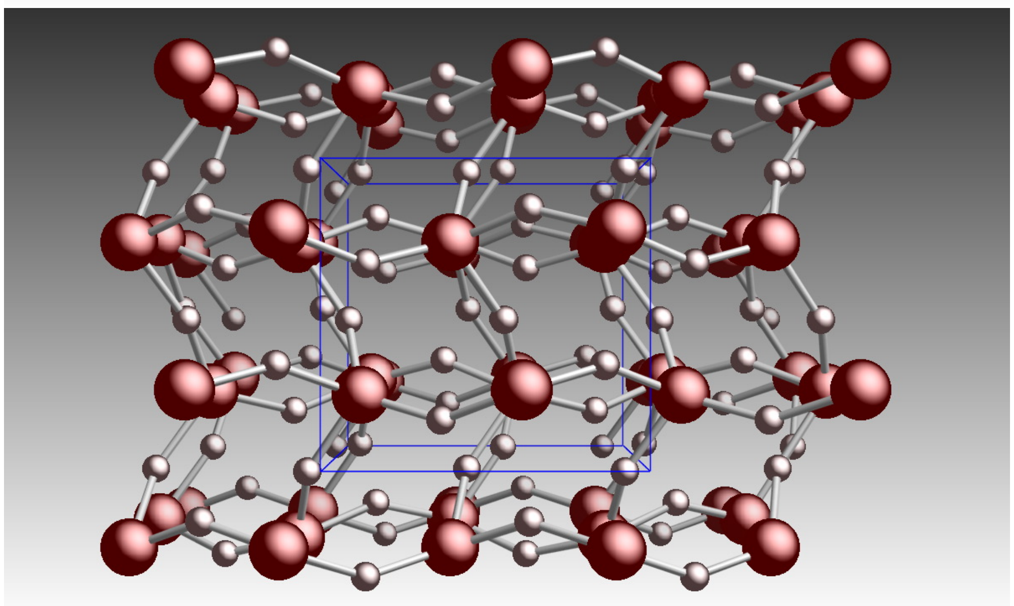
# Phase Diagram of water ice

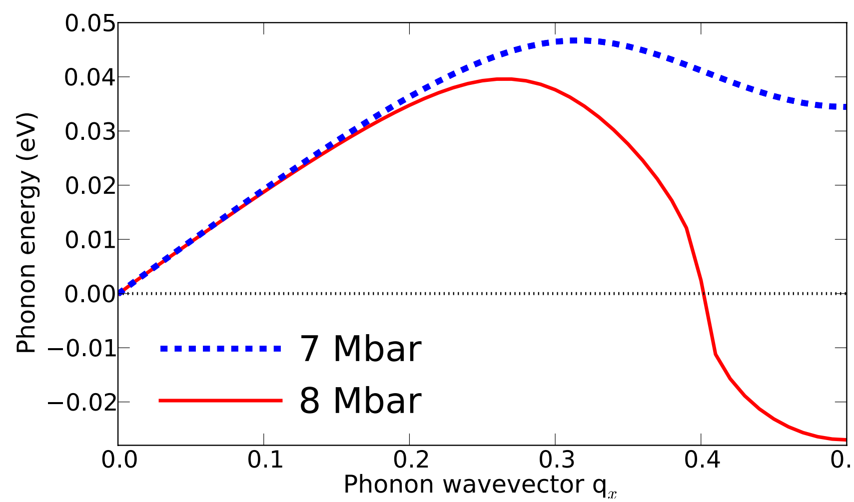



*Pbcm* phase predicted with ab initio simulations by Benoit *et al.* (1996)

# Phonon instability leads to new phase of water ice at 7.6 megabar

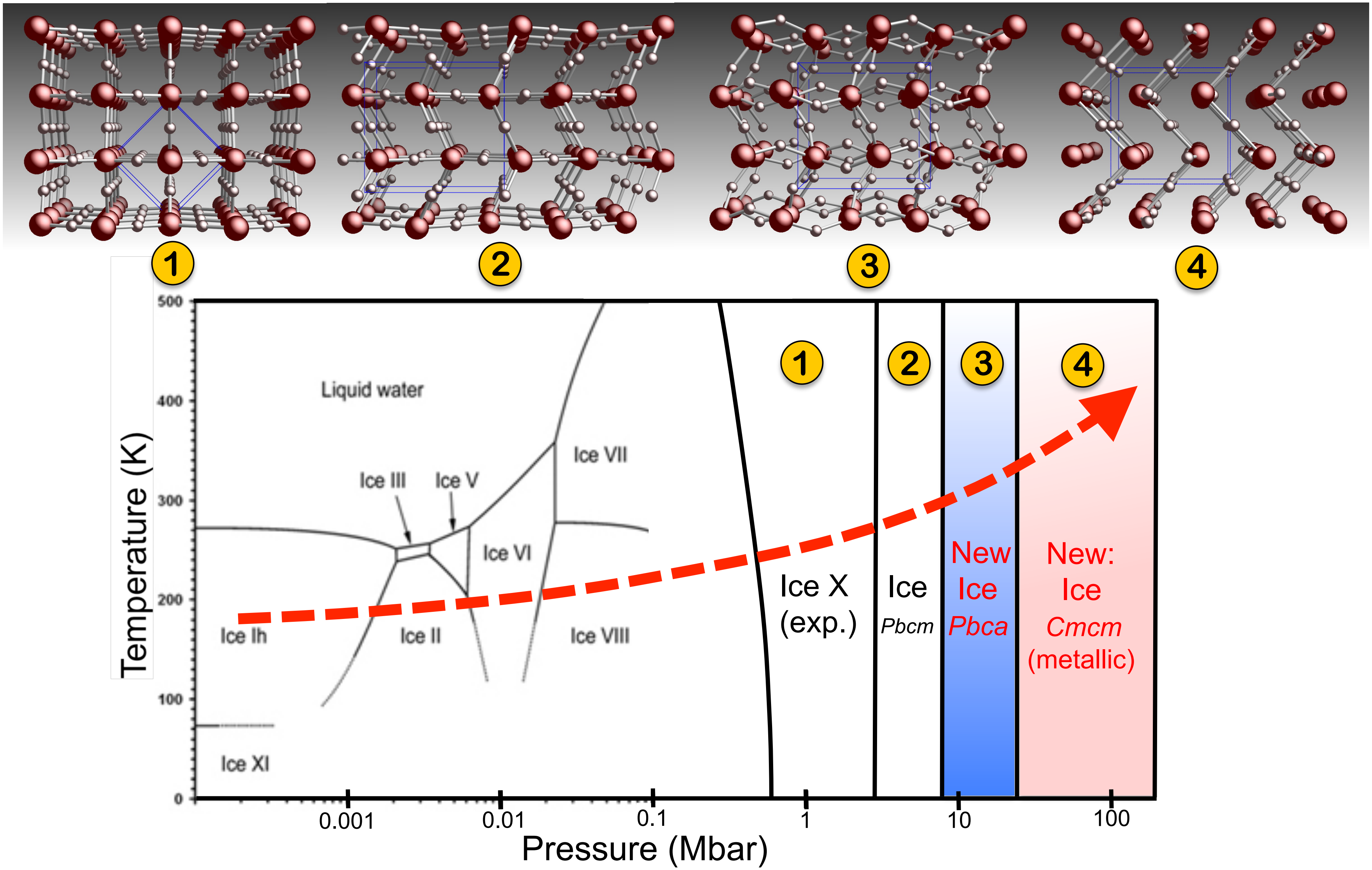






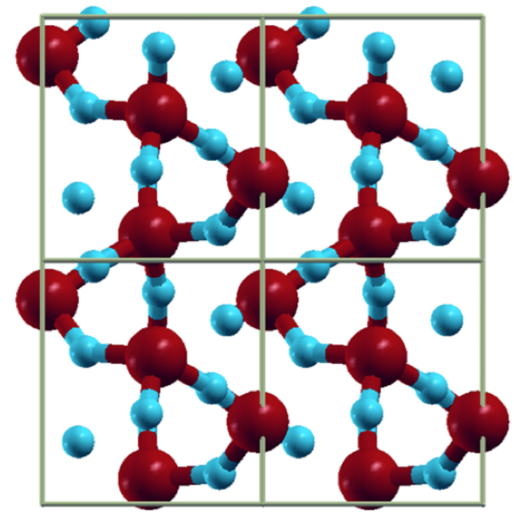

Militzer and Wilson, *PRL* 105 (2010) 195701

# Extended Phase Diagram of Water Ice



# Improved Structural Search Methods revealed six additional ice structures at yet higher pressures

| Name/Symmetry | Author,Year | Pressure (Mbar) | #mol. |
|---|---|---|---|
| Ice X (Pn-3m) | Polian,1984 | 0.44 | 2 |
| Pbcm | Benoit, 1996 | 3 | 4 |
| Pbca | **Militzer, Wilson, 2010** | 7.6 | 8 |
| I-42d | **Wang, 2011** | 8.1 | 8 |
| $P2_1$ | **McMahon,2011** | 11.7 | 4 |
| | Ji, 2011 | 11.4 | 4 |
| | Wang, 2011 | 14 | 4 |
| | Hermann, 2011 | 11.7 | 4 |
| $P2_1/c$ | **Ji, 2011** | 19.6 | 8 |
| C2/m (metallic) | **McMahon, 2011** | 56.2 | 2 |
| | Hermann, 2011 | 60 | 2 |
| $P2_1/m$ | **Zhang, Militzer, 2012** | 135 | 4 |
| I4/mmm | **Zhang, Militzer, 2012** | 330 | 2 |

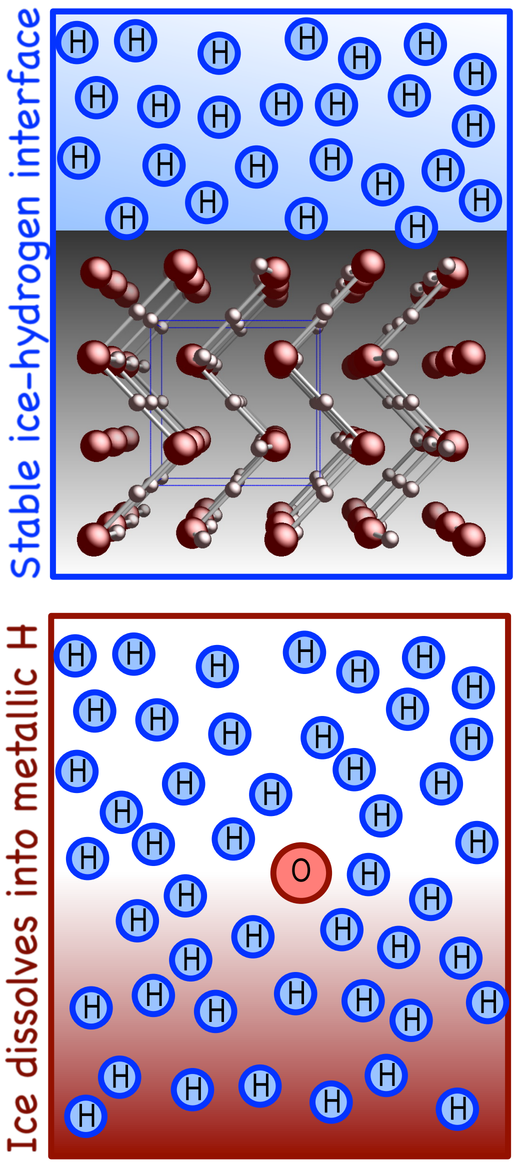


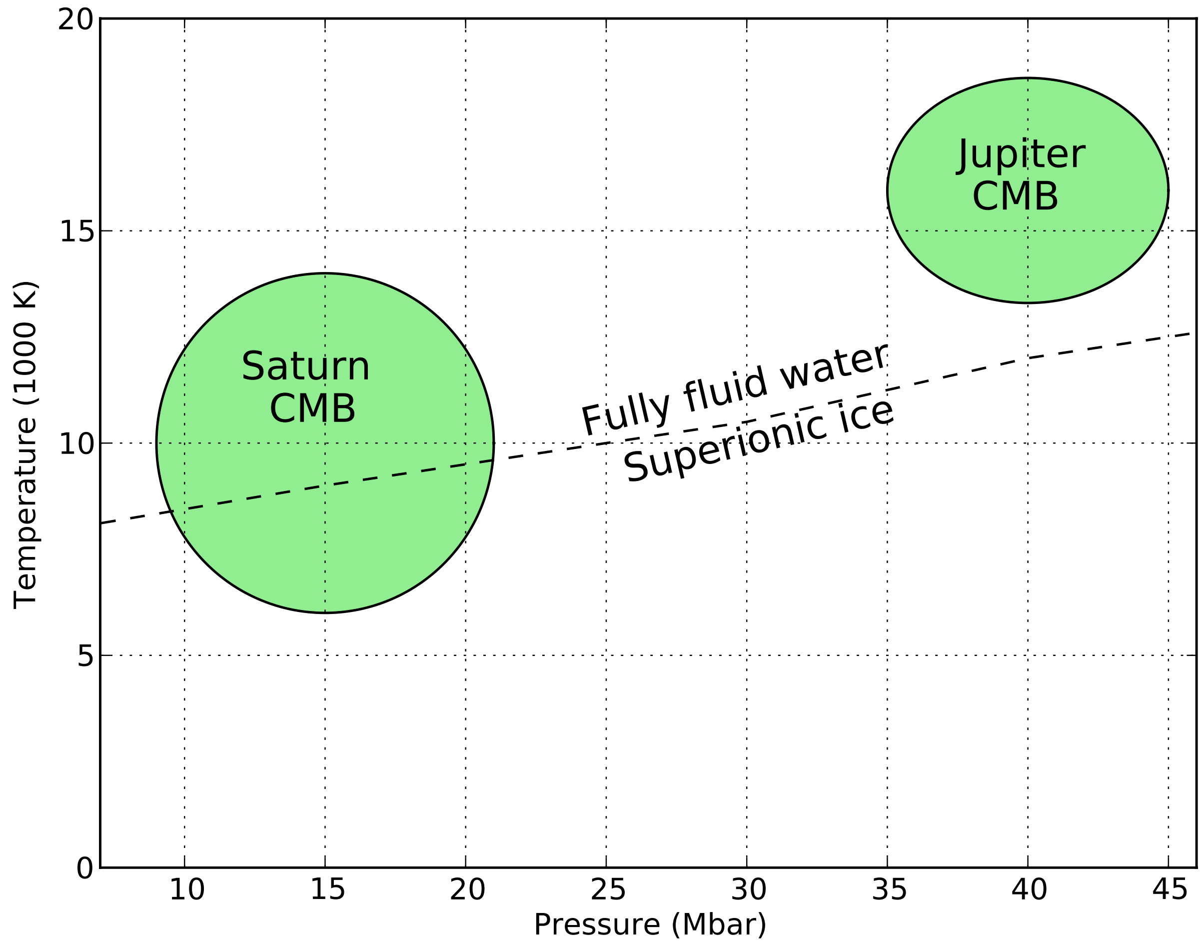
$P2_1$ symmetry


**Militzer, Wilson, PRL *105*, 195701 (2010)**.
Wang et al., *Nature Commun.*, *2*, 563 (2011).
McMahon, PRB *84*, 220104(R) (2011).
Ji et al., PRB, *84*, 220105(R) (2011).
Hermann et al., PNAS *109*, 745 (2011)
**Zhang, Wilson, Driver, Militzer,** arXiv:1209.3448

# IV. Is Ice Stable in Cores of Giant Planets?

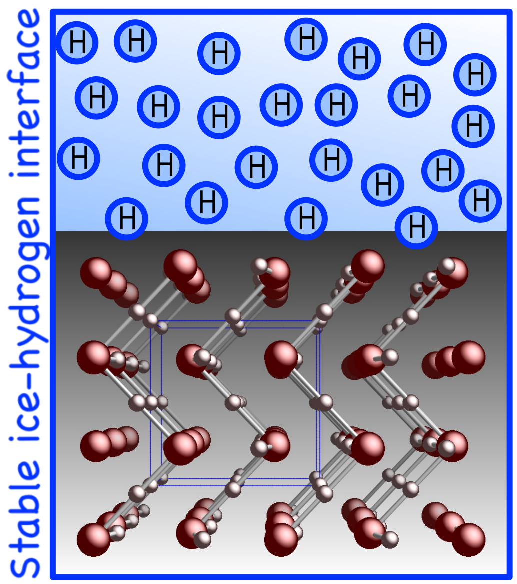
# Is the interface between ice and metallic hydrogen stable in giant planet cores?

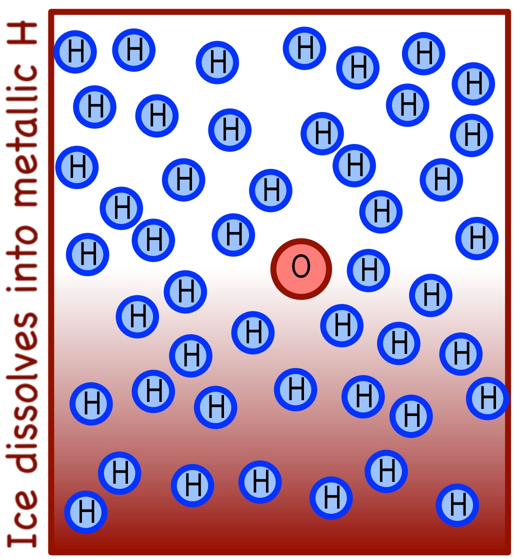


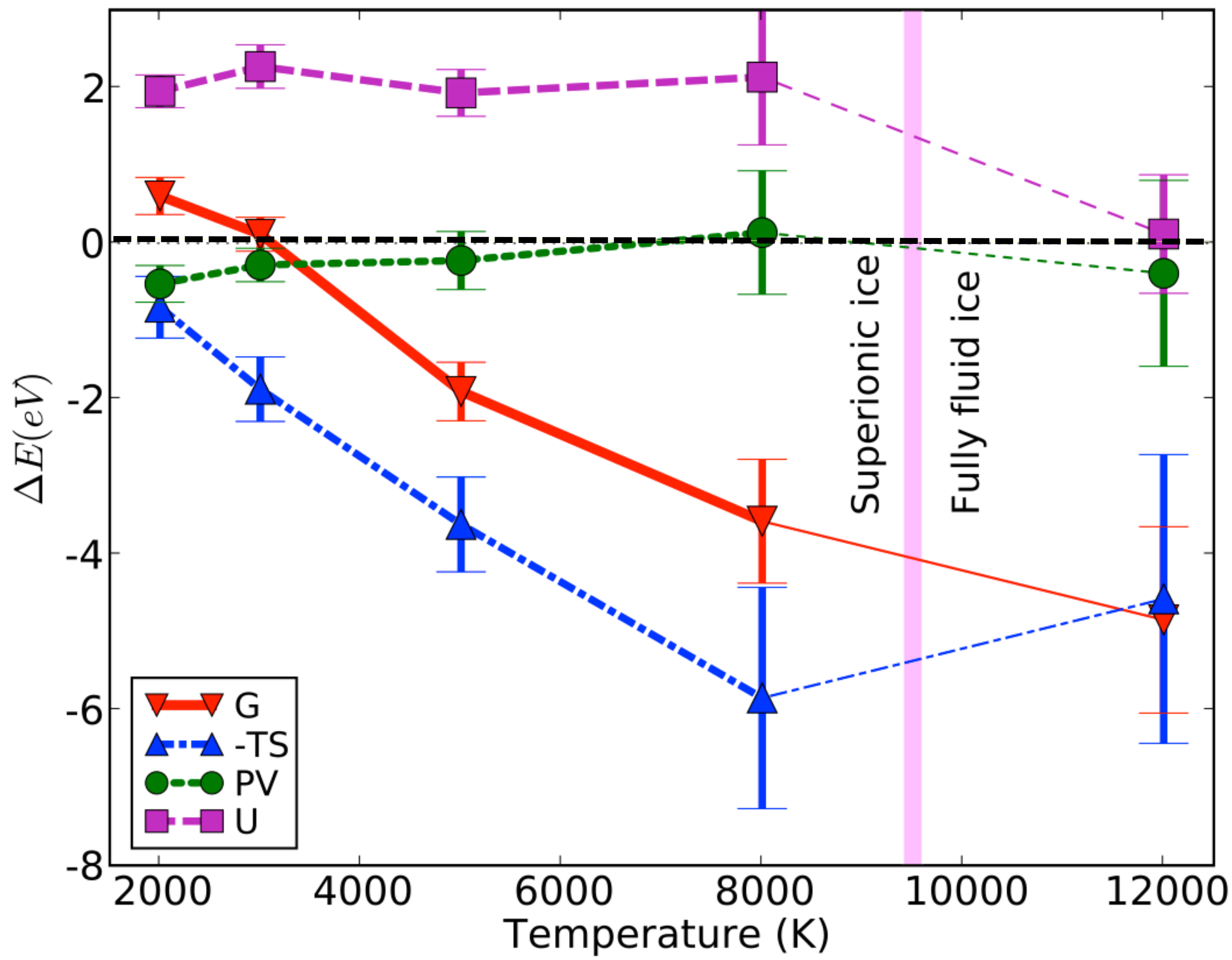




Wilson and Militzer, Astrophys. J. 745 (2012) 54

# Analysis of Gibbs Free Energy differences shows ice erosion is an entropy driven process



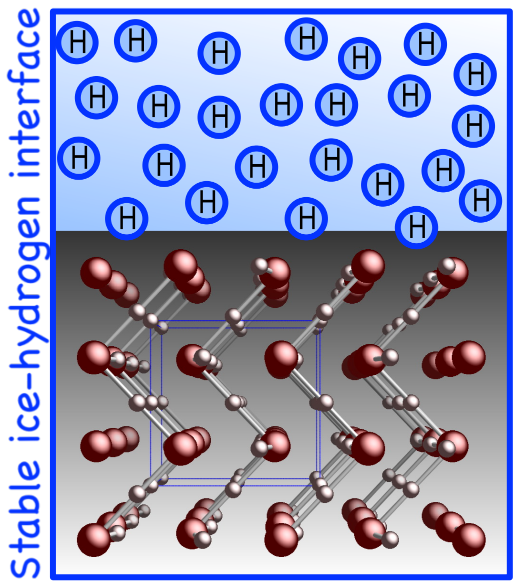



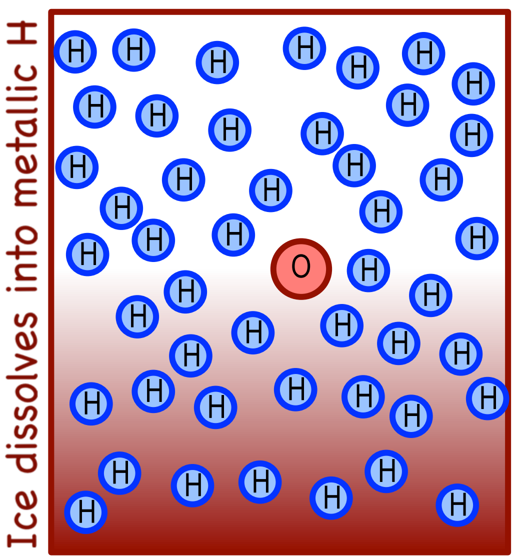



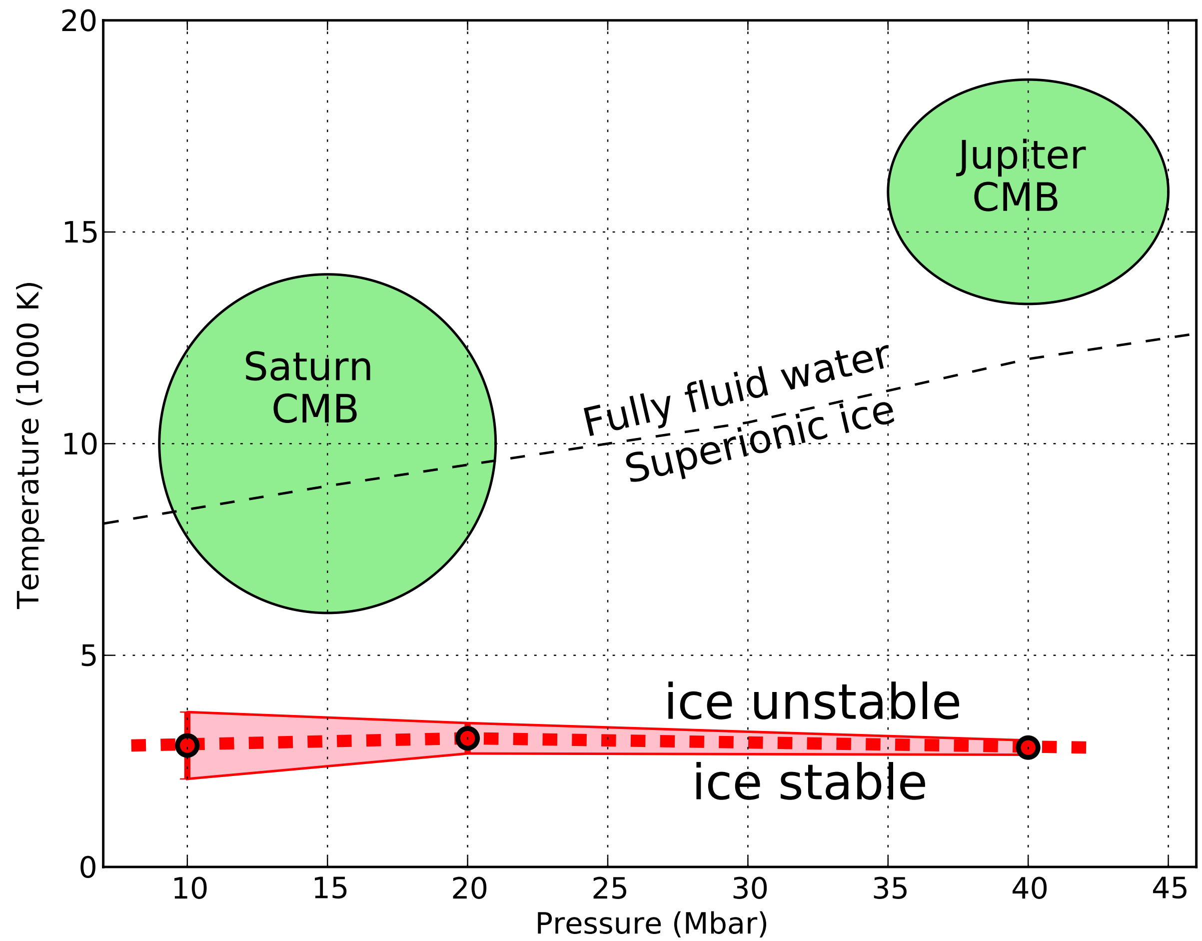

**Predict core erosion in both Saturn and Jupiter**

Wilson, Militzer, Astrophys. J. 745 (2012) 54

# Computer simulations predict erosion of icy cores in Saturn and Jupiter



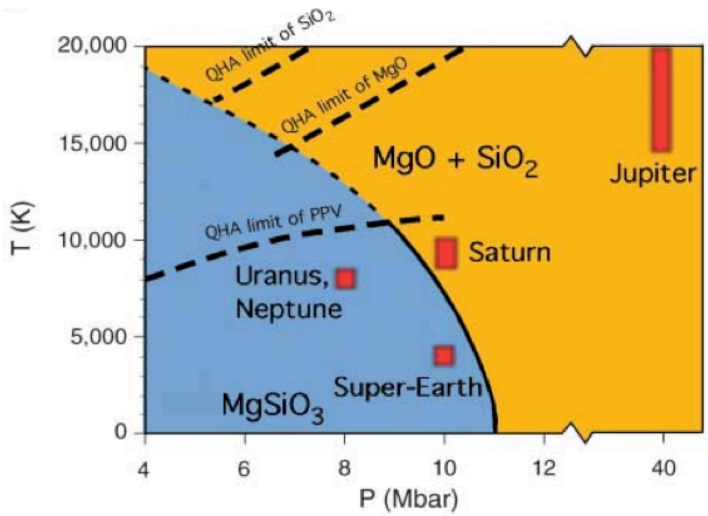



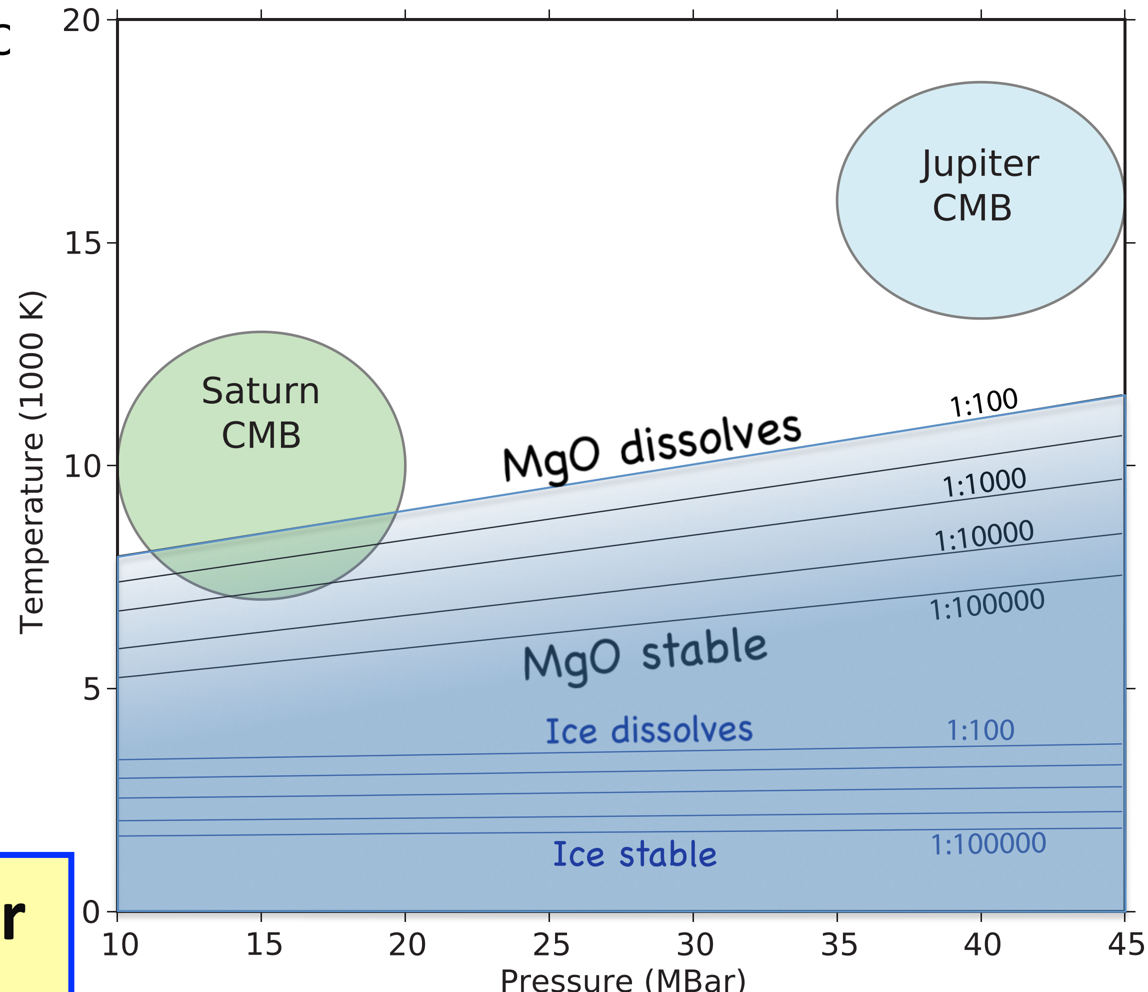

**Predict core erosion in both Saturn and Jupiter**

Wilson, Militzer, Astrophys. J. 745 (2012) 54

# Erosion of other core materials: silicates and iron

$MgSiO_3$ dissociates into $SiO_2$ and MgC at 11 Mbar (Umemoto, 2006):




**MgO dissolves in Jupiter and hot exoplanets but maybe not in Saturn.**

Wilson, Militzer, Phys. Rev. Lett. (2012)

# Implications of our Core-Erosion Calculations for Jupiter and Saturn

**Three core-erosion scenarios:**

- **Rapid in Jupiter and Saturn: homogenized envelops, core were much bigger originally**
- **Slow in J & S: inefficient up-convection, gravity wins, Juno cannot distinguish a slowly eroding core and a stable one**
- **Fast in J, slow in S: This could explain the difference in core size in the Guillot models for J and S.**

Recent core erosion model using double-diffusive convection:
Leconte and Chabrier, A&A (2012)

*The End*