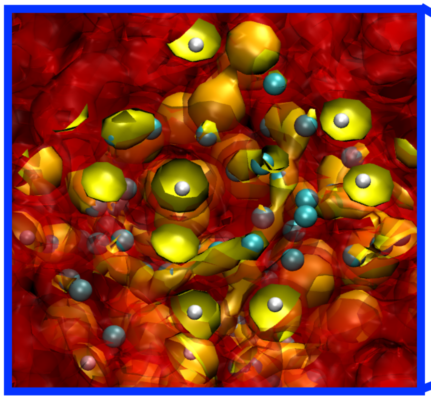
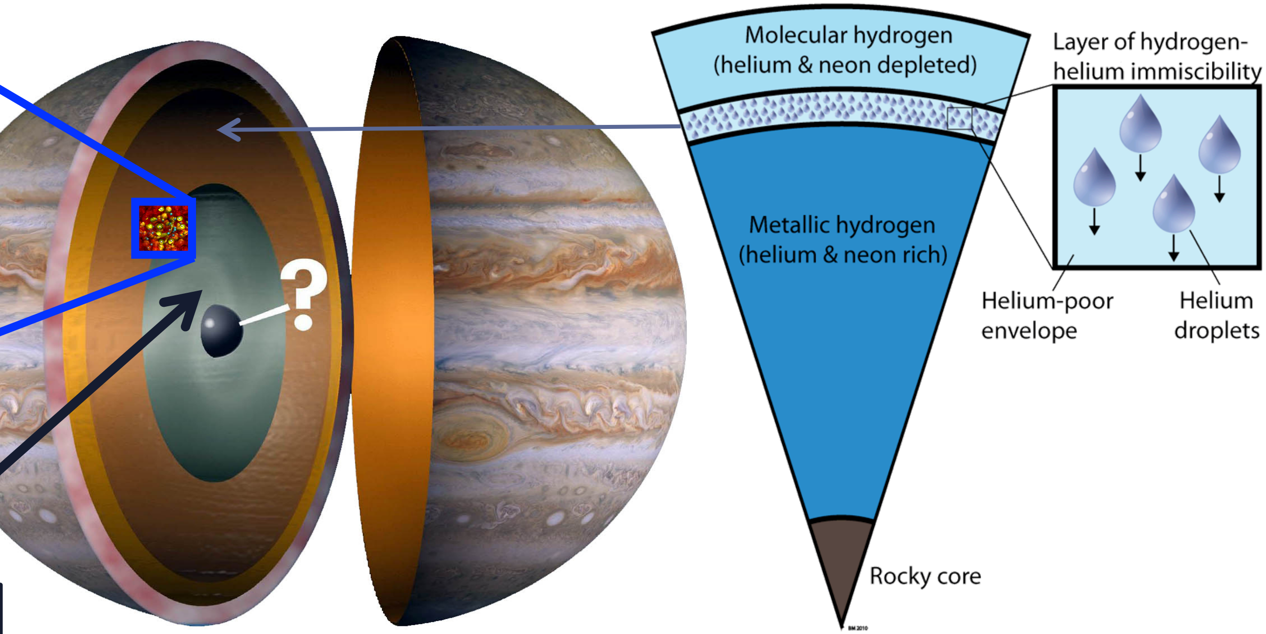
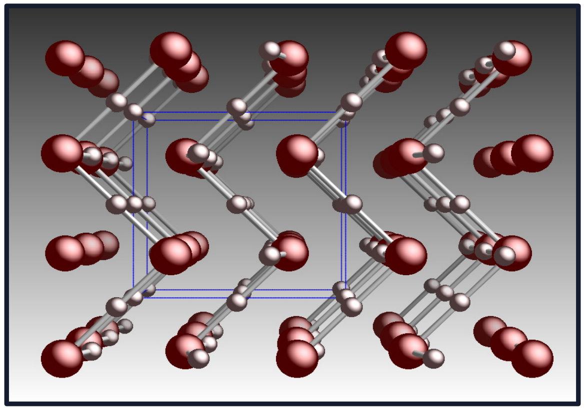
Helium Rain and The State of Water Ice in Giant Planets Predicted with Ab Initio Simulations







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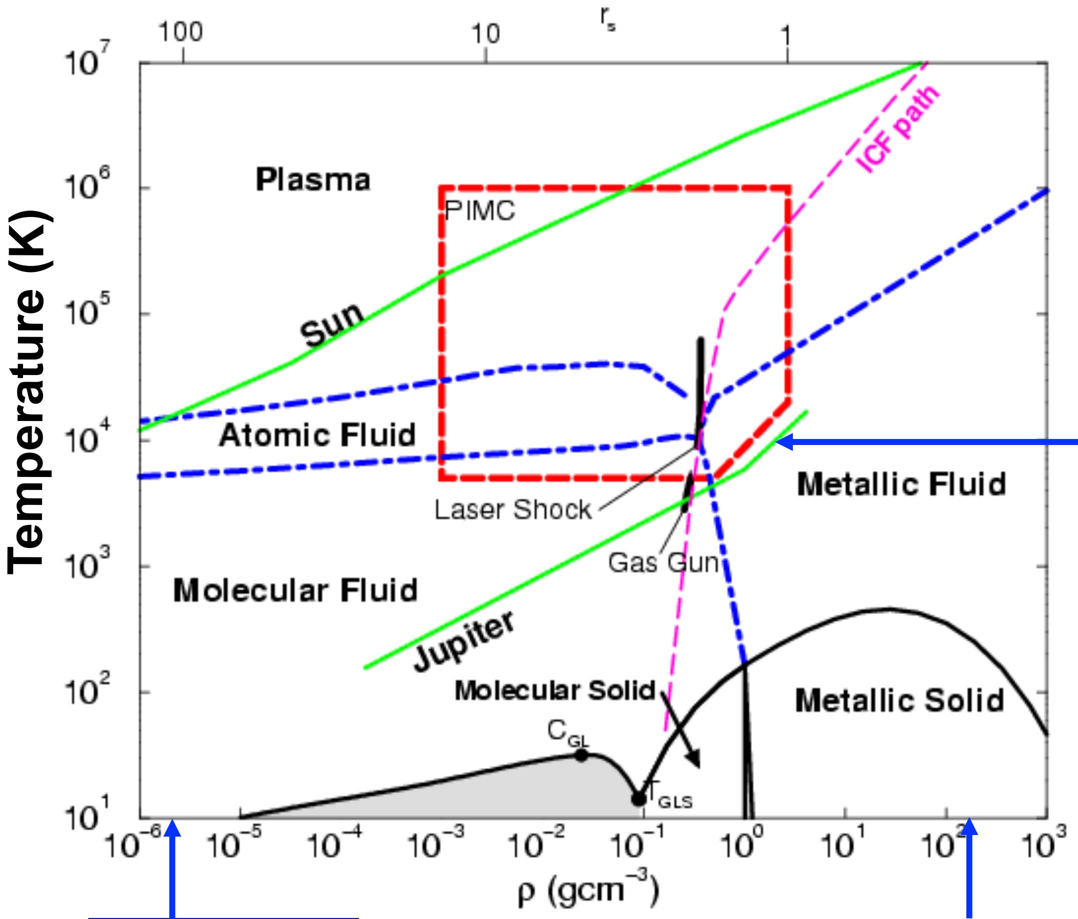
Outline

1. Introduction to Simulations
2. Helium rain on Jupiter
3. Phase diagram of water ice
4. Erosion of icy and rocky materials in cores in giant planets
5. Do iron and rocks ever mix in planetary interiors

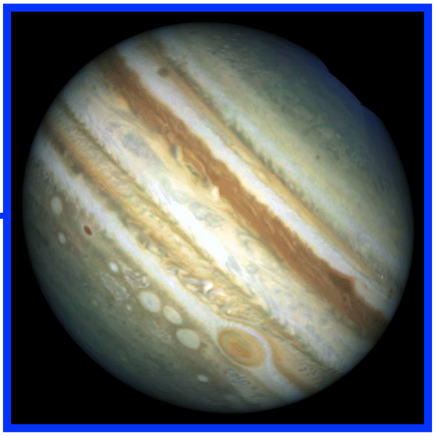
Supported by NASA and NSF.

I. Ab Initio Simulations of Materials at High Pressure

Focus: Characterization of the Interior of Solar and Extrasolar Giant Planets



Solar GP: Jupiter, Saturn

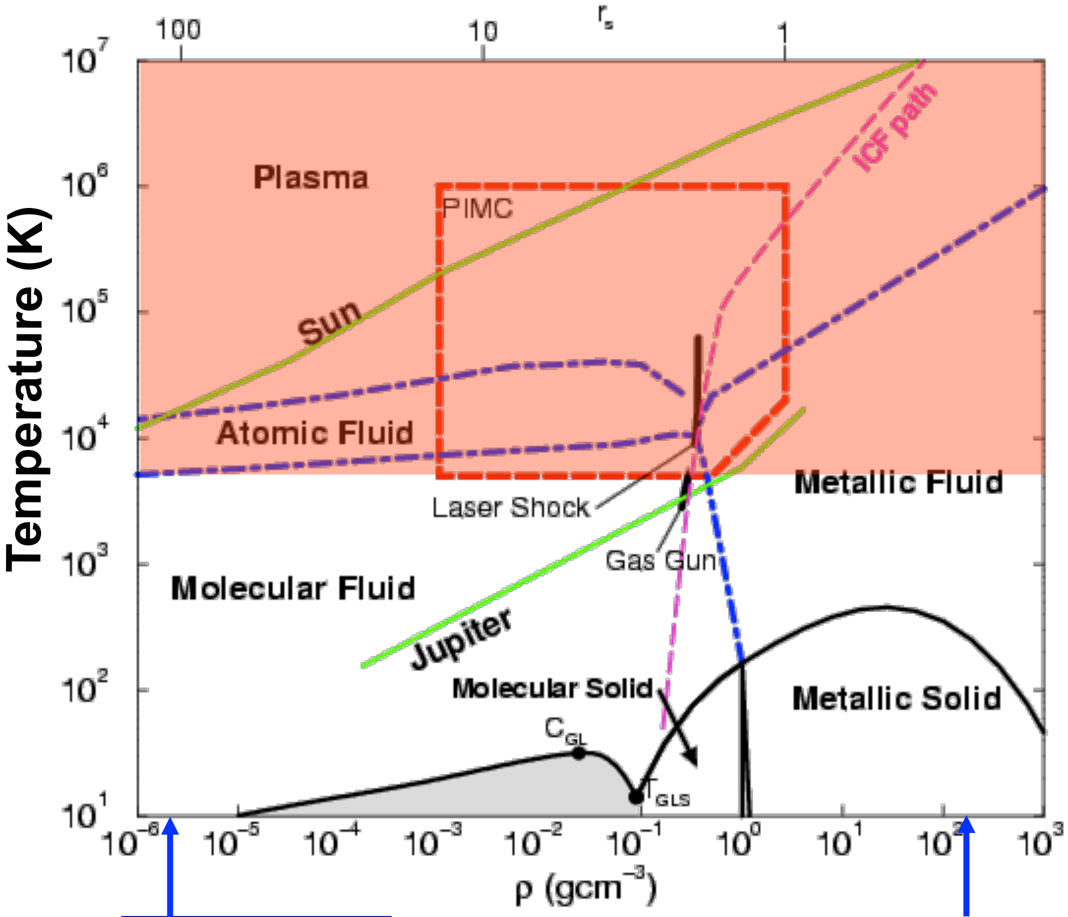


n=10^{18} cm^{-3}

Density

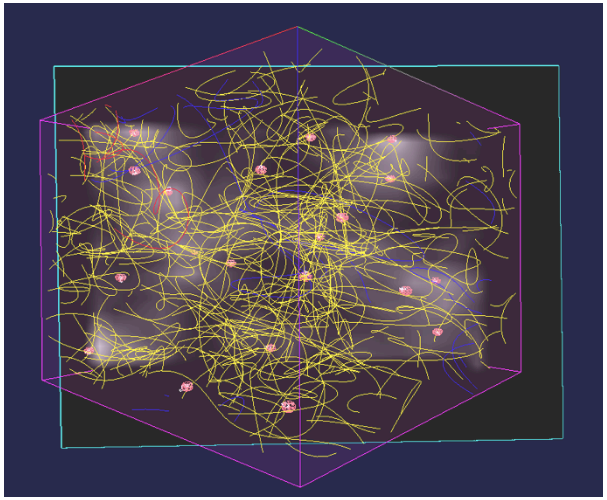
n=10^{26} cm^{-3}

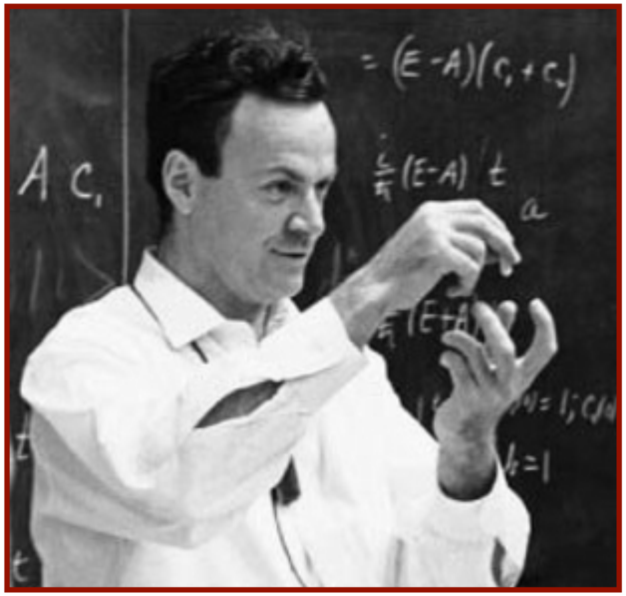
1) Path integral Monte Carlo for T>5000K



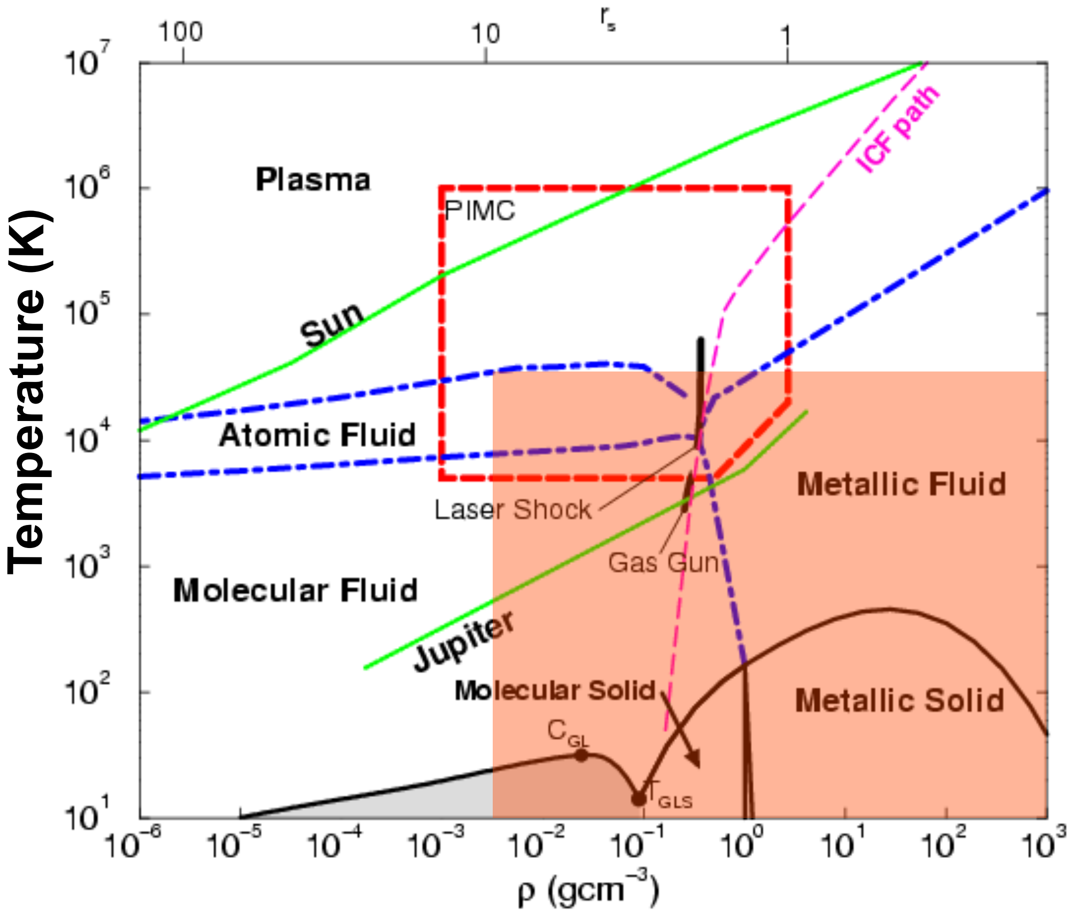
n=10^{18} cm^{-3}

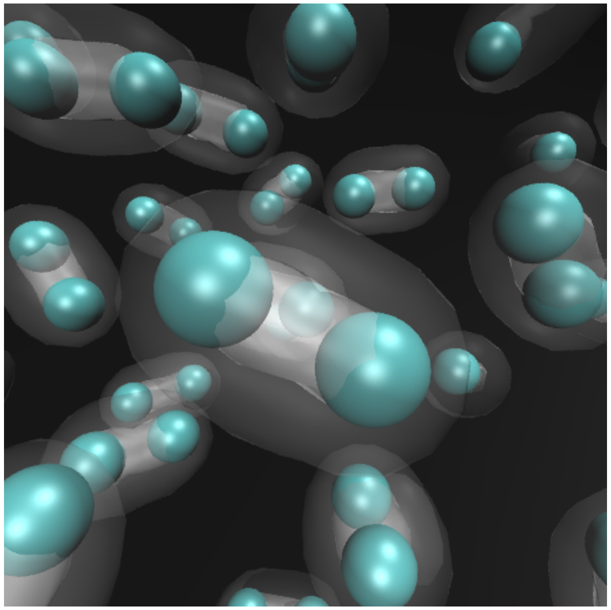
n=10^{26} cm^{-3}





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.

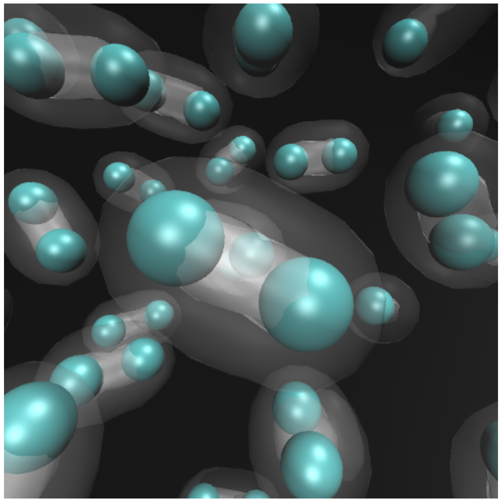
What is meant by first-principles simulations?

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

Density functional theory:

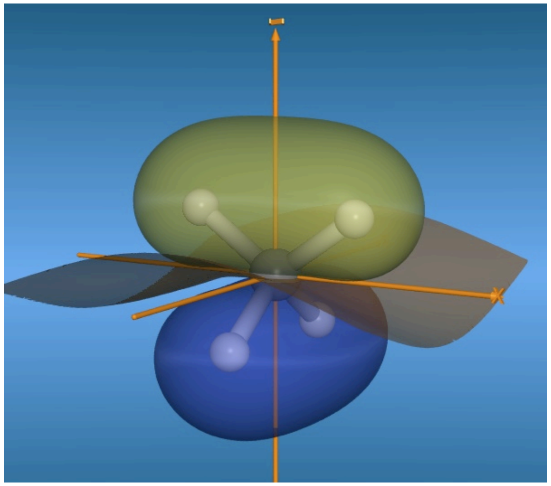
Local density approximation (LDA)

Gen. Gradient approximation (GGA)

Hybrid functionals

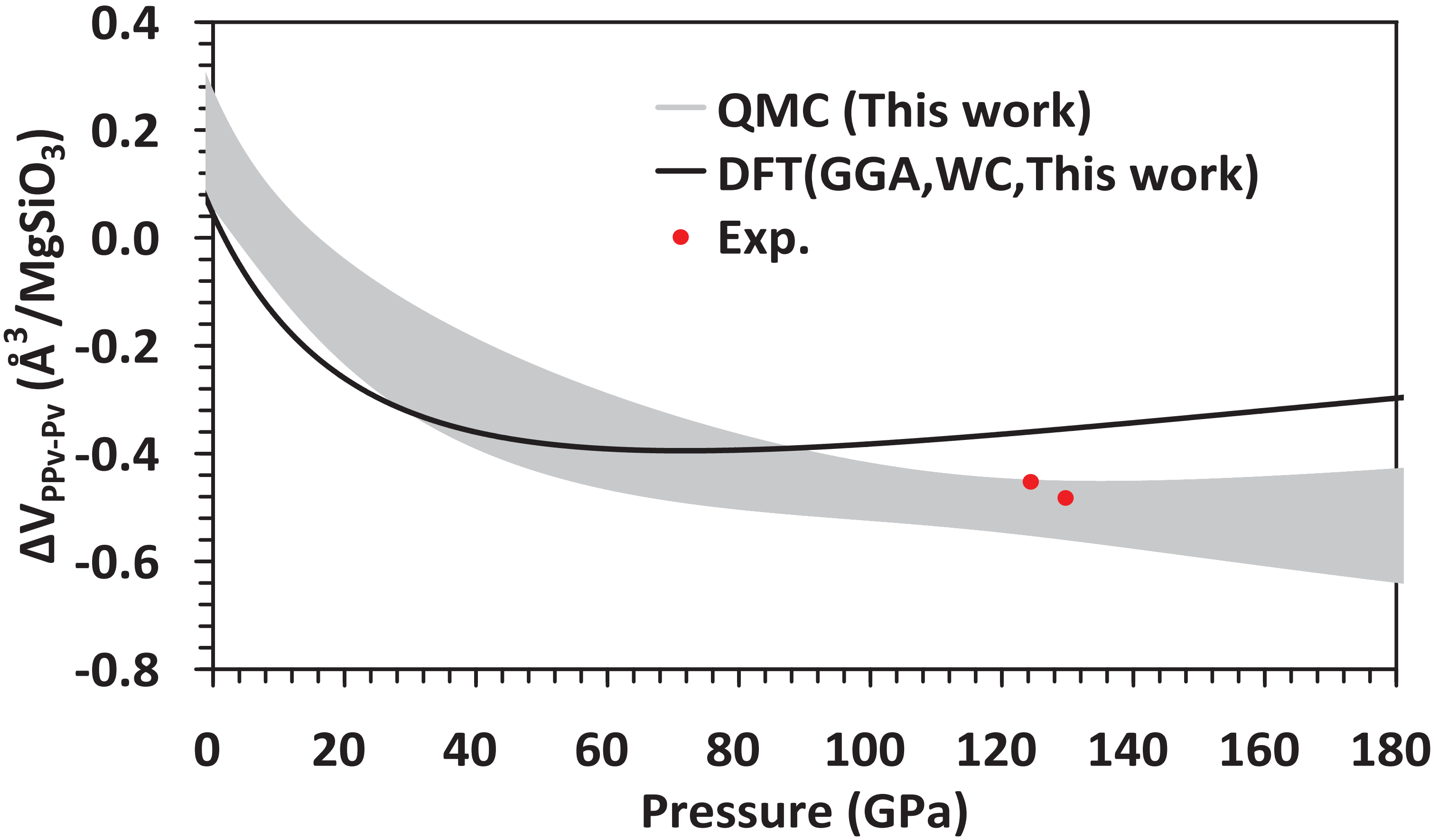
Van der Waals functionals

Quantum Monte Carlo



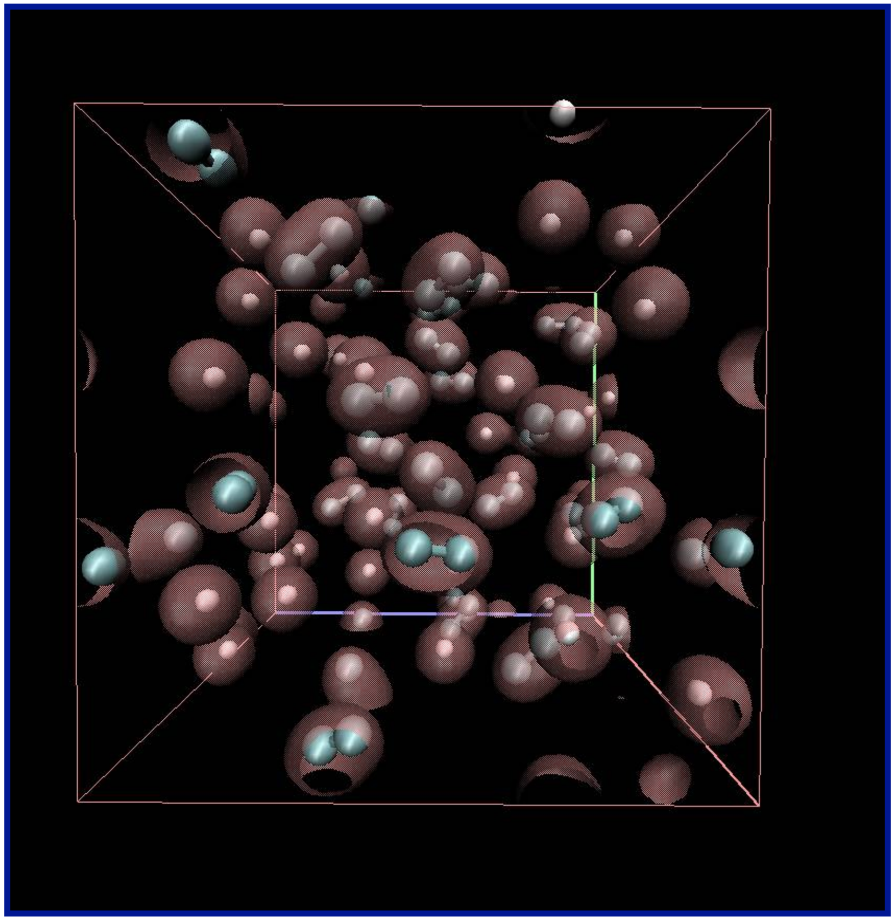
Methane - molecular orbitals

Quantum Monte Carlo Calculations of $MgSiO_3$ Perovskite and Post-Perovskite

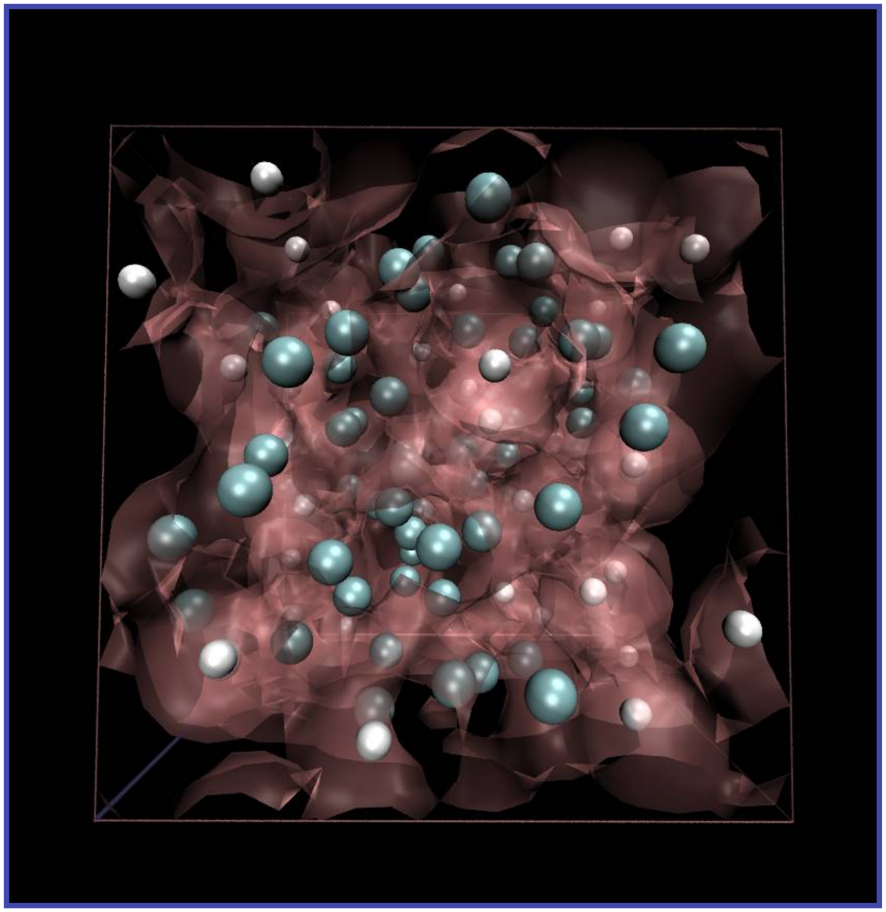


Y. Lin, R. E. Cohen, S. Stackhouse, K. P. Driver, B. Militzer, L. Shulenburger, J. Kim
Phys. Rev. B, in press (2014)

Comparison of molecular and metallic hydrogen

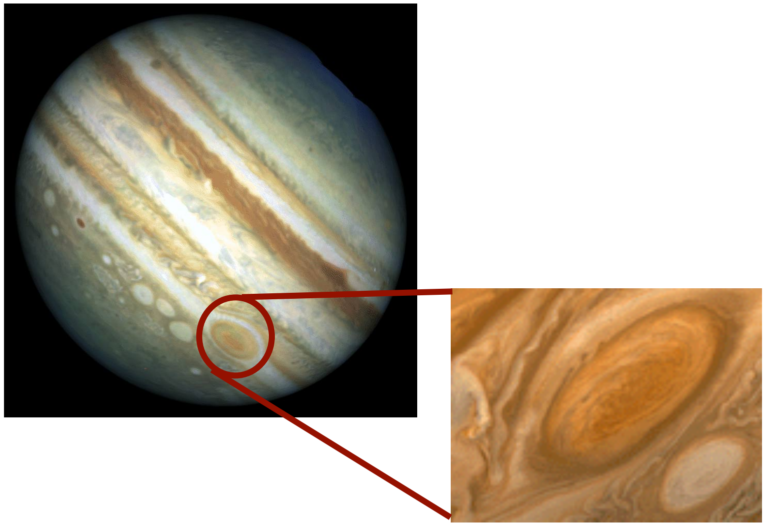


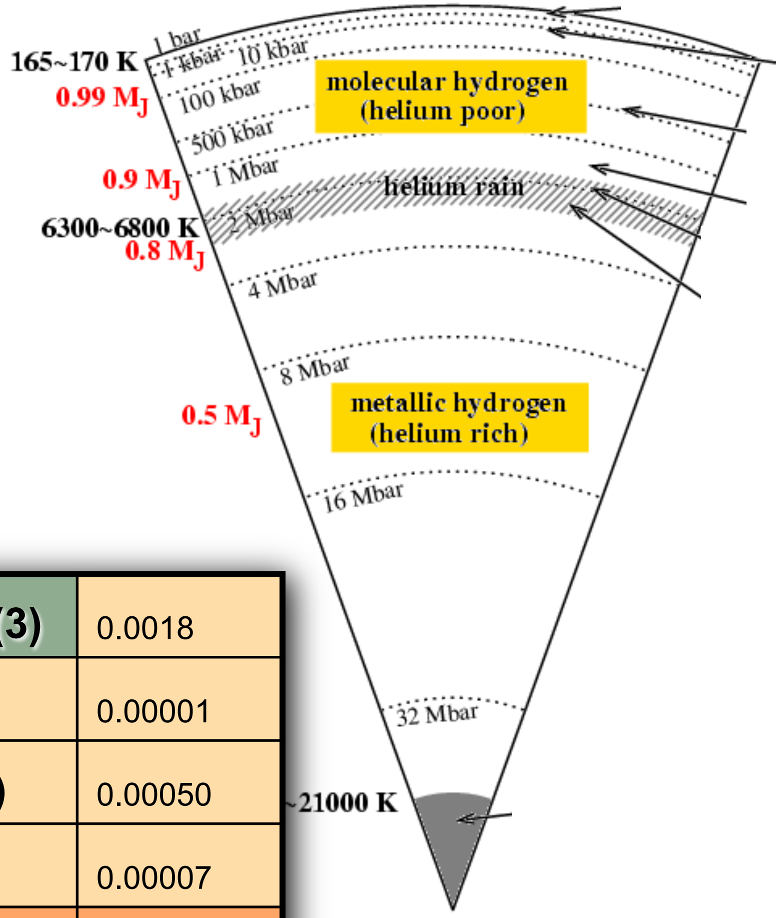
Molecular hydrogen



Metallic hydrogen

Jupiter’s Composition



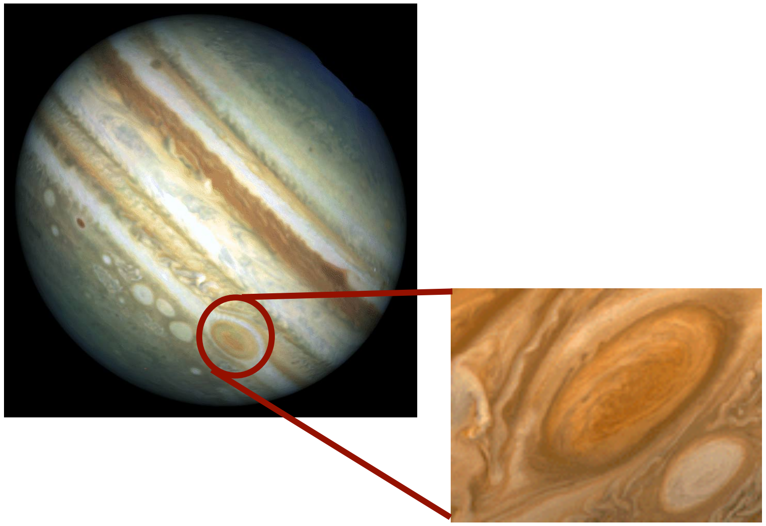


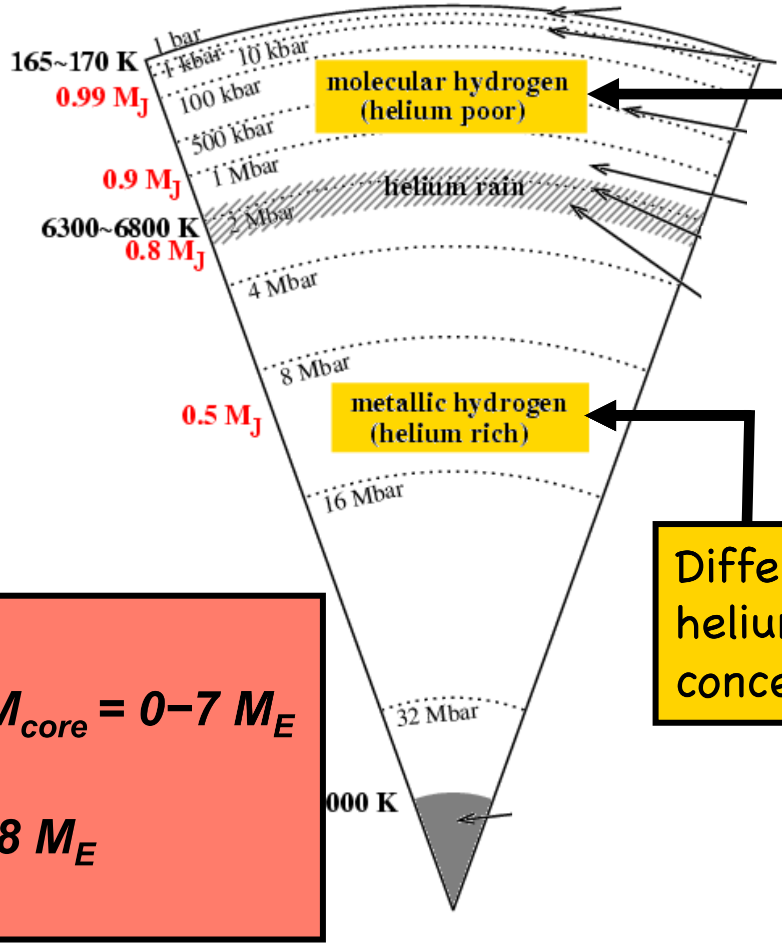
Composition on the surface (solar):

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





Different helium concentration

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

B) We derived a model: M_{core} = 14−18 M_E

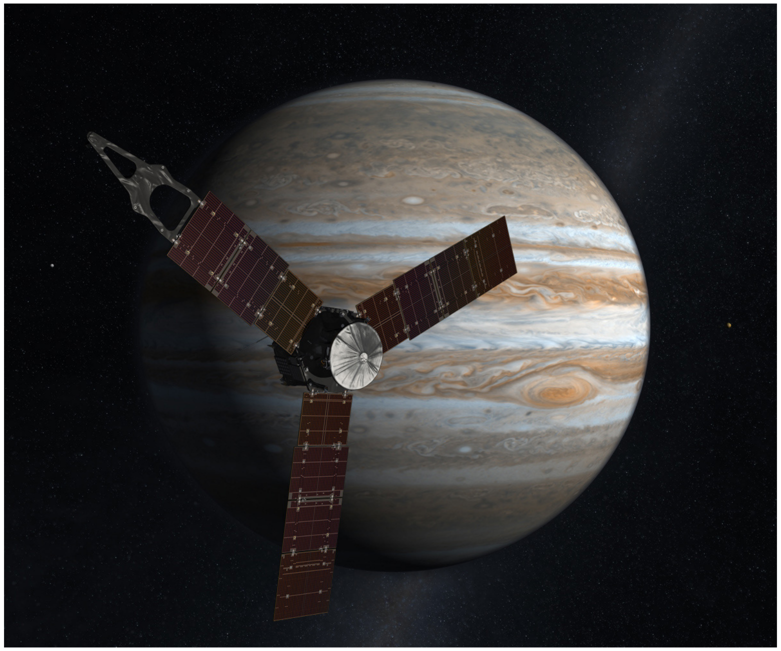
Guillot et al. (Jupiter book, 2002, chap.3)

Juno Mission

launched successfully August 2011

My contribution:

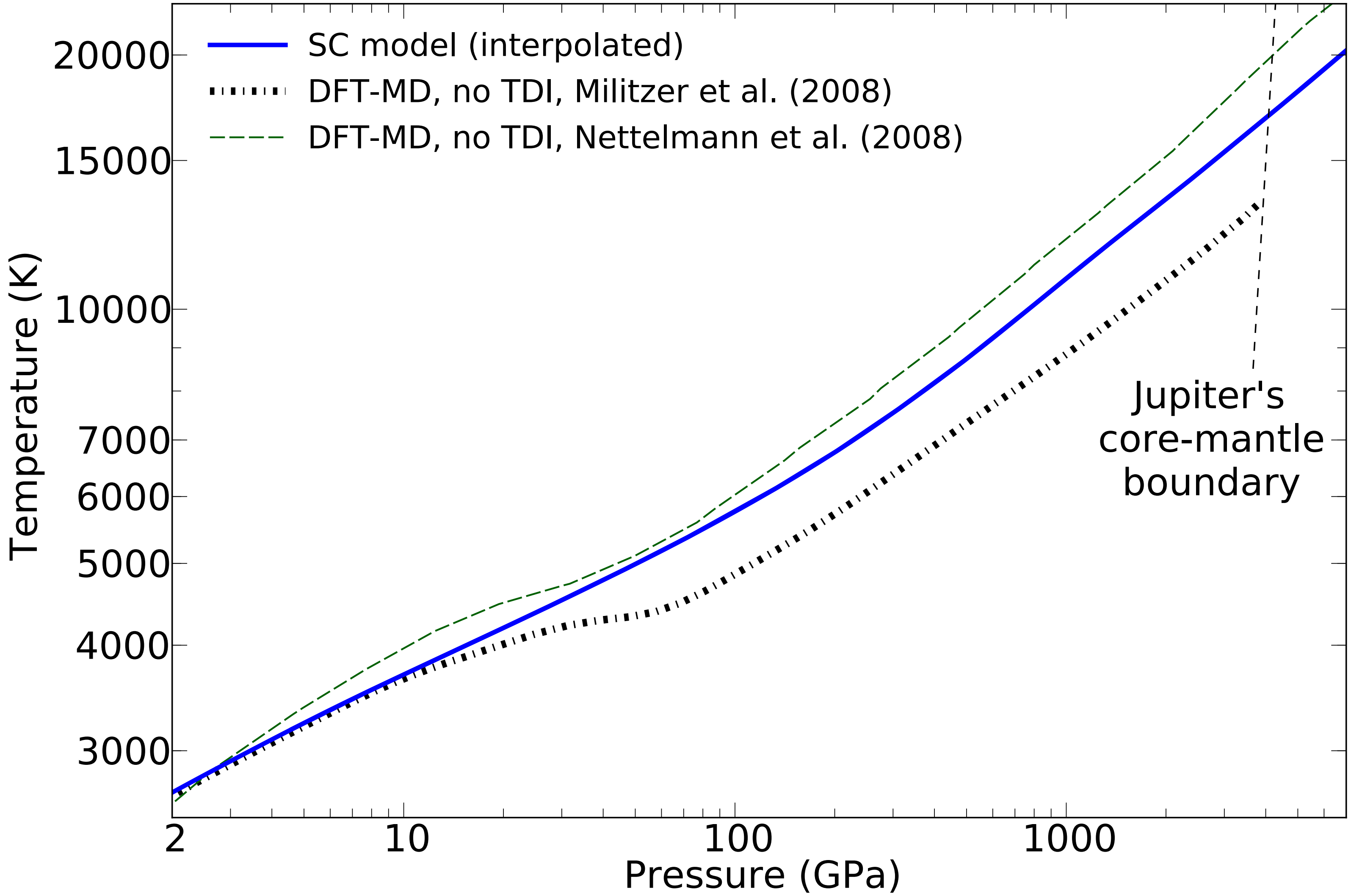
- Equation of state calculations for hydrogen-helium mixtures
- Thermodynamics of heavier elements



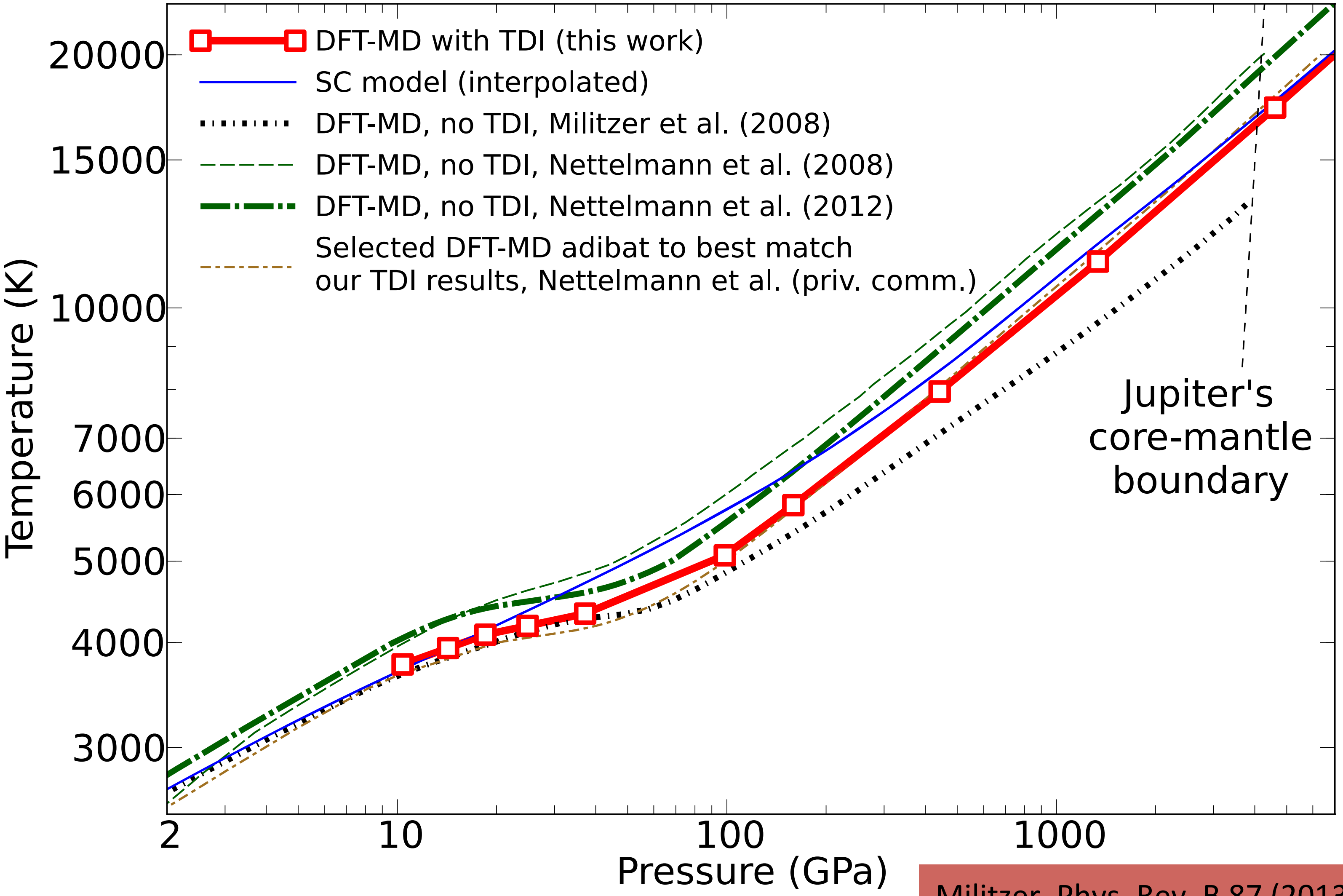
Mission Timeline:

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

Jupiter’s Interior Temperature Profile

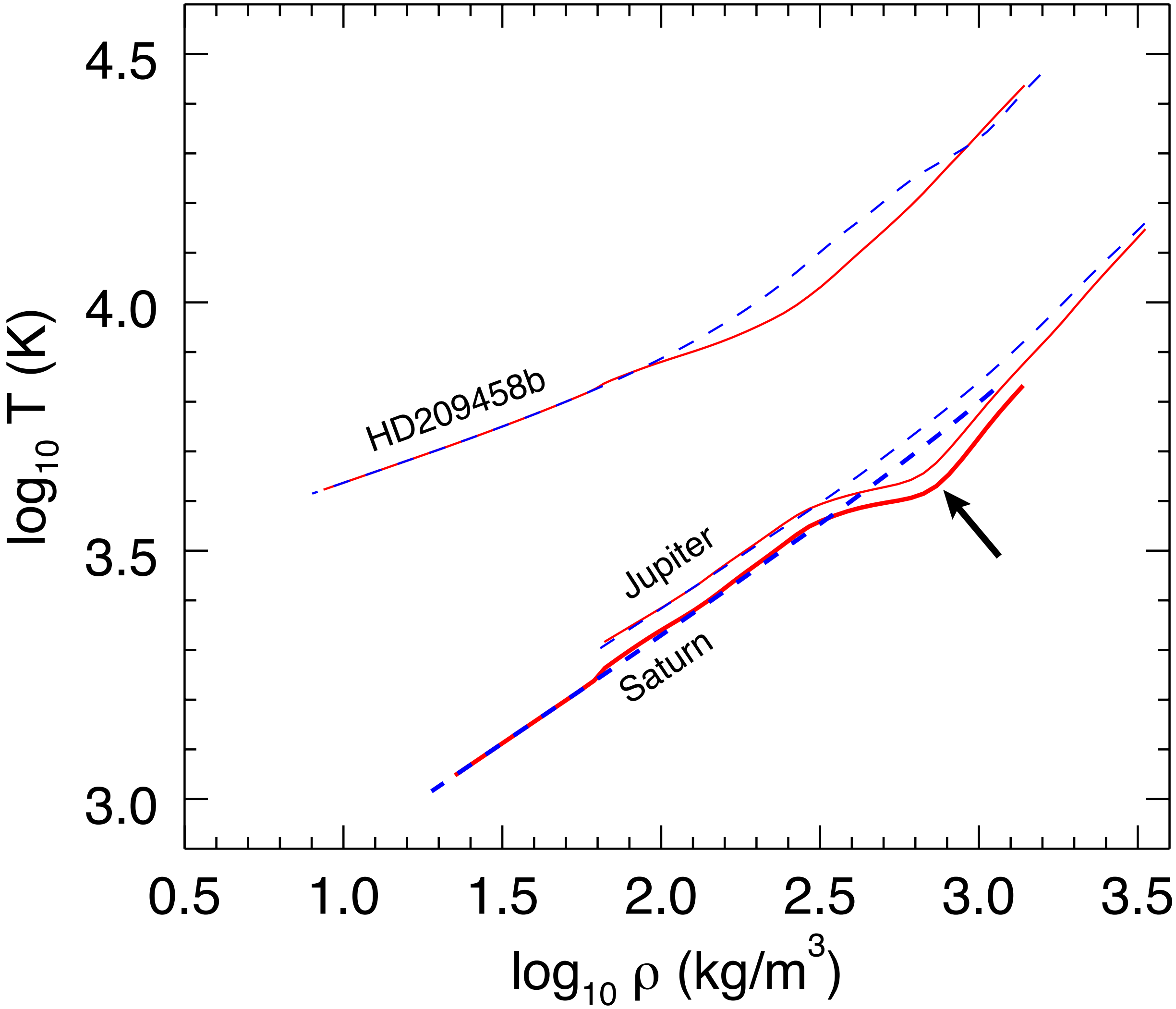


Jupiter's Interior Temperature Profile



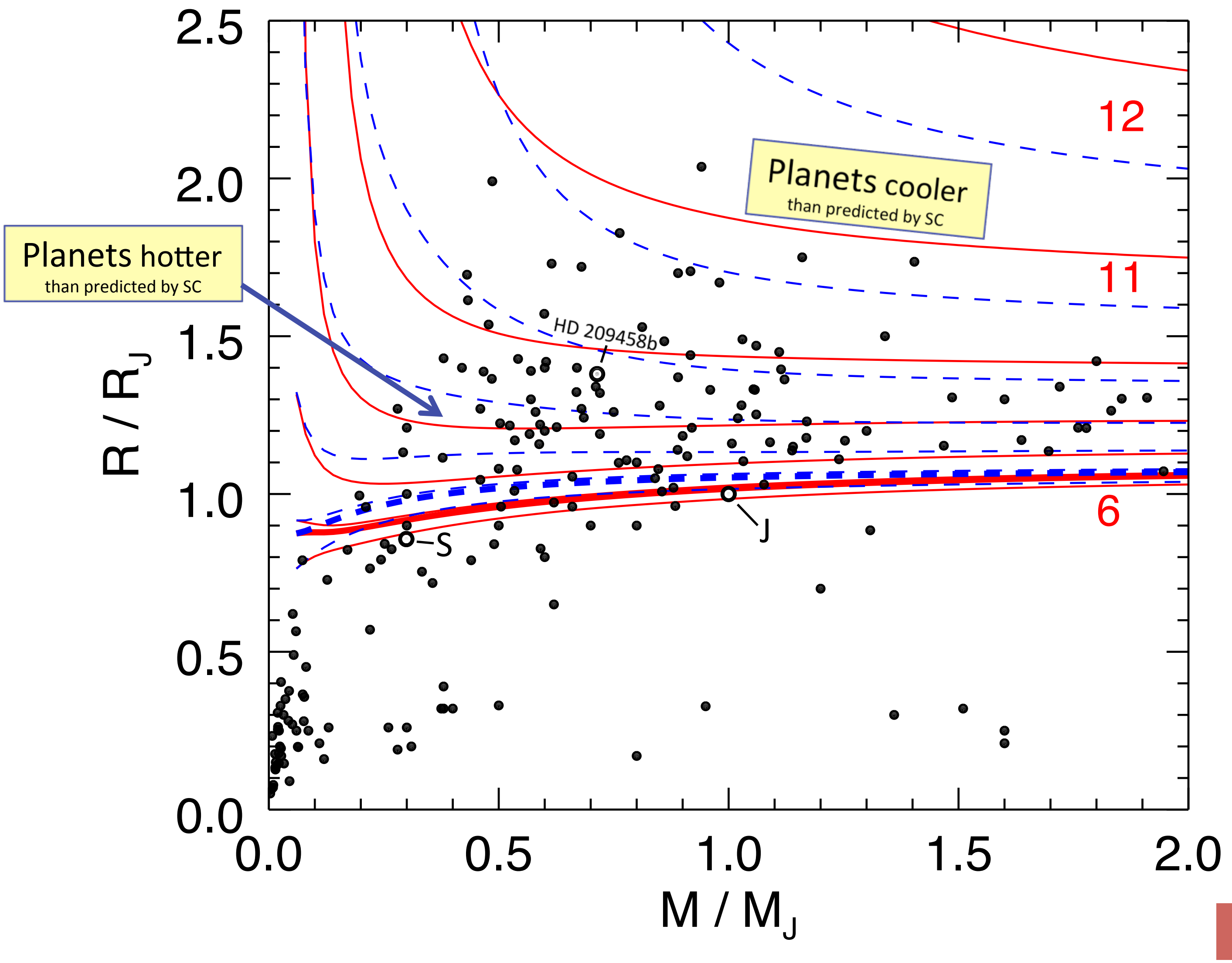
Militzer, Phys. Rev. B 87 (2013) 014202

Interiors of Saturn and Jupiter are more dense



Militzer, Hubbard, Apj (2013)

Recalibration of Mass-Radius Relationship of Hot Jupiters



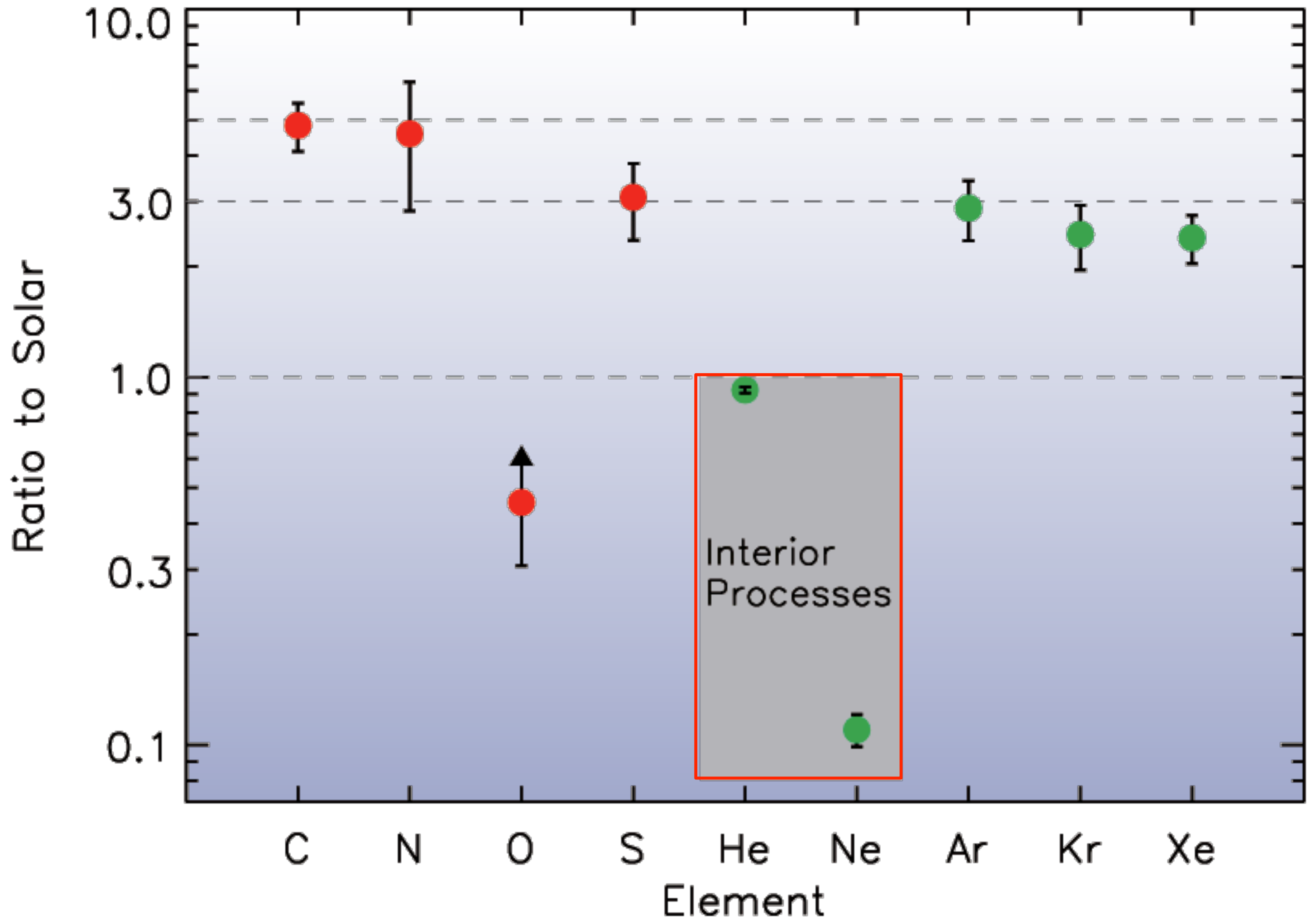
Planets hotter
than predicted by SC

Planets cooler
than predicted by SC

Militzer, Hubbard, Apj (2013)

II. Helium Rain on Jupiter

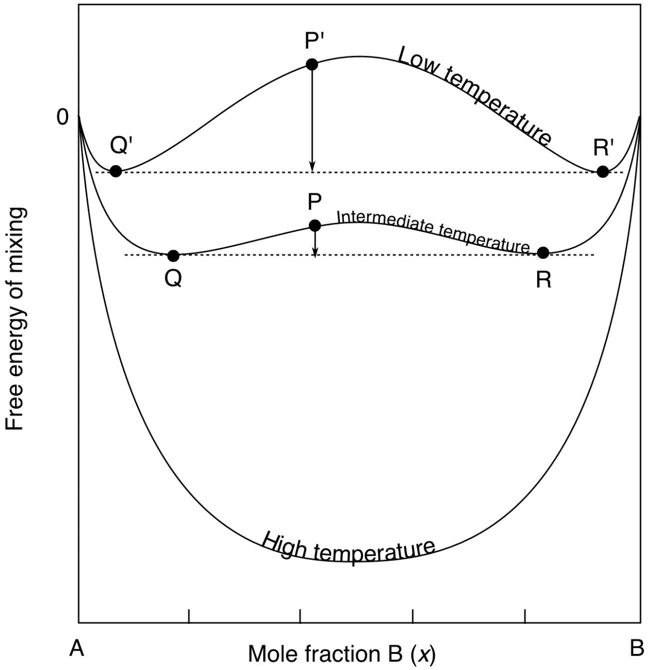
Galileo Entry Probe found: Helium and Neon depleted in Jupiter's Atmosphere

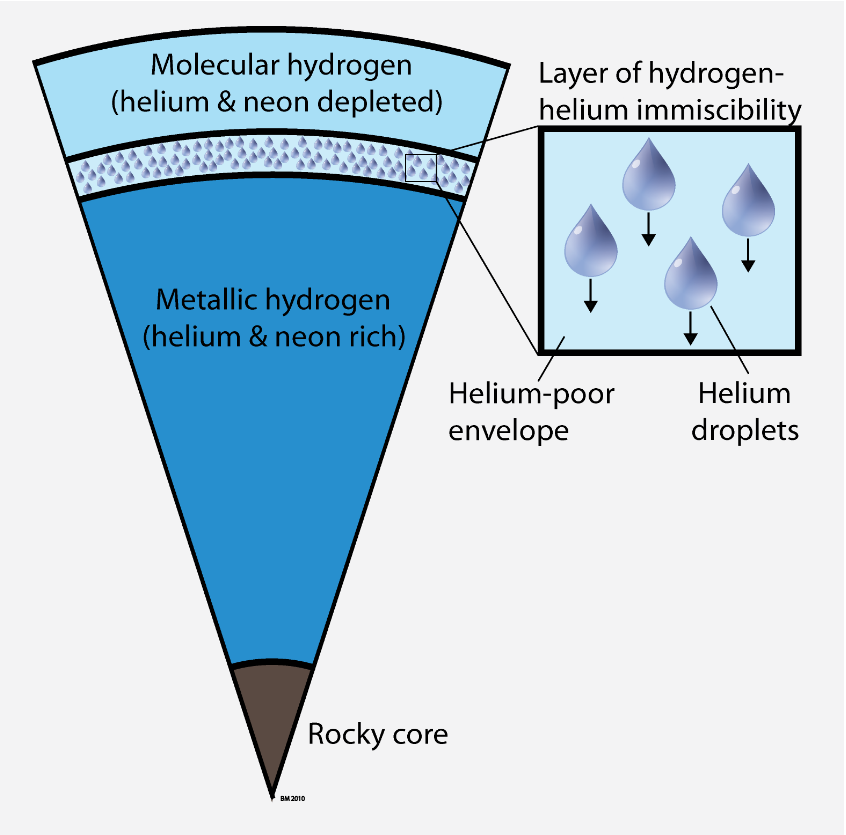


Can hydrogen and helium become immiscible? Helium rain inside Saturn?

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

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



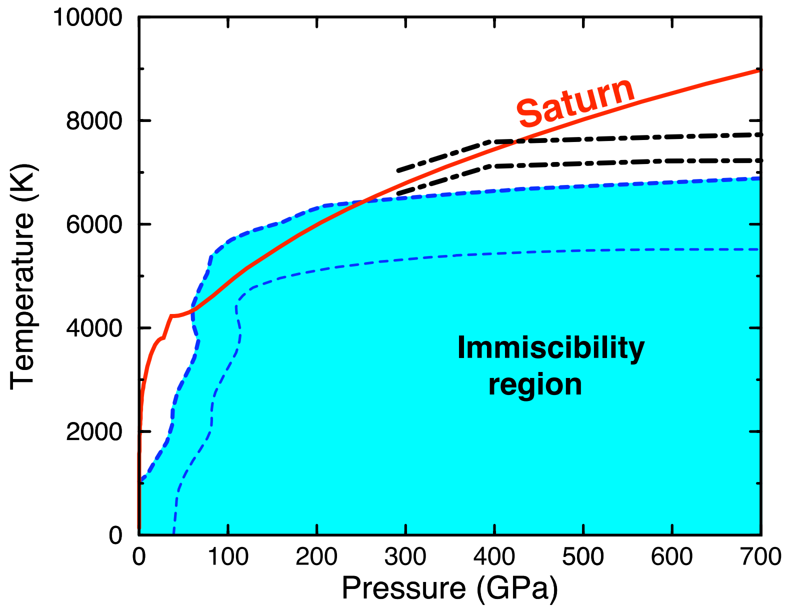


$G(\mathrm{P,T}) = \mathrm{E+PV-TS}$ Main difficulty is to calculate the mixing entropy!

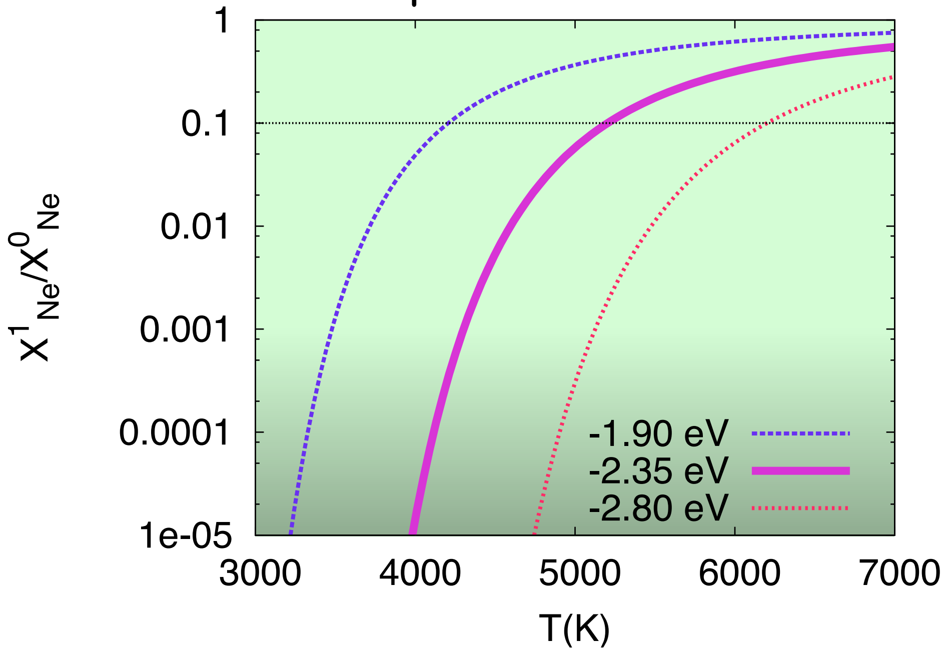
Neon depletion is consistent with helium depletion in Jupiter

Quantitative agreement between:

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



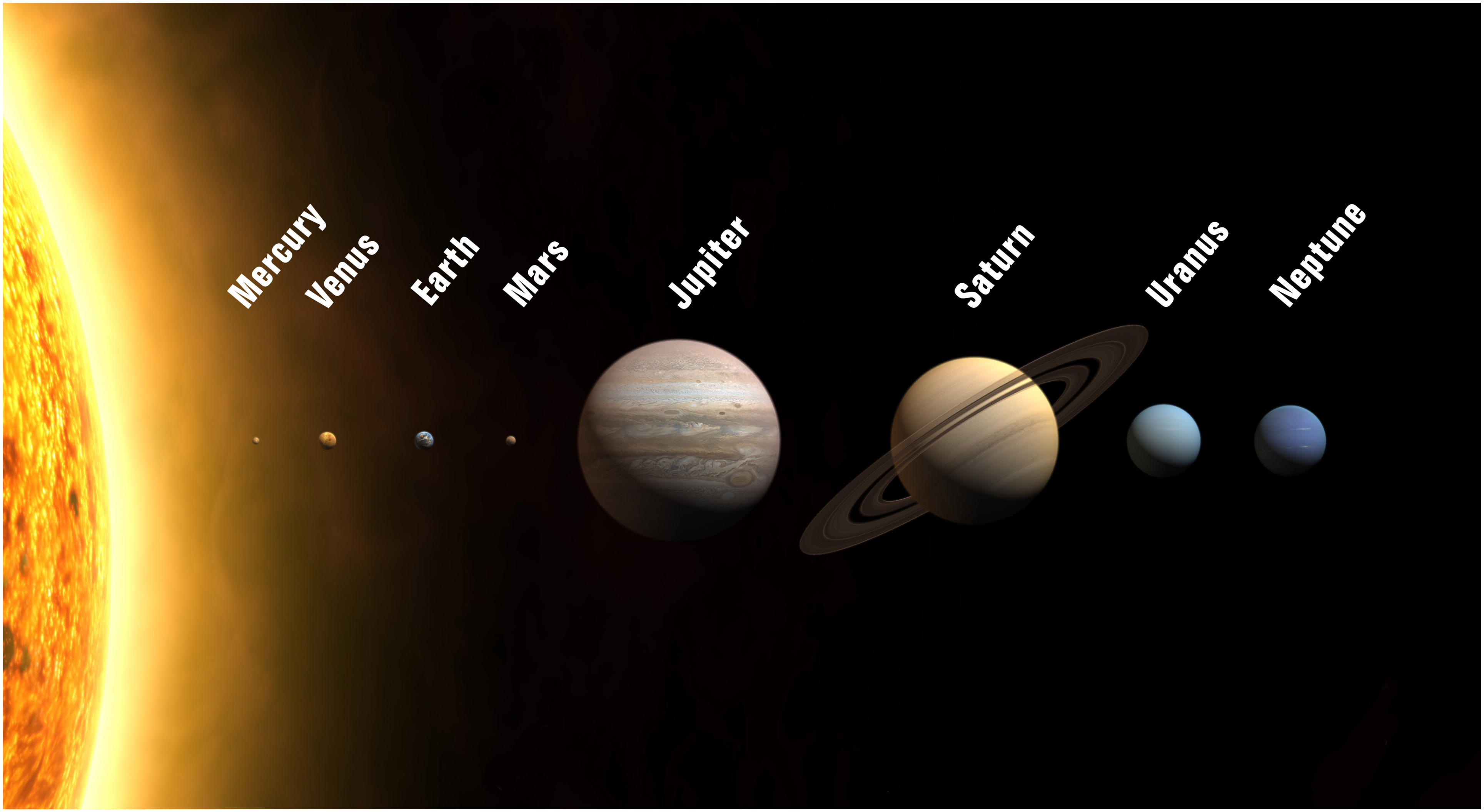
Neon depletion vs temperature at fixed helium depletion of $X^0_{He} - X^1_{He} = 1.2\%$



Roulston and Stevenson (1995)

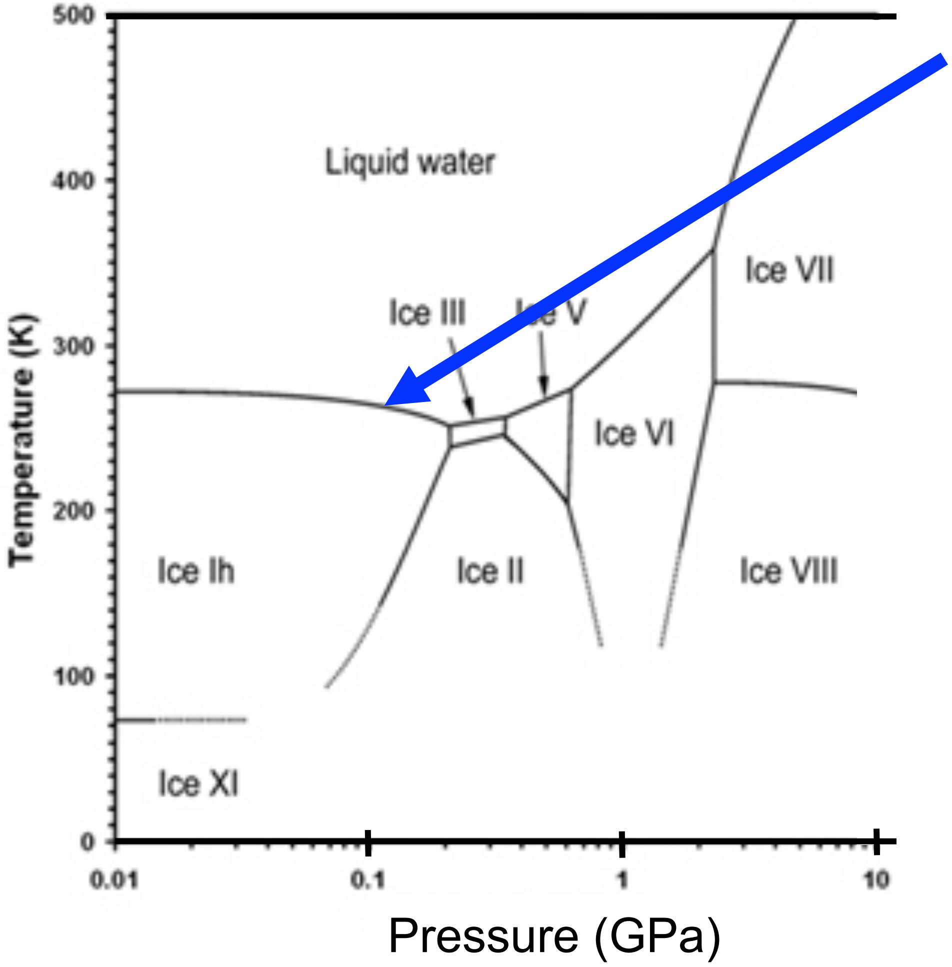
$$\frac{dX_{Ne}}{dt} = X_{He}\ \exp\left(\frac{\Delta G}{k_B T}\right)\ \frac{dX_{He}}{dt}$$

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

Phase Diagram of water ice

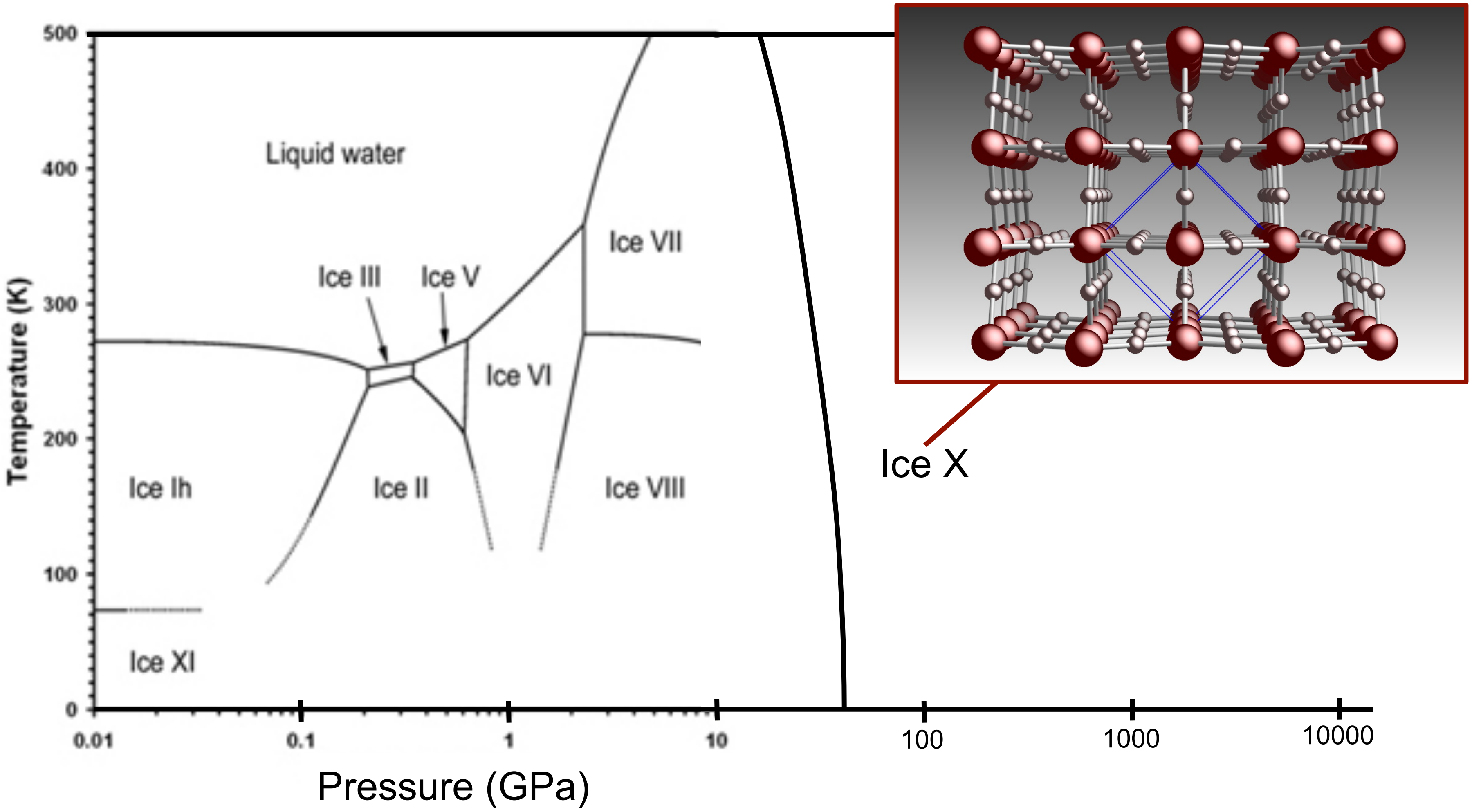


Ice 1h has negative Clapeyron slope:

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

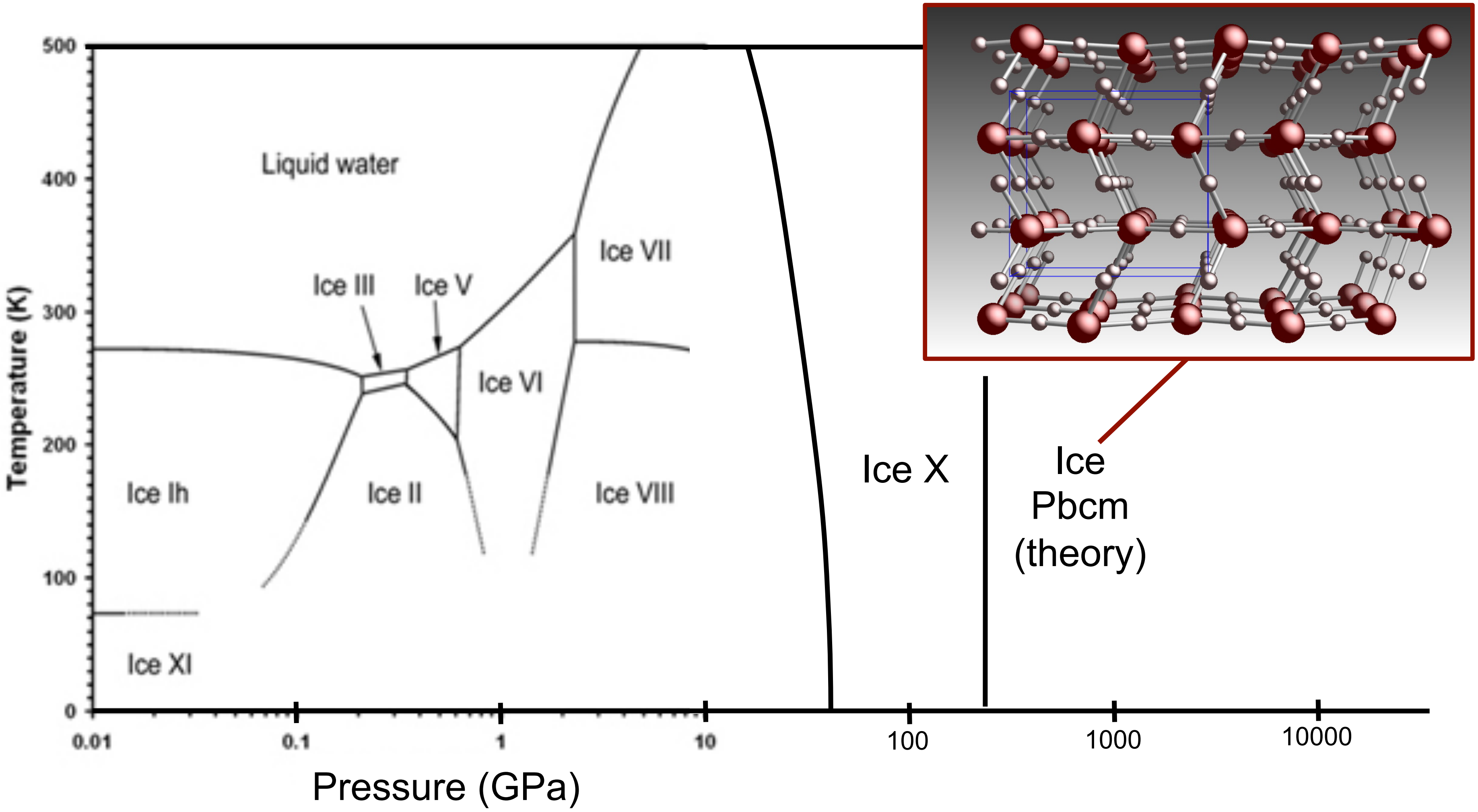
$$\boxed{G(P,T)=E+PV-TS}$$

Phase Diagram of water ice



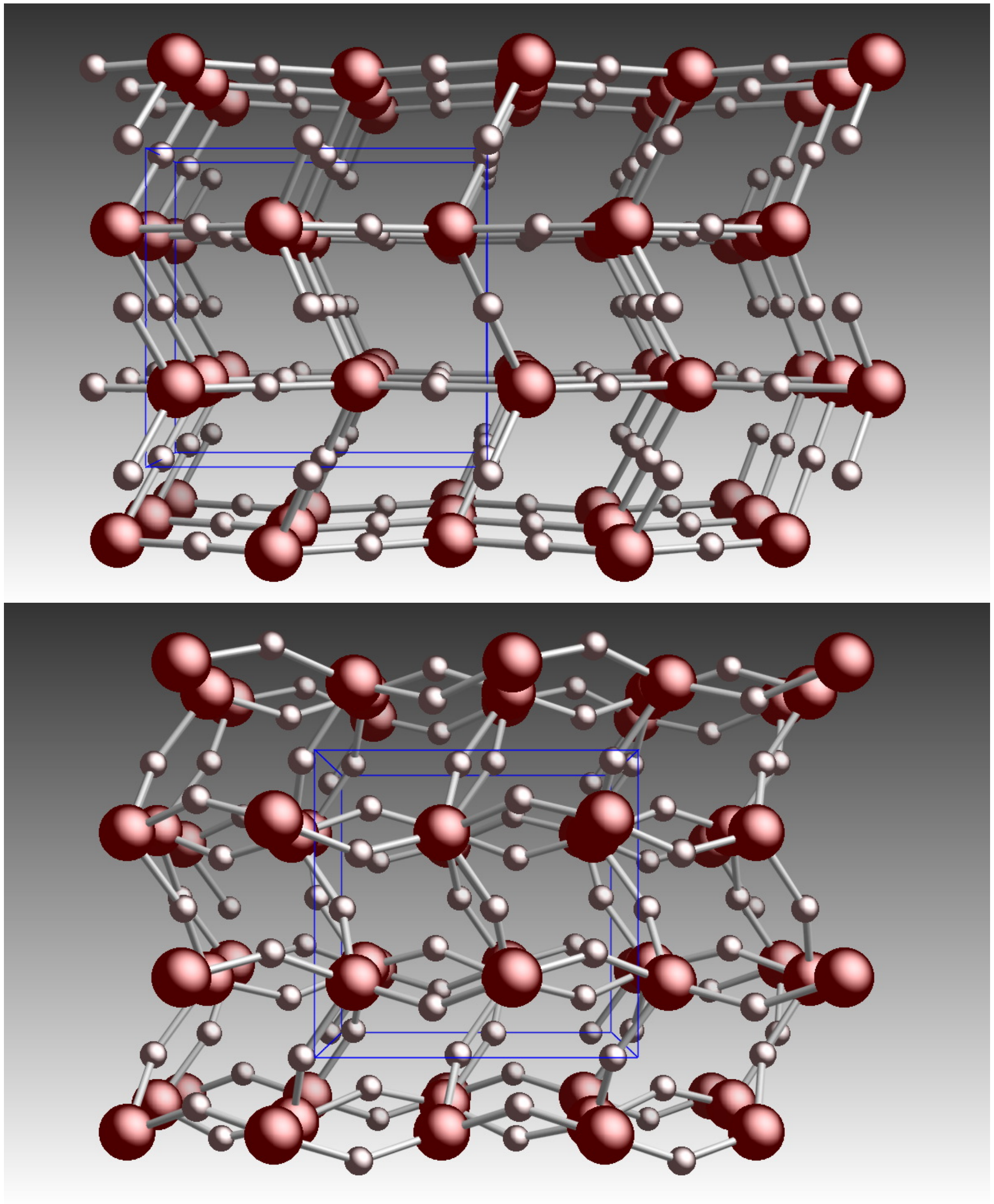
Ice X: the highest pressure phase seen in experiments.

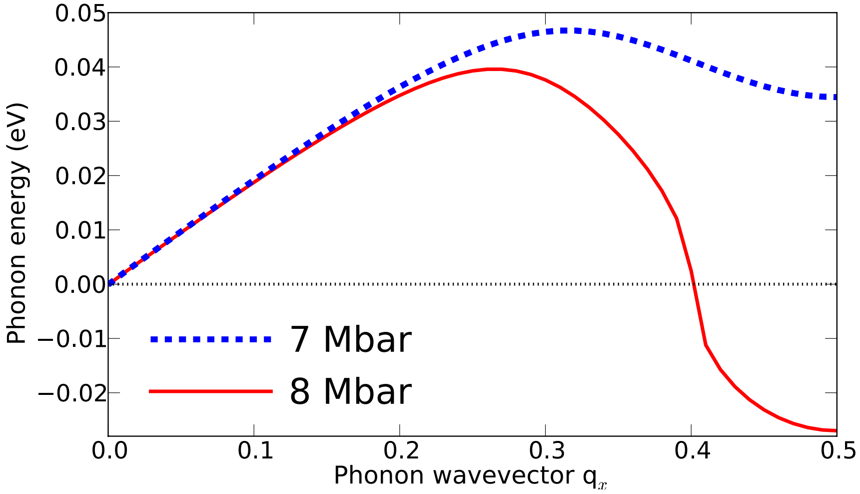
Phase Diagram of water ice



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

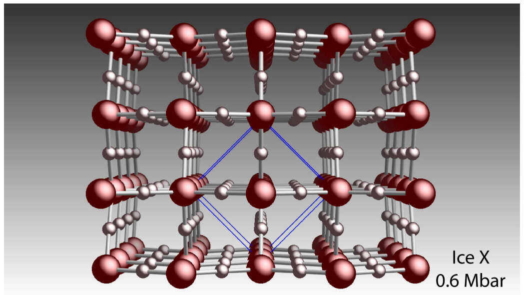


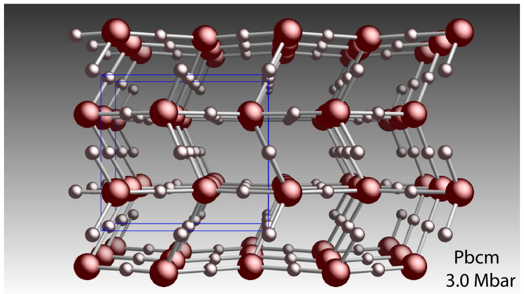


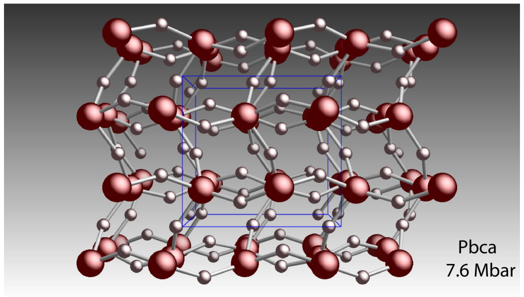
Militzer and Wilson, *PRL* 105 (2010) 195701

2013: Ab Initio Structure Search Methods predict Two New Ice Structures at Megabar Pressure

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**	7.7	8
$P3_121$	**Pickard, Needs, 2013**	8.1	12
Pcca	**Pickard, Needs, 2013**	14.4	12
$P2_1/c$	**Ji, 2011**	19.6	8
C2/m (metallic)	**McMahon, 2011**	56.2	2
	Hermann, 2011	60	2
H_2O_2	**Pickard, Needs 2013**	~50	
H_4O	**Zhang, Militzer, 2013**	~50	





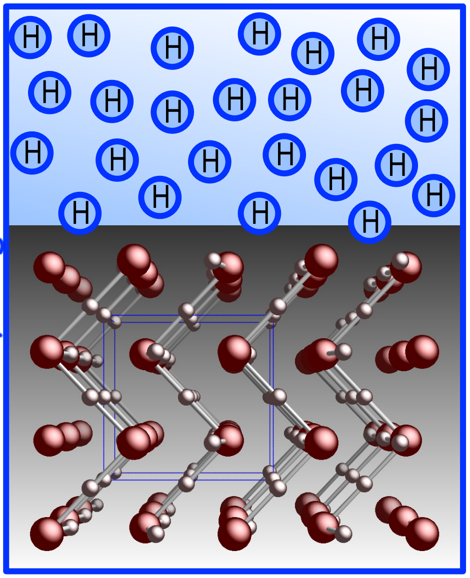


Militzer, Wilson, *Phys. Rev. Lett. 105*, 195701 (2010).
McMahon, *PRB 84*, 220104(R) (2011).
Pickard, Needs 110 (2013) 245701

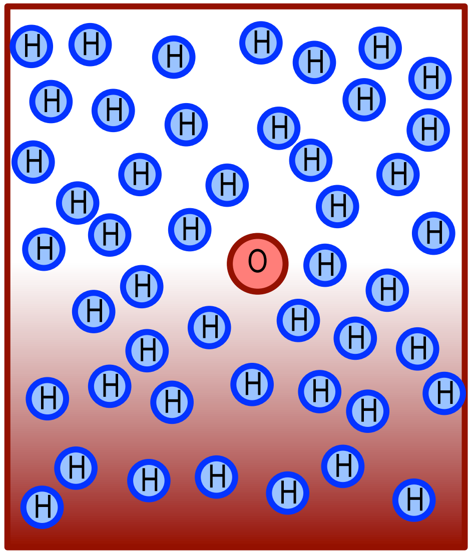
Ji *et al.*, *PRB*, 84, 220105(R) (2011).
Hermann *et al.*, *PNAS 109*, 745 (2011).
Zhang, Wilson, Driver, Militzer, *PRB* 87, 02411 (2013).

IV. Is Ice Stable in Cores of Giant Planets?

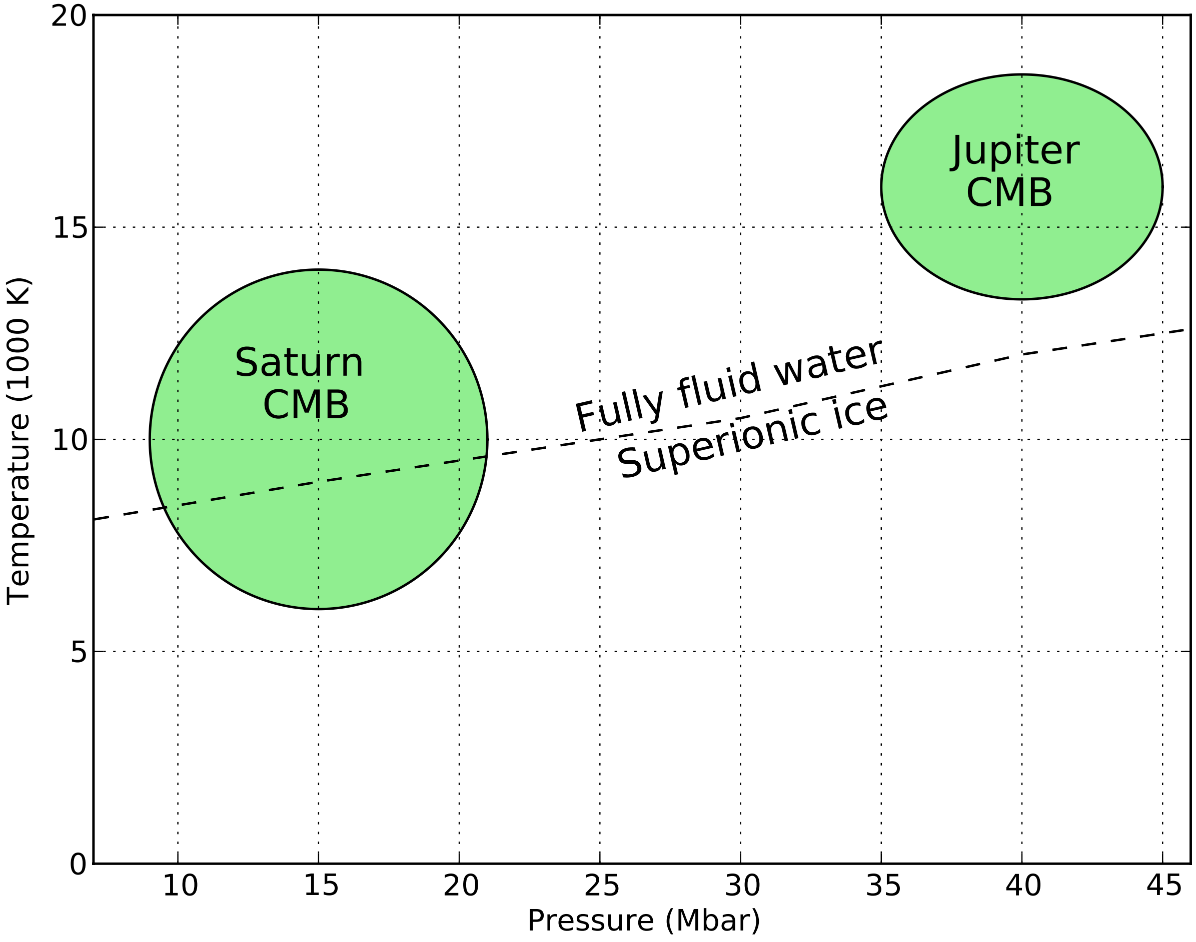
Is the interface between ice and metallic hydrogen stable in giant planet cores?



Stable ice-hydrogen interface

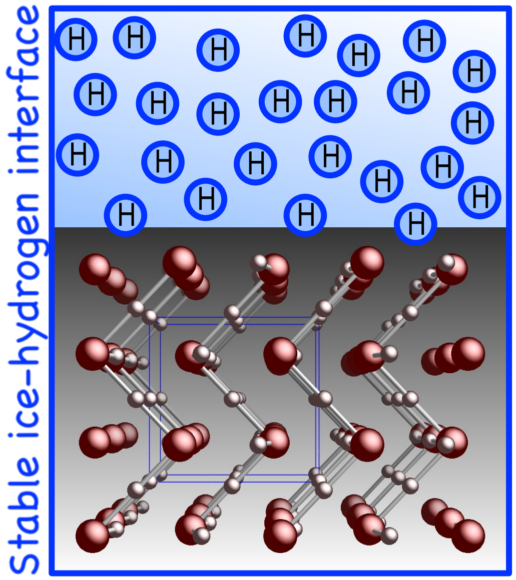


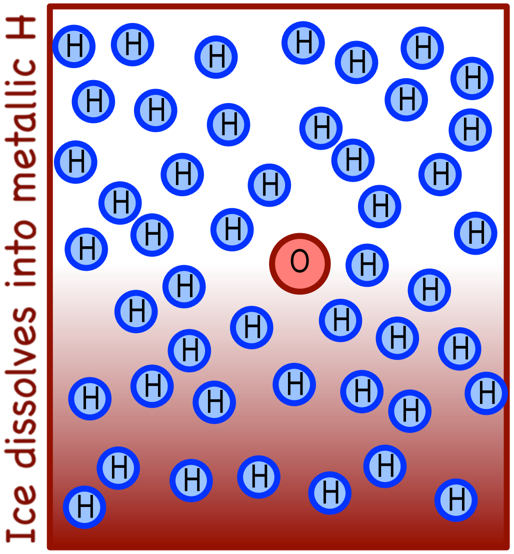
Ice dissolves into metallic H

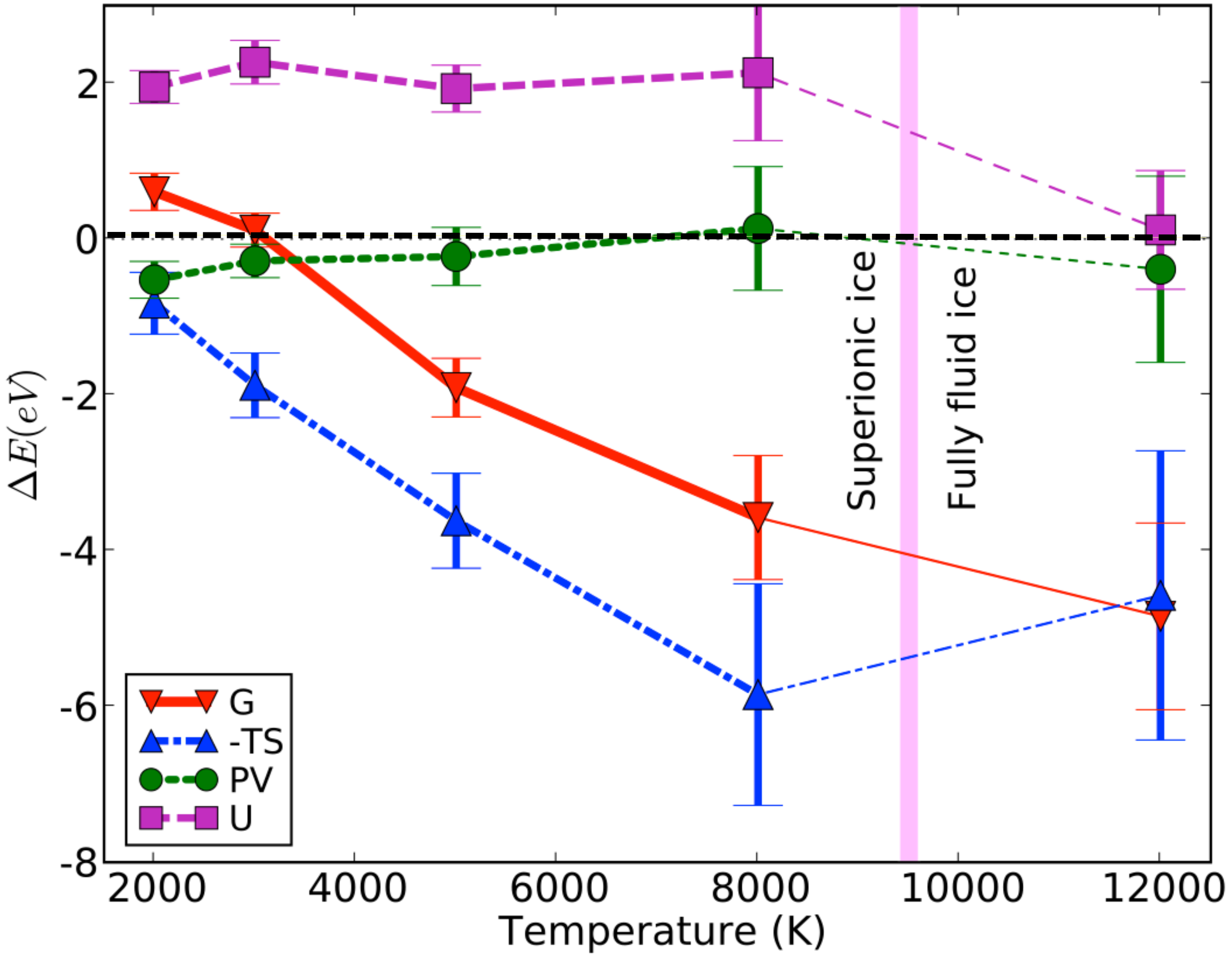


Wilson and Militzer, Astrophys. J. 745 (2012) 54

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



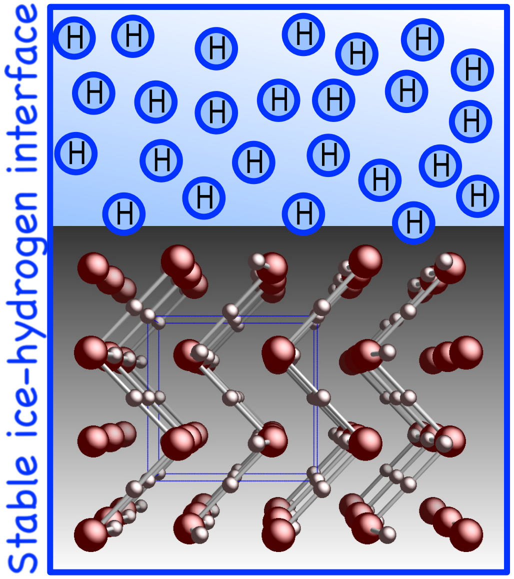


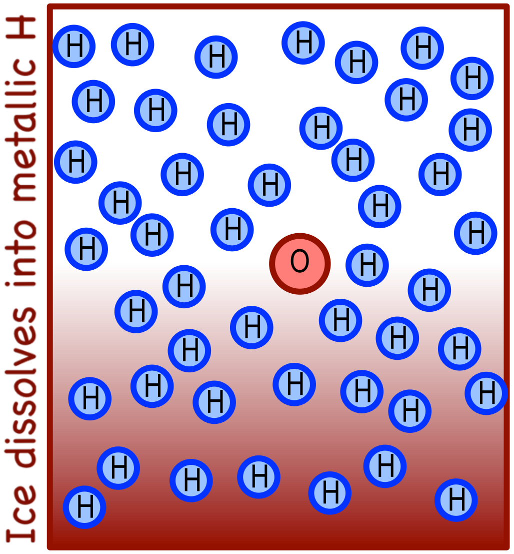


Predict core erosion in both Saturn and Jupiter

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

Computer simulations predict erosion of icy cores in Saturn and Jupiter


Stable ice-hydrogen interface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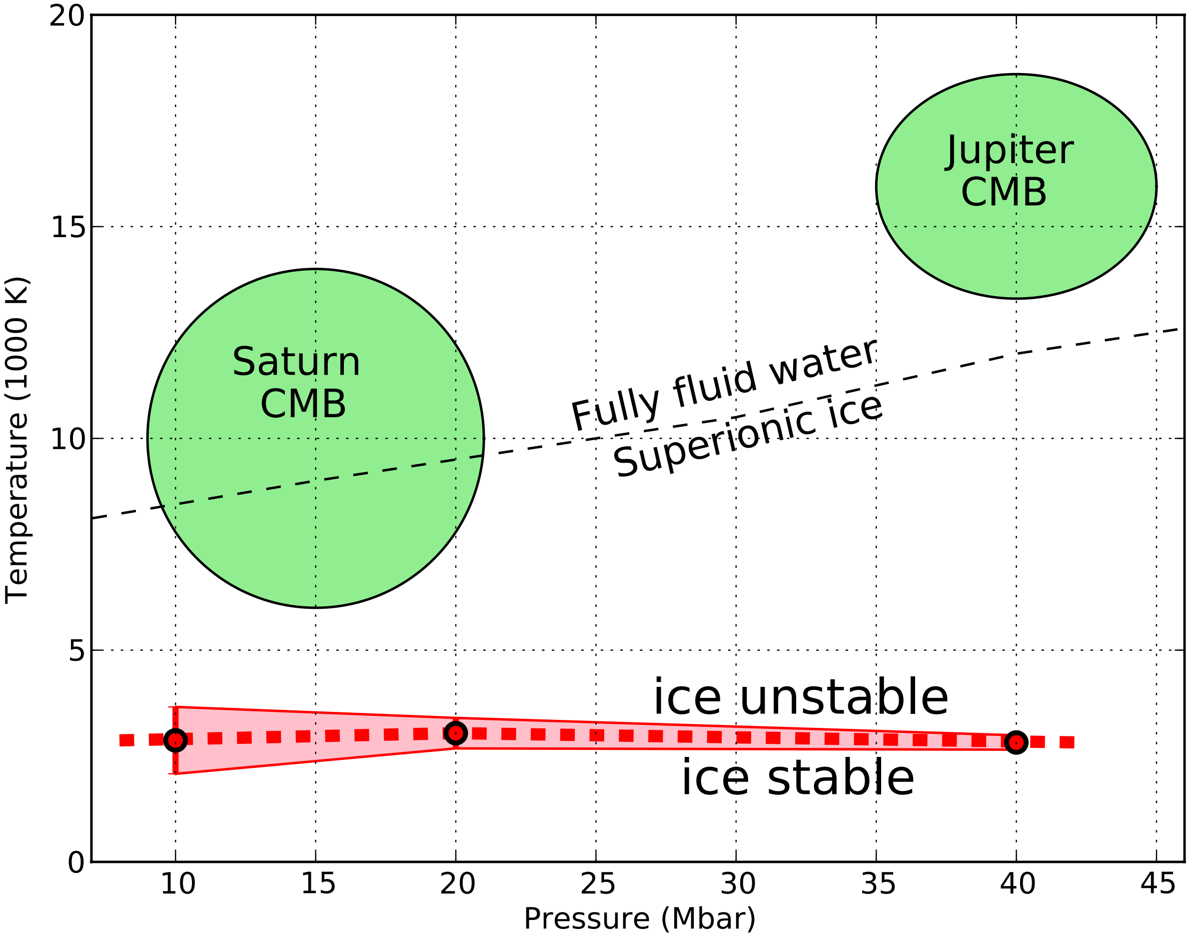

Predict core erosion in both Saturn and Jupiter

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

Conclusions

- Indirect evidence for helium rain on Jupiter based on low neon abundances in atmosphere
- Superionic H_2O water could be relevant for Uranus and Neptune
- All core materials such as ices, rocks and iron are thermodynamically unstable – core erosion timescale unclear
- Iron and rocks mix at temperatures 4,000-10,000 K.

The End