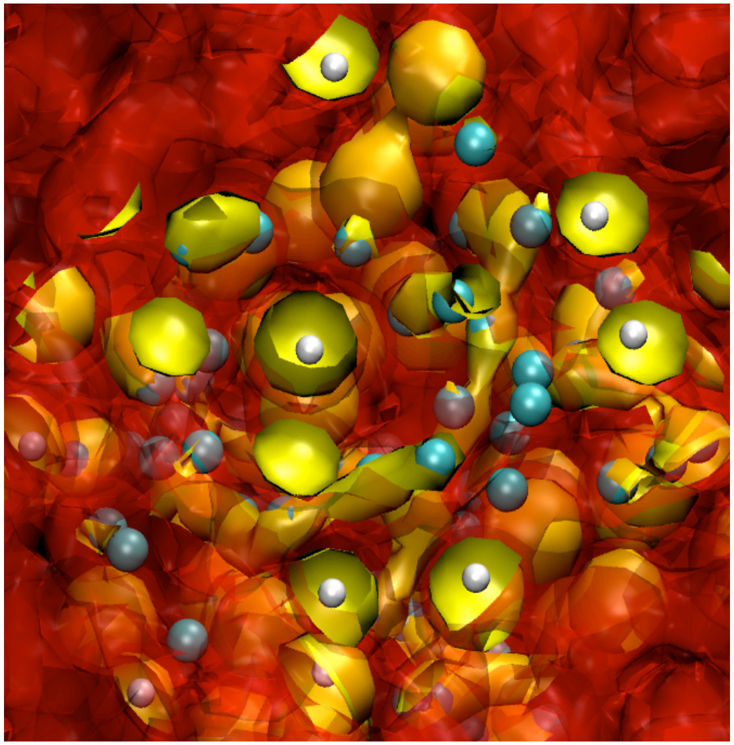
First-Principles Simulations in Planetary Science



Burkhard Militzer

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June 20, 2008

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Outline and Acknowledgements

Hydrogen-helium calculation:

Path Integral Monte Carlo (PIMC)

Density Functional Theory

Jan Vorberger (University of Warwick, UK)
Isaac Tamblyn (Dalhousie Univ., Halifax)

Modeling of Jovian planets:

Bill Hubbard (LPL, University of Arizona, Tucson)
David Stevenson (Caltech)

QMC of solid helium:

Saad Khairallah (UC Berkeley)

Supported by NASA and NSF.

Outline and Acknowledgements

Main points:

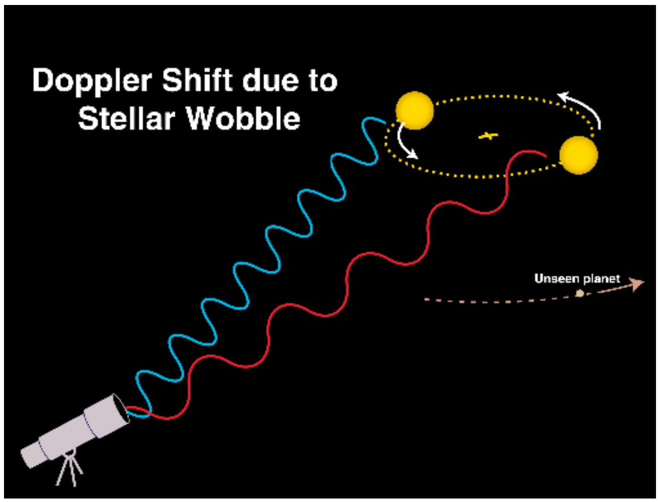
I. Jupiter has a solid core of 16 Earth masses.

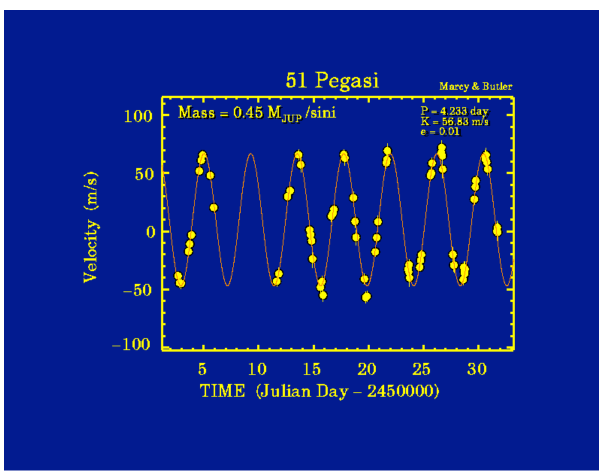
II. It does not rotate as a ``solid'' body $\Rightarrow$ differential rotation on cylinders.

Supported by NASA and NSF.

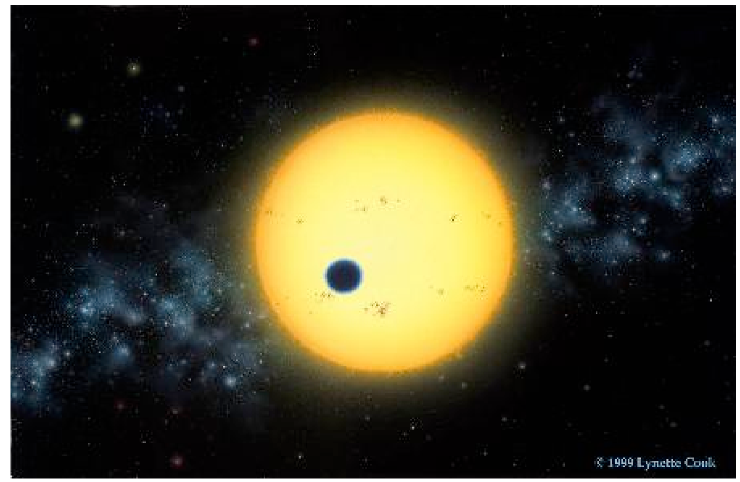
Detection techniques for extrasolar planets: radial velocity technique, transient method, …

270+ planets found with radial velocity meas.





14 planets seen with transient technique



First planet detected:

Mayor & Queloz, Nature 378 (1995) 355
(Geneva Observatory)

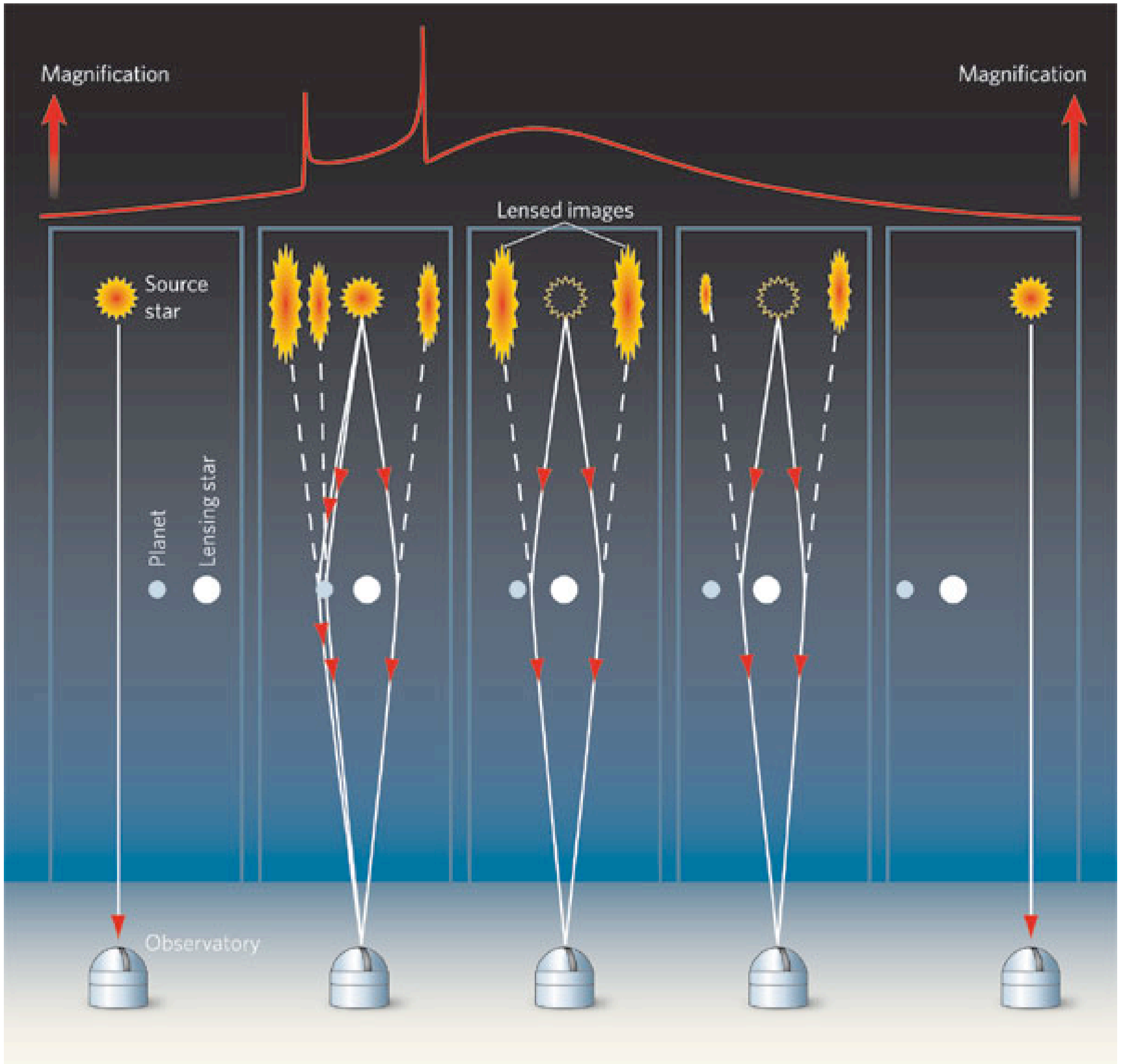
Orbital period: 4.23 days !
Msin(i) = 0.46
a = 0.05 AU

2006: Third technique finds extrasolar planets: observation of gravitational microlensing events

So far, 4 planets found by observation of gravitational microlensing events.

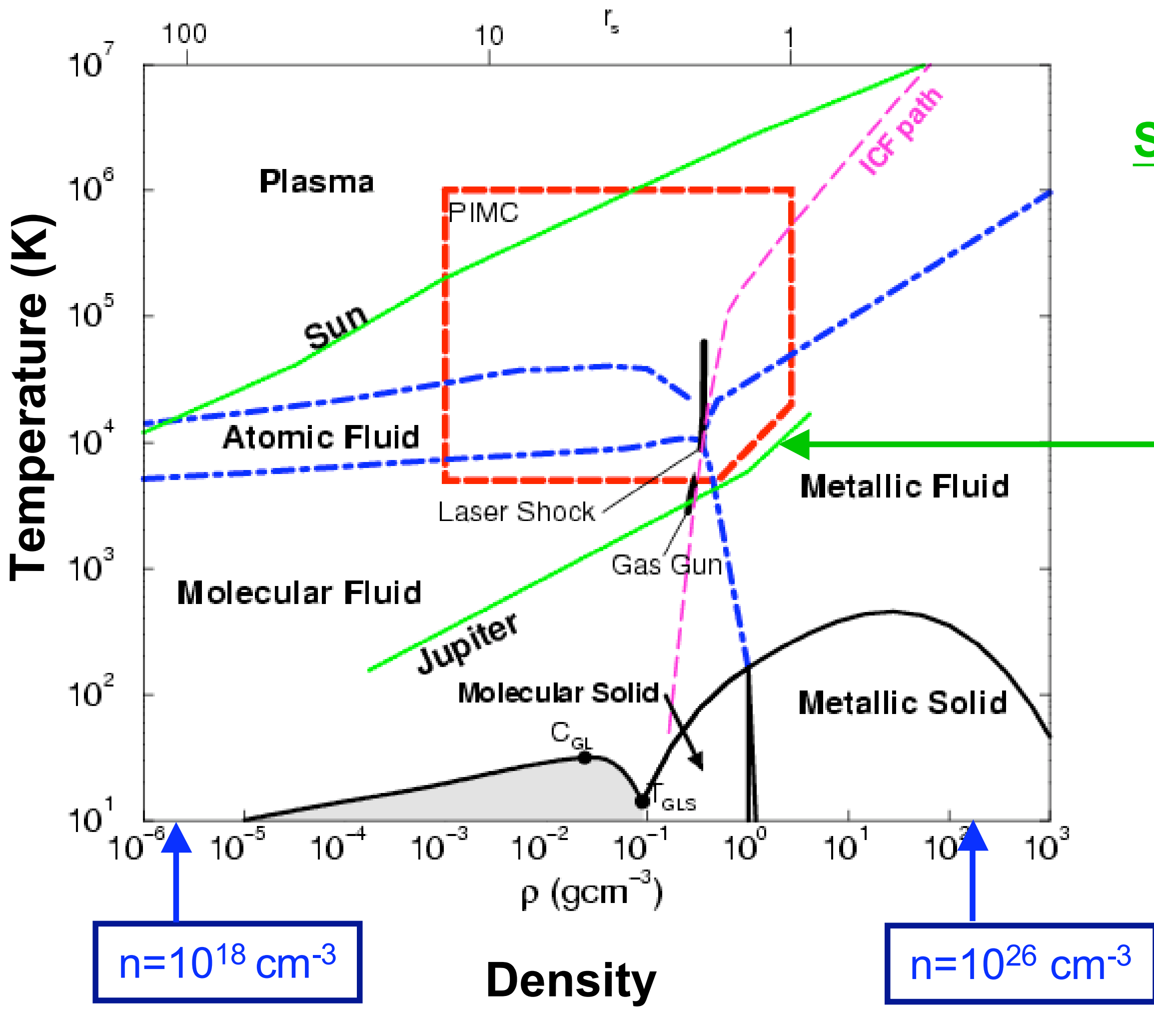
J.P. Beaulieu et al, Nature (2006).

Detected planet well below the Doppler detection limit.

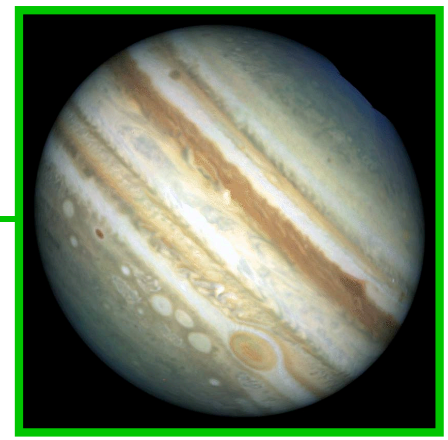


D. Queloz, Nature, New & Views (2006).

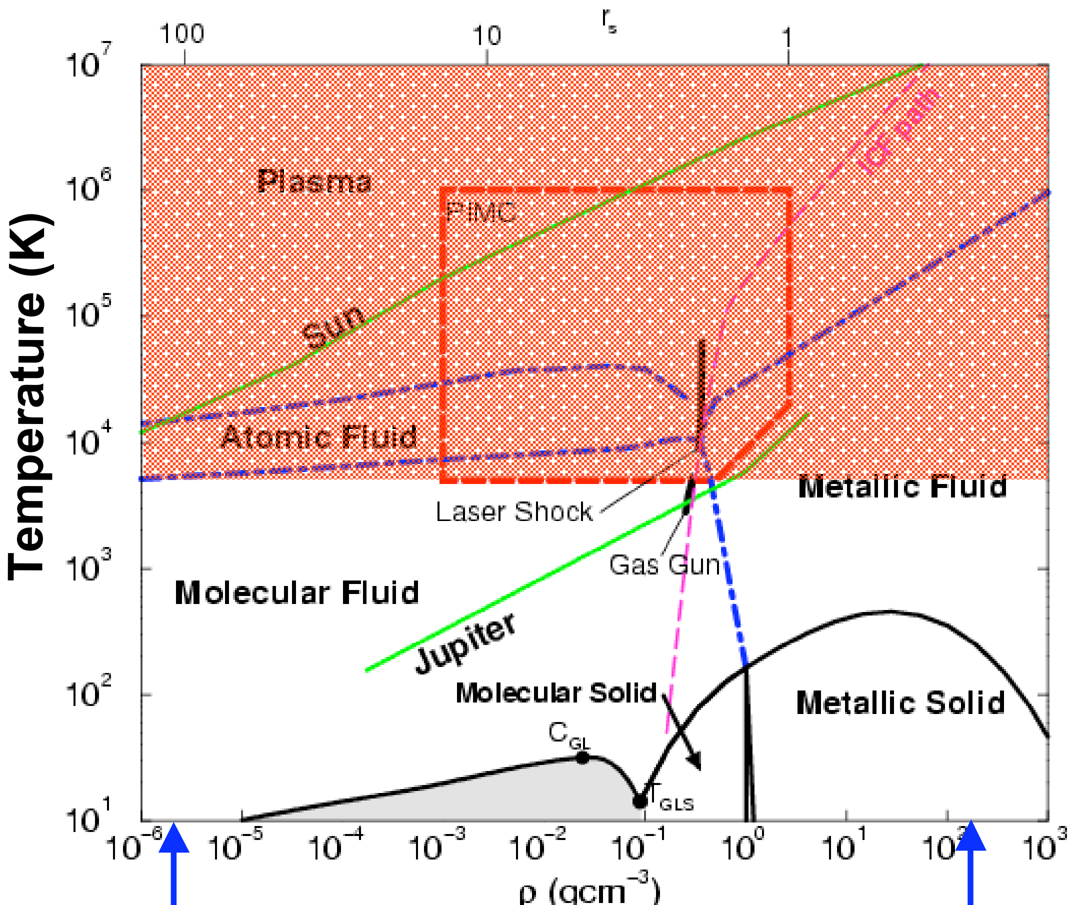
Focus: Characterization of the Interior of Solar and Extrasolar Giant Planets



Solar GP: Jupiter, Saturn

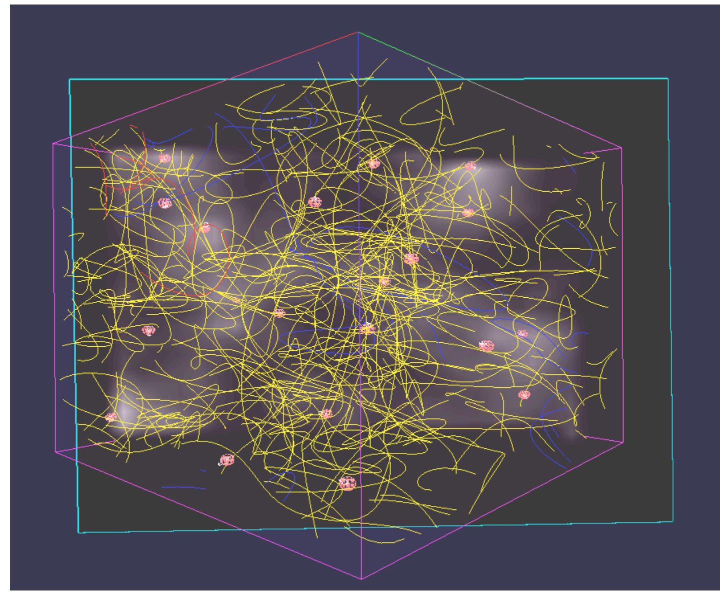


1) Path integral Monte Carlo for T>5000K



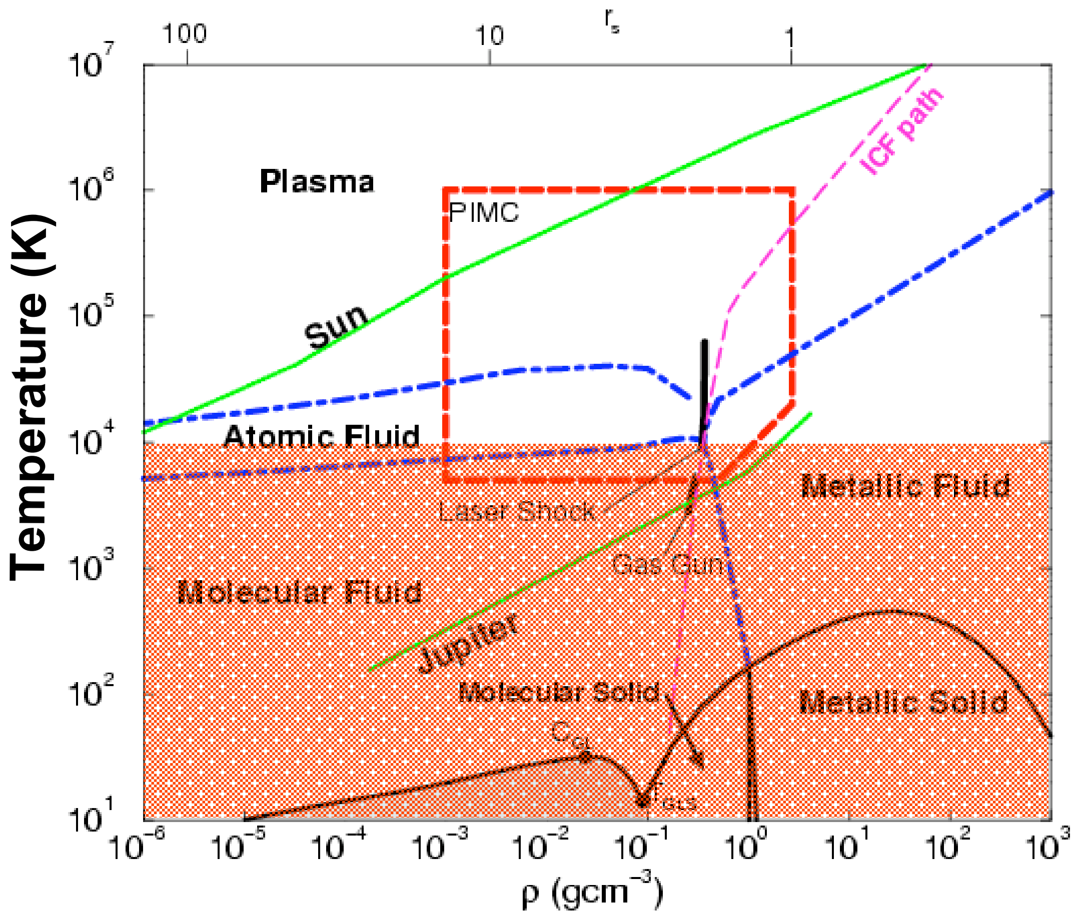
n=10^{18} cm^{-3}

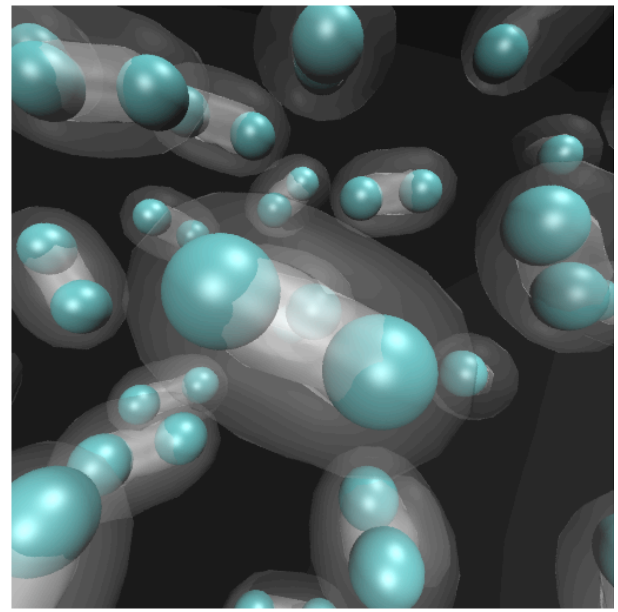
n=10^{26} cm^{-3}



PIMC applicable at:
T>5000K

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



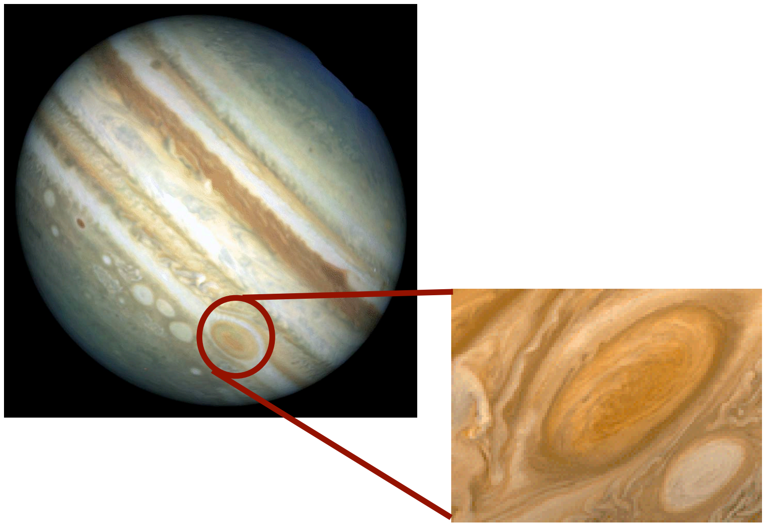


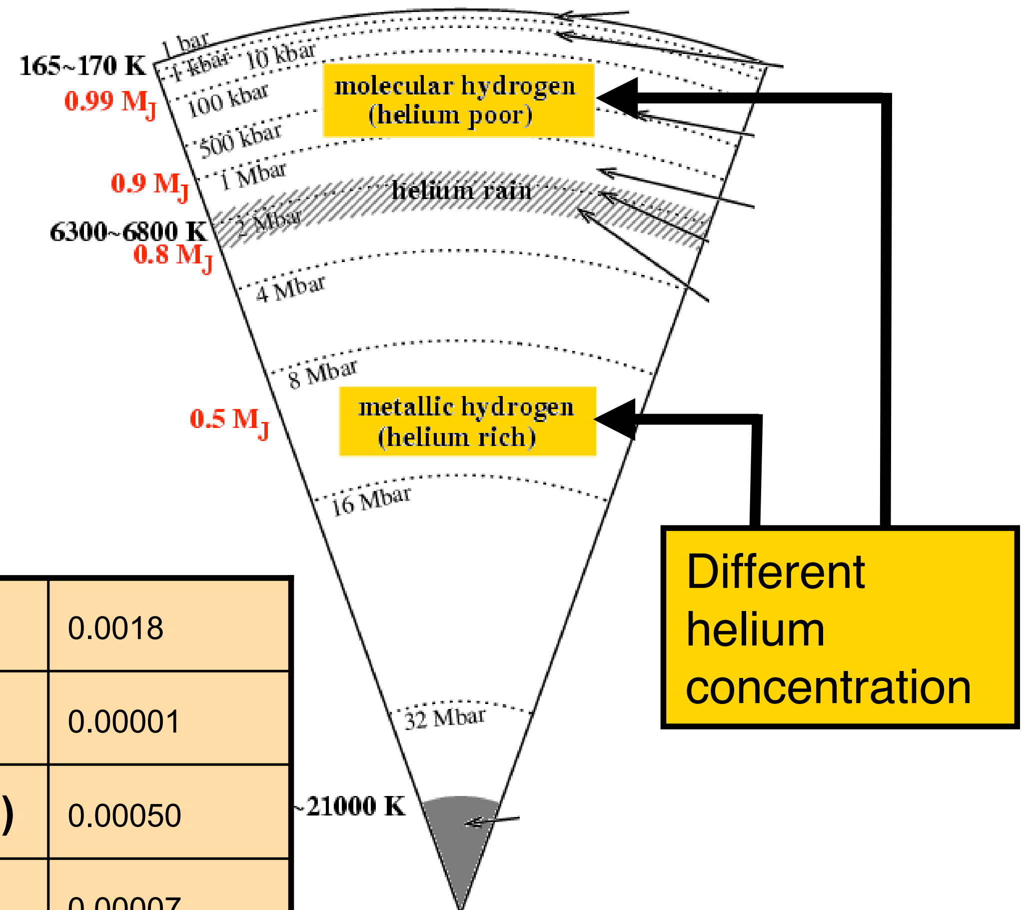
Born-Oppenheimer approx.
MD with classical nuclei:

F = m a

Forces derived DFT with electrons in the instantaneous ground state.

Previous Jupiter Models with 3 Layers



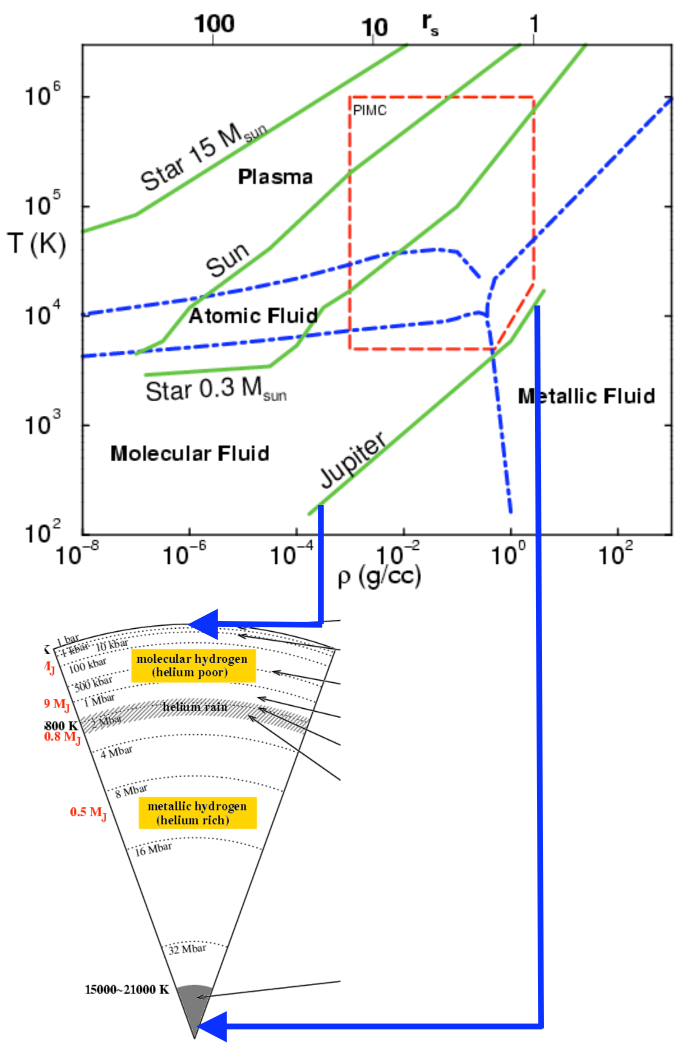


Guillot et al. (Jupiter book, 2002, chap.3)

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

H	**0.742**	0.736	**Ne**	**< 0.0002**	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

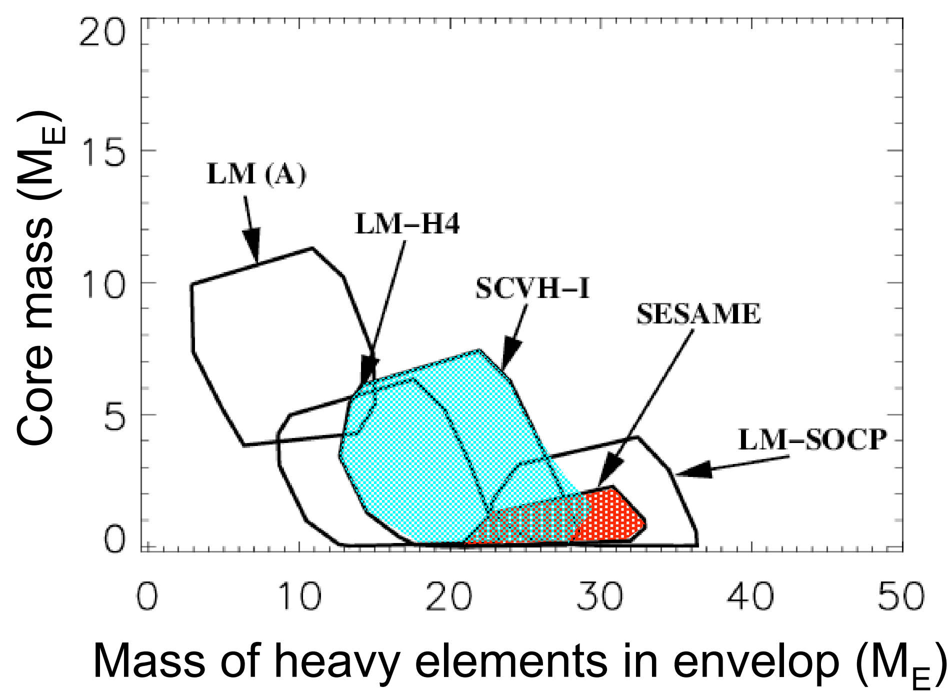
T. Guillot's model: Uncertainties in EOS do not allow to determine if Jupiter has a rocky core



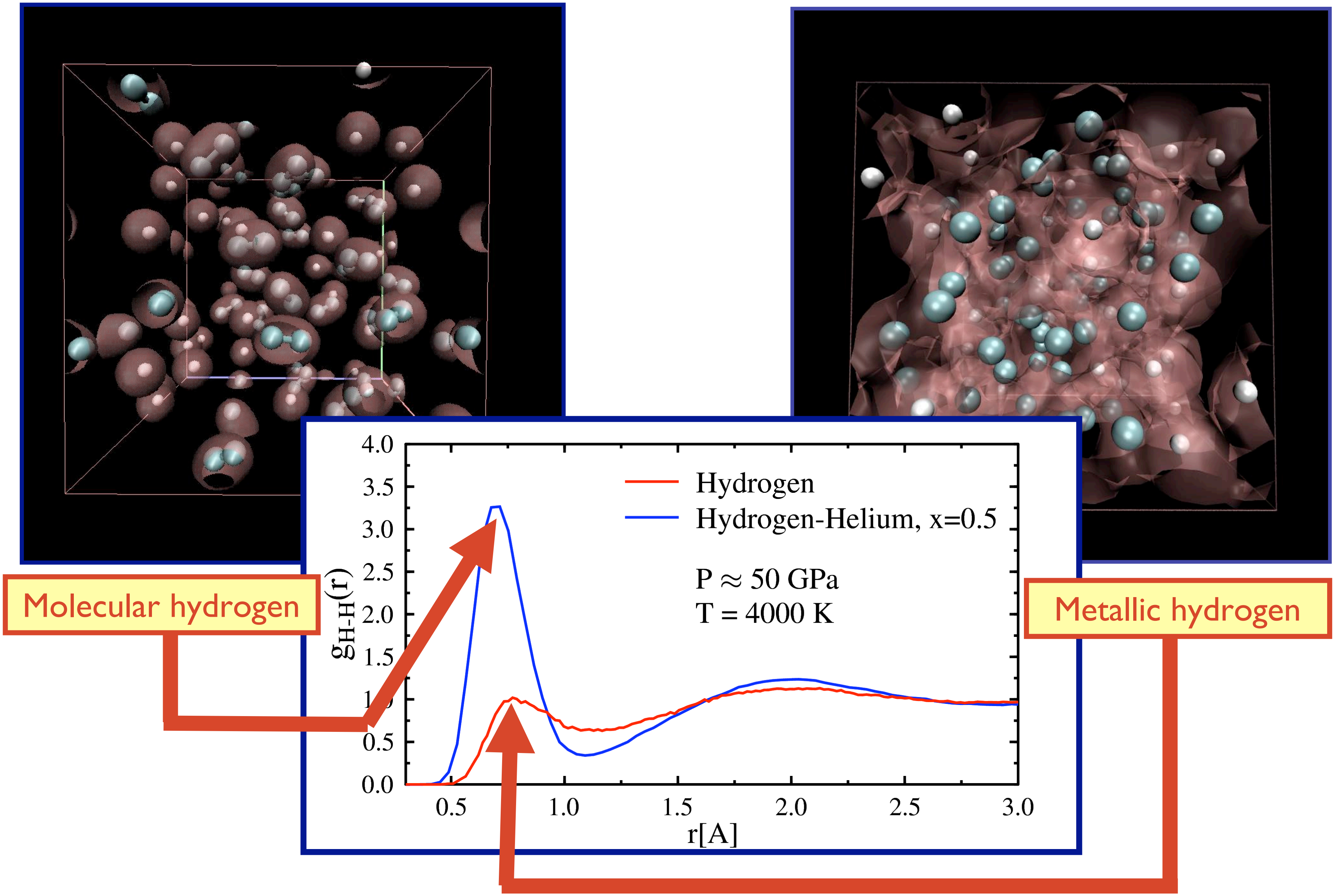
T. Guillot's three layer model is based on

1) Hydrogen-helium EOS
2) Surface composition
3) Gravitational moments inferred from fly-by trajectories (Cassini mission)

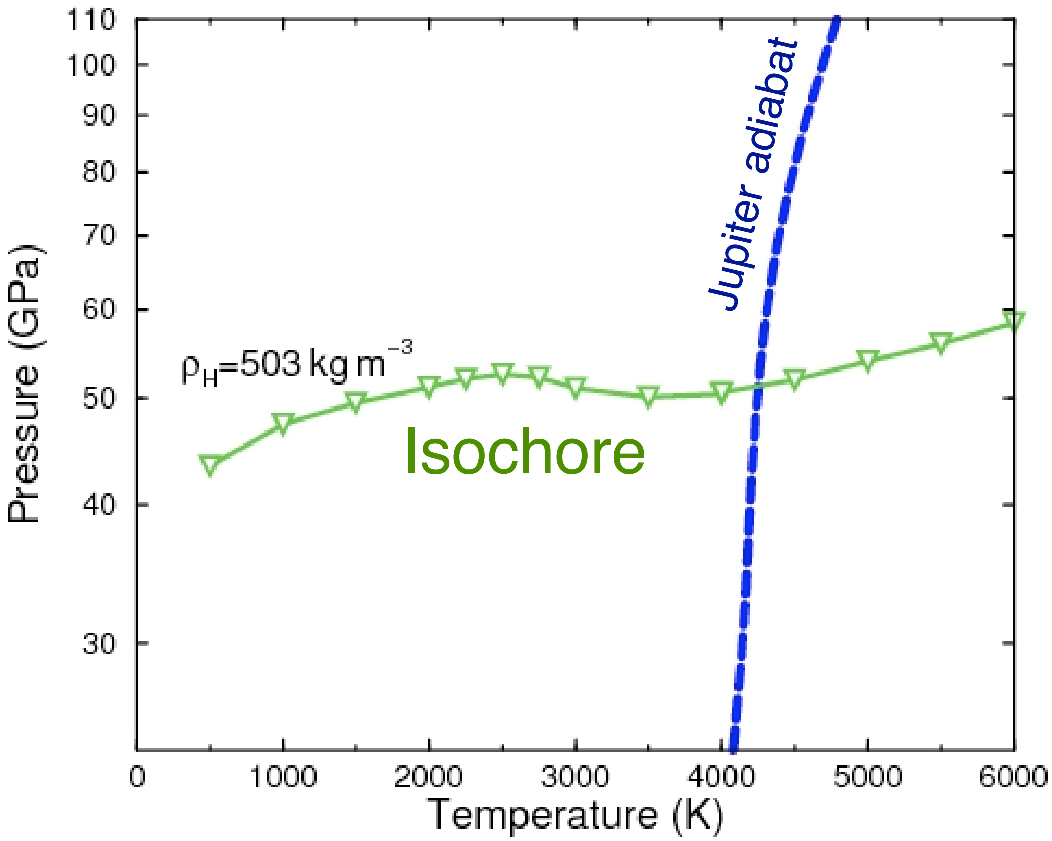
Parameters like core mass or amount of heavier



Simulations show that helium stabilizes H_2 molecules



Molecular-to-metallic transition in fluid hydrogen studied with DFT simulations



- Molecular to atomic transition is continuous as function of T (must use BOMD not CPMD)
- Negative $dP/dT|_V < 0$ region for pure hydrogen

J. Vorberger, I. Tamblyn, B. Militzer, S. Bonev, "Hydrogen-helium mixtures in the interior of giant planets", *Phys. Rev. B* **75** (2007) 024206.

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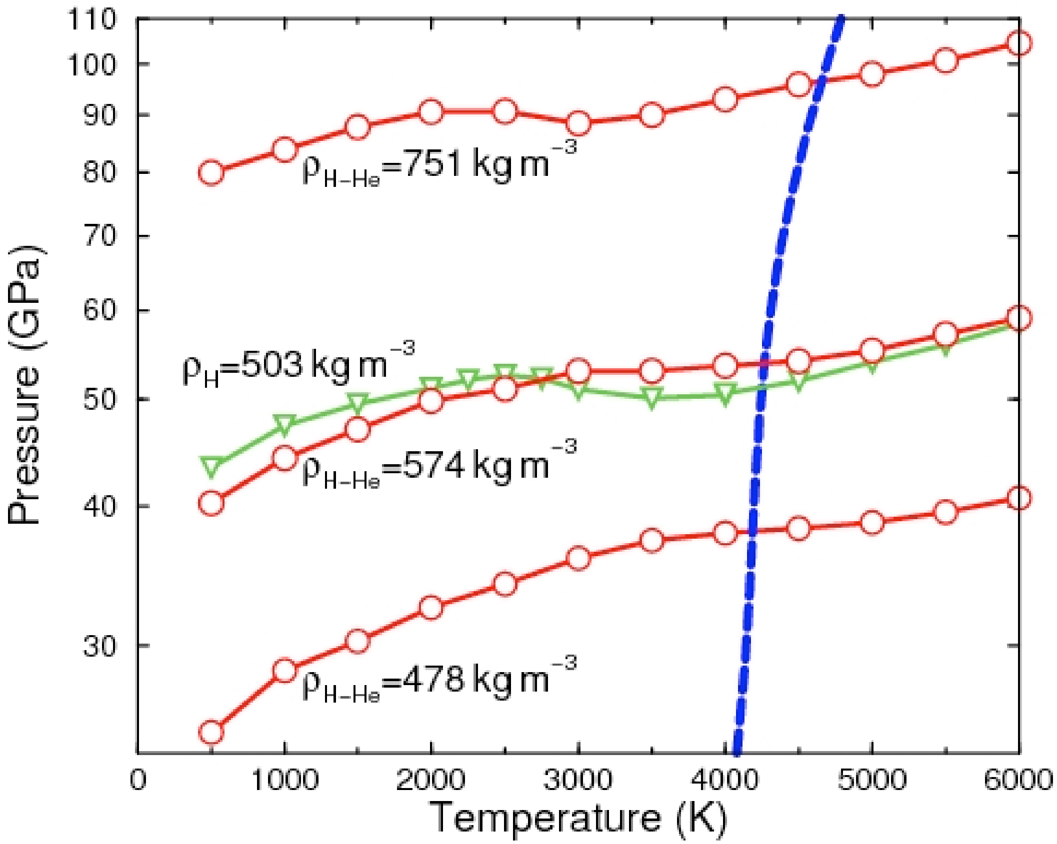
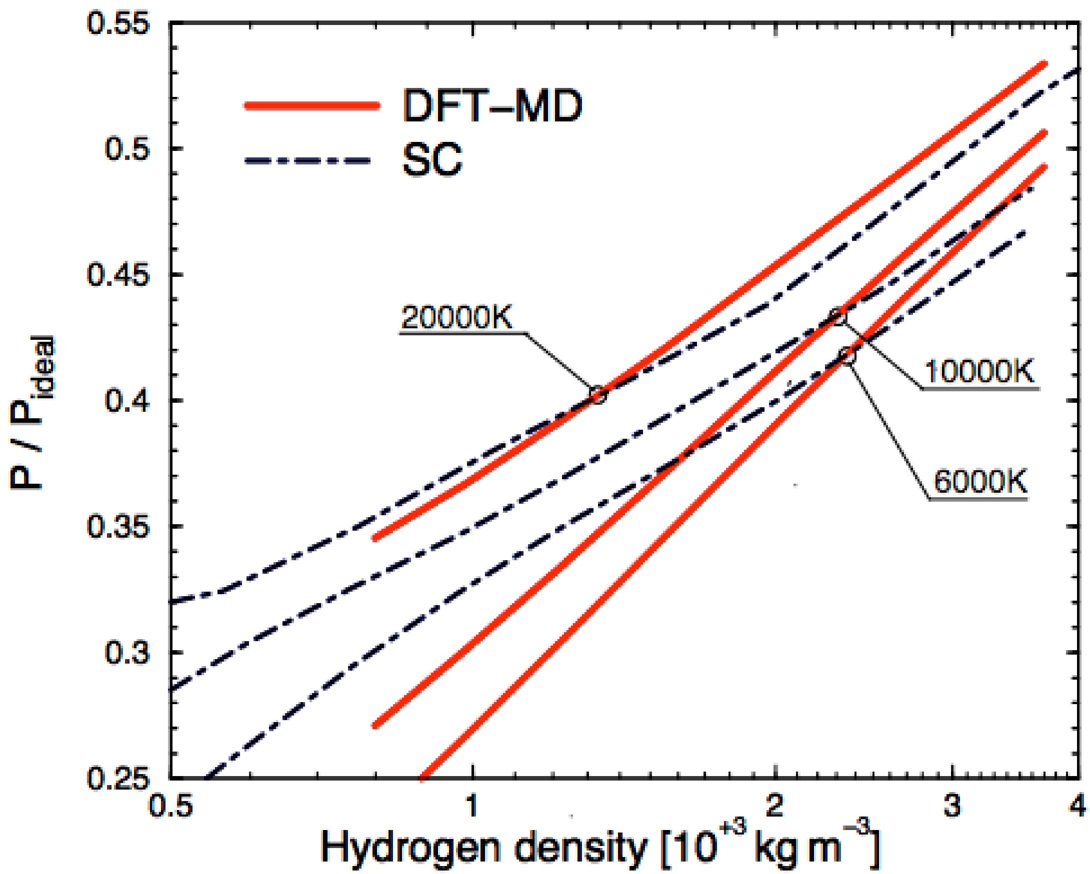


- Molecular to atomic transition is continuous as function of T (must use BOMD not CPMD)
- Negative $dP/dT|_V < 0$ region for pure hydrogen
- No such region: H-He mixtures
- *Jupiter envelope is isentropic, fully convective and of constant chemical composition.*

J. Vorberger, I. Tamblyn, B. Militzer, S. Bonev, "Hydrogen-helium mixtures in the interior of giant planets", *Phys. Rev. B* **75** (2007) 024206.

Comparison of first-principles EOS with analytical Saumon-Chabrier-Van Horn model



The most important difference were found in the regime of metallic hydrogen where little experimental EOS data are available.

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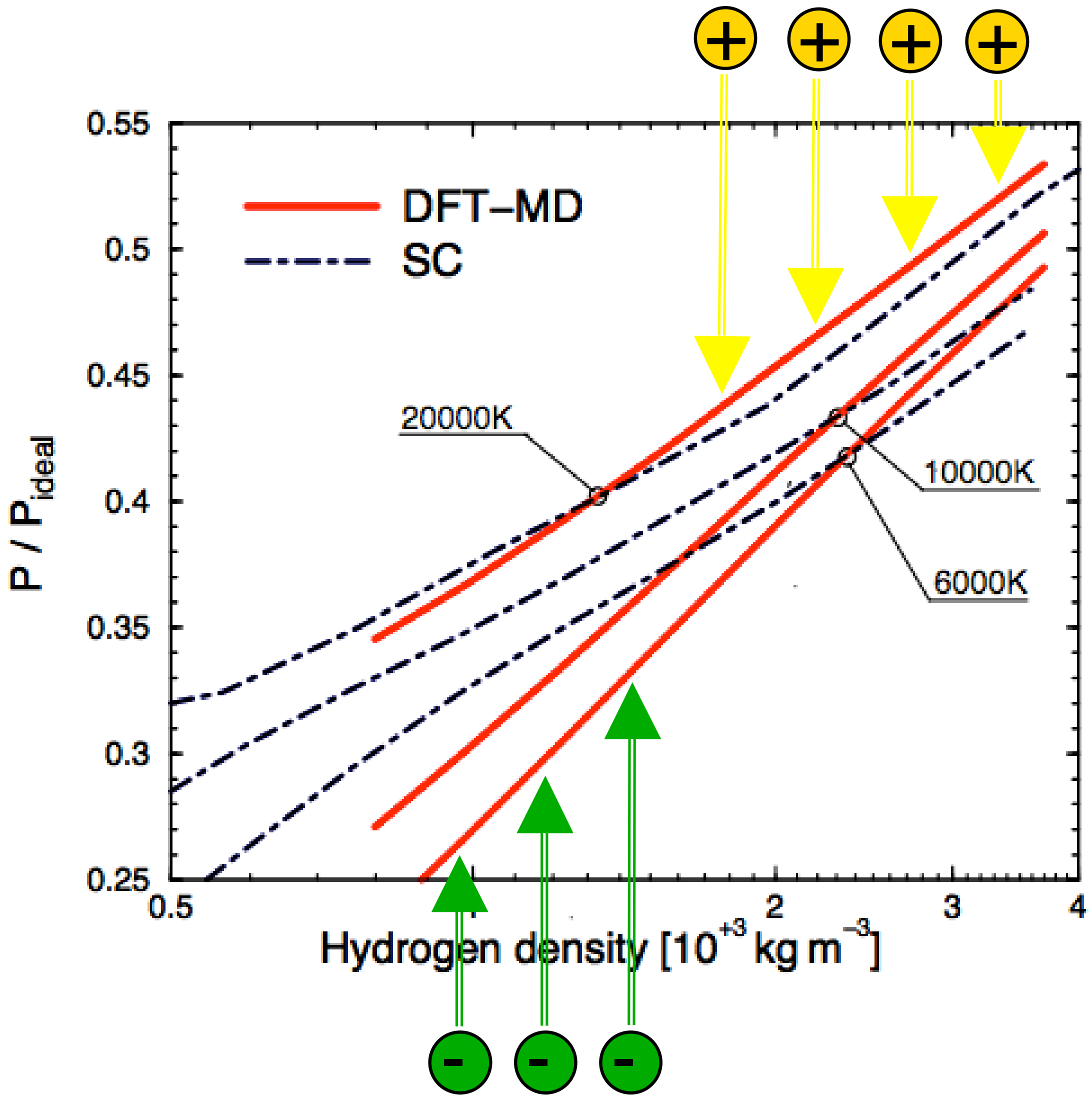

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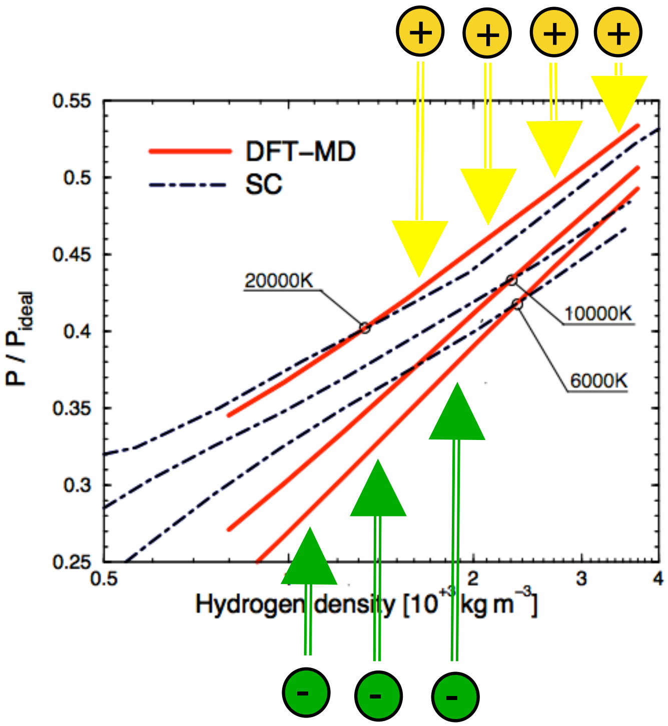
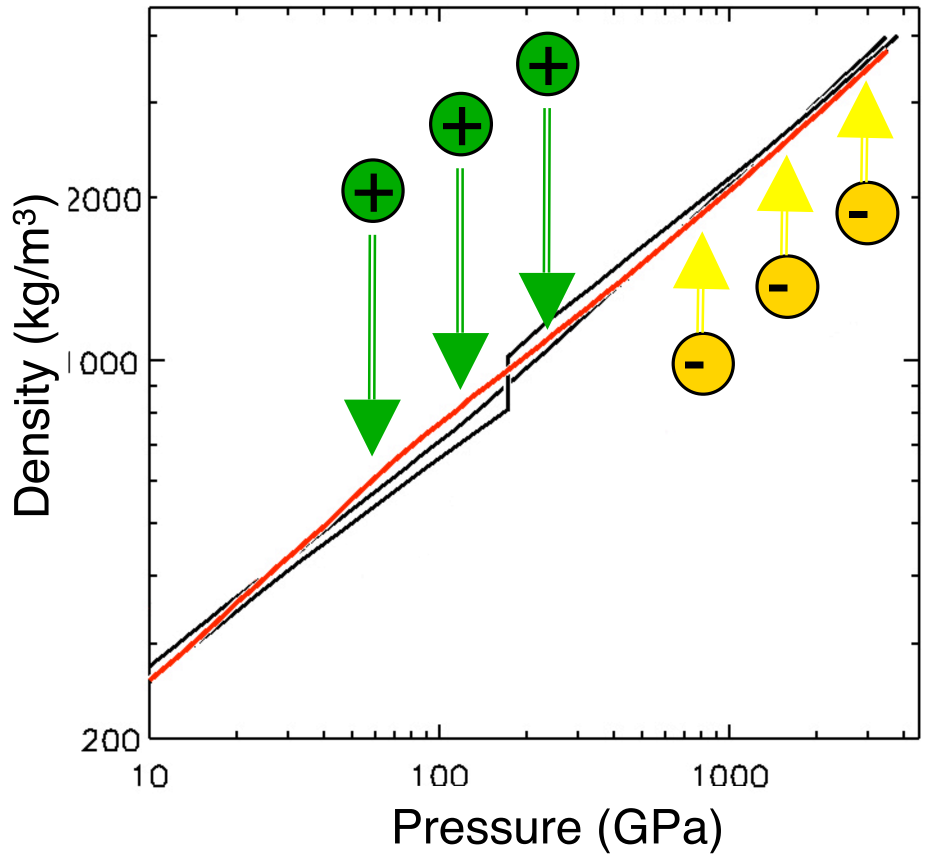
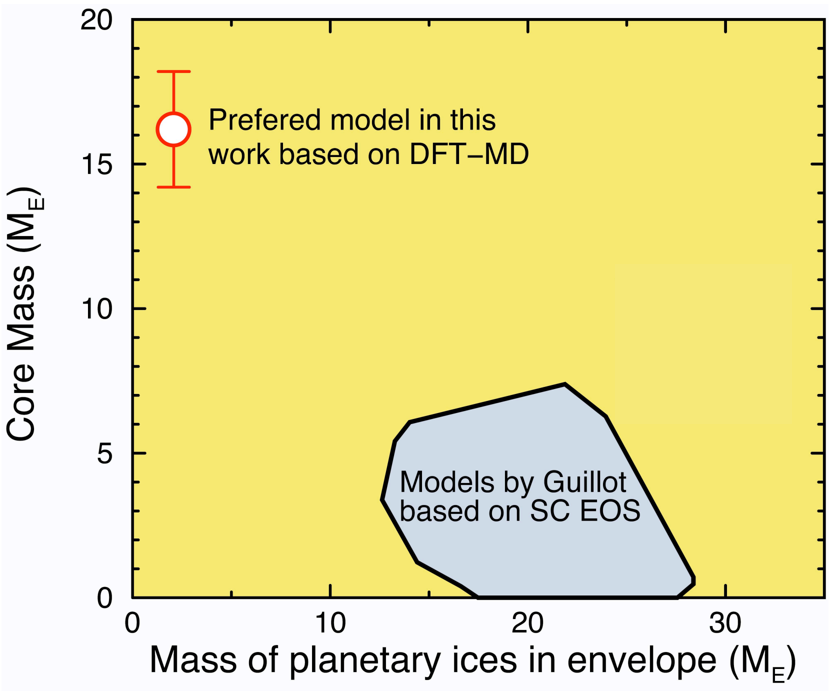


Direct EOS comparison

Comparison of the resulting Jupiter models
⇒ Different density profile

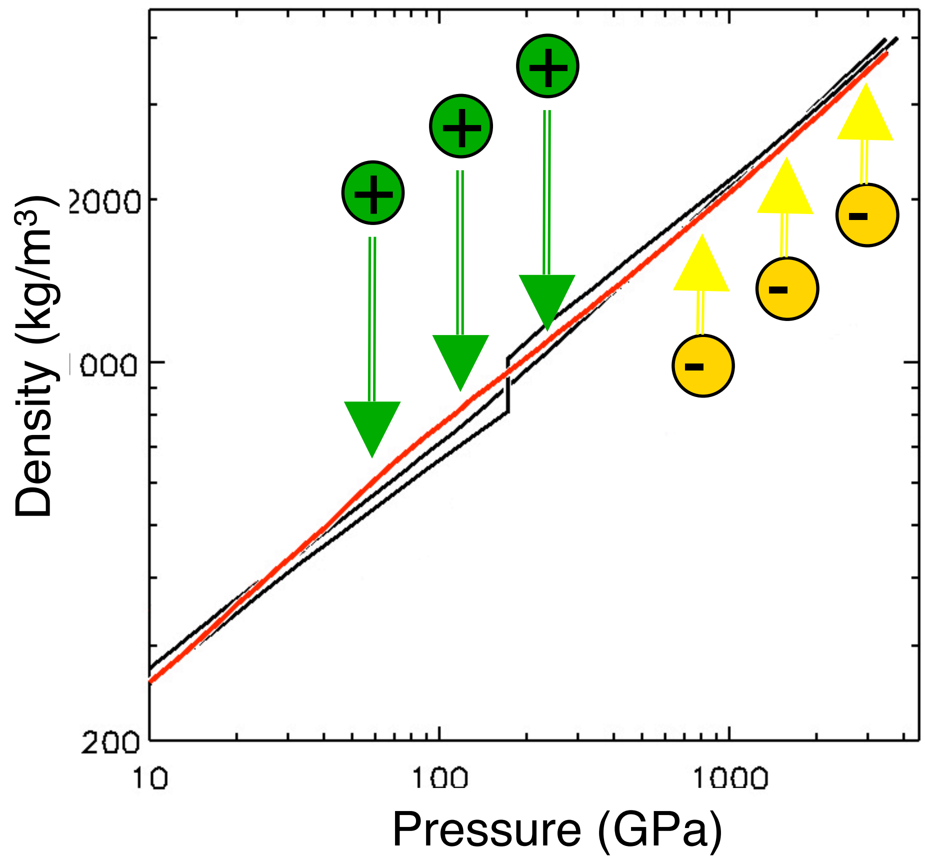


DFT-MD Simulations Predict A Massive Core in Jupiter

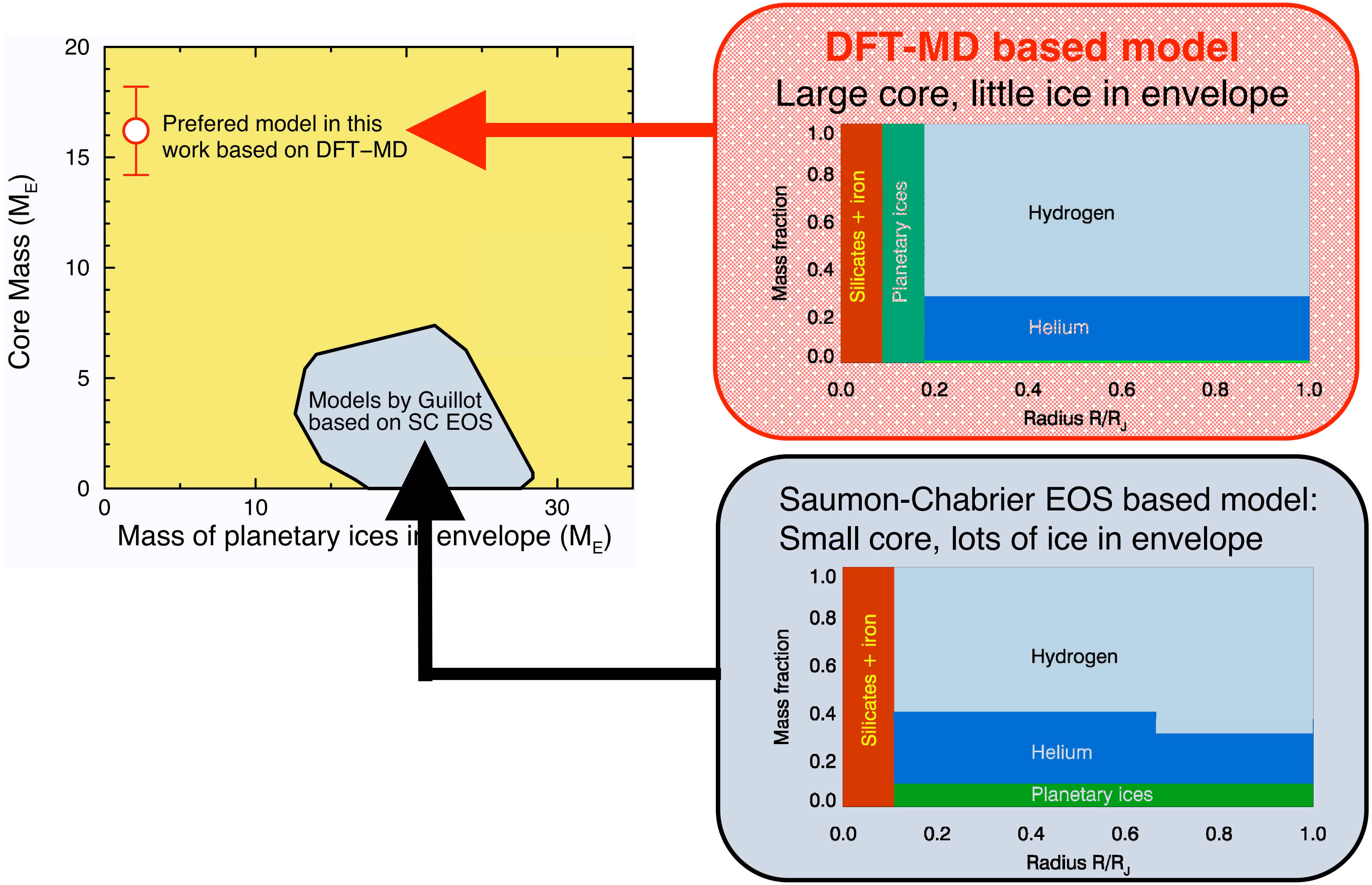


Core mass of 16 M_E predicted!

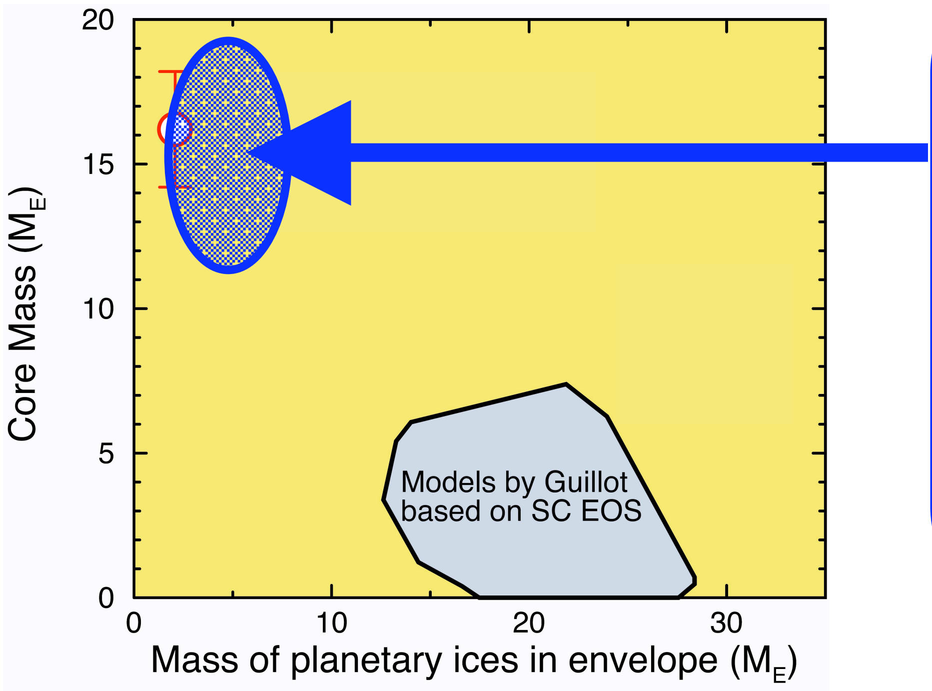
Comparison of the resulting Jupiter models
⇒ Different density profile



Our new 2-layer Jupiter model



Jupiter and Saturn made by same formation mechanism?



Saturn:

All models predict as large core of 10-20 Earth masses

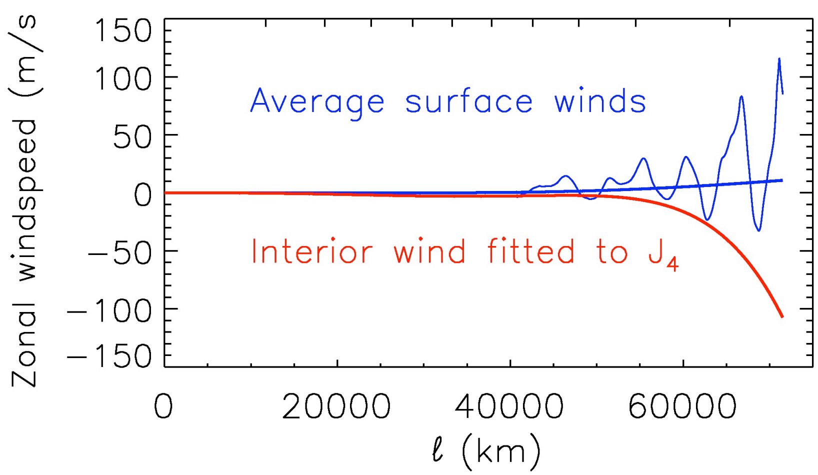
Small amount of ices in envelope 2-8 Earth masses

Guillot (2004)

Nasa mission to Jupiter: Juno, a low periapse orbiter
High quality gravity and magnetic field data expected during 2016.

Predictions: Jupiter does not rotate as a solid body ⇒ deep interior winds

Model	Equatorial radius (km)	$J_2 \times 10^6$	$J_4 \times 10^6$	$J_6 \times 10^6$
Observed	71492	14696.43 ± 0.21	-587.14 ± 1.68	34.25 ± 5.22
Solid-body rotation	Matched	Matched	-620	37.5
Preferred model: deep winds	Matched	Matched	Matched	23.9



Summary: New Jupiter Model

- EOS from first-principles simulations (DFT-MD)
- Continuous molecular-to-metallic transition
  ⇒ the planet is fully convective
- Massive core of 16 Earth masses predicted
- Small amount of ices in evelope
- Favored formation mechanism: core-accretion
- To match J_4, we propose differential rotation

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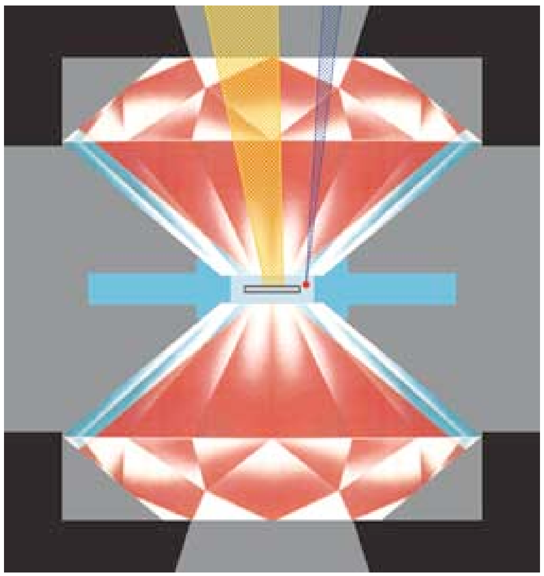
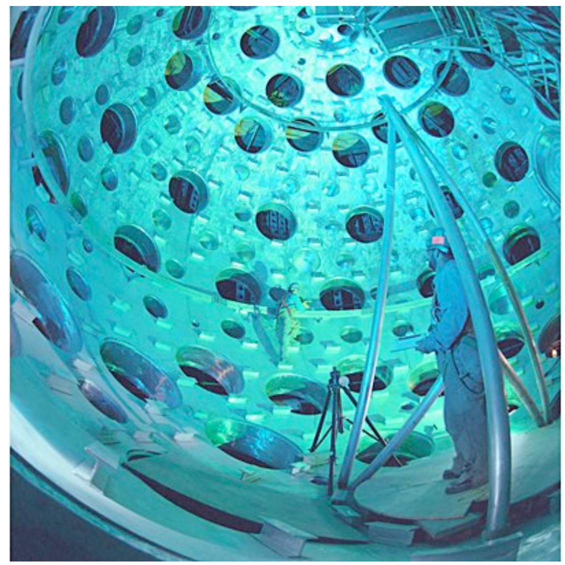
New Experimental Technique: Combination of Static and Dynamic Compression

1) Static compression
Diamond anvil cell

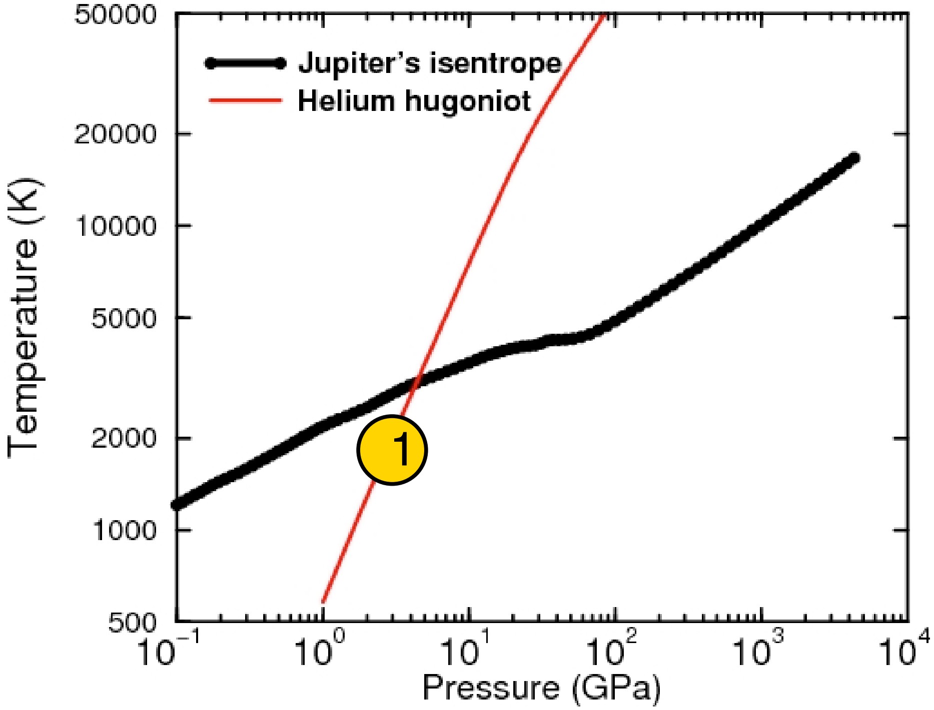


2) Dynamic shock comp.
Laser shocks

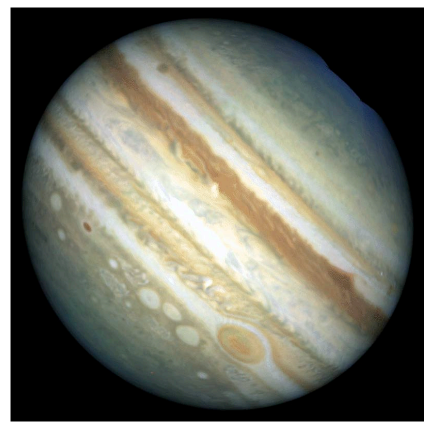


- LLNL-CEA collaboration
- Samples are **precompressed** in modified diamond anvil cell
- Precompression up to 1.5 GPa = 15 kbar

How far into in Jupiter's interior can be probed with precompressed shocks?

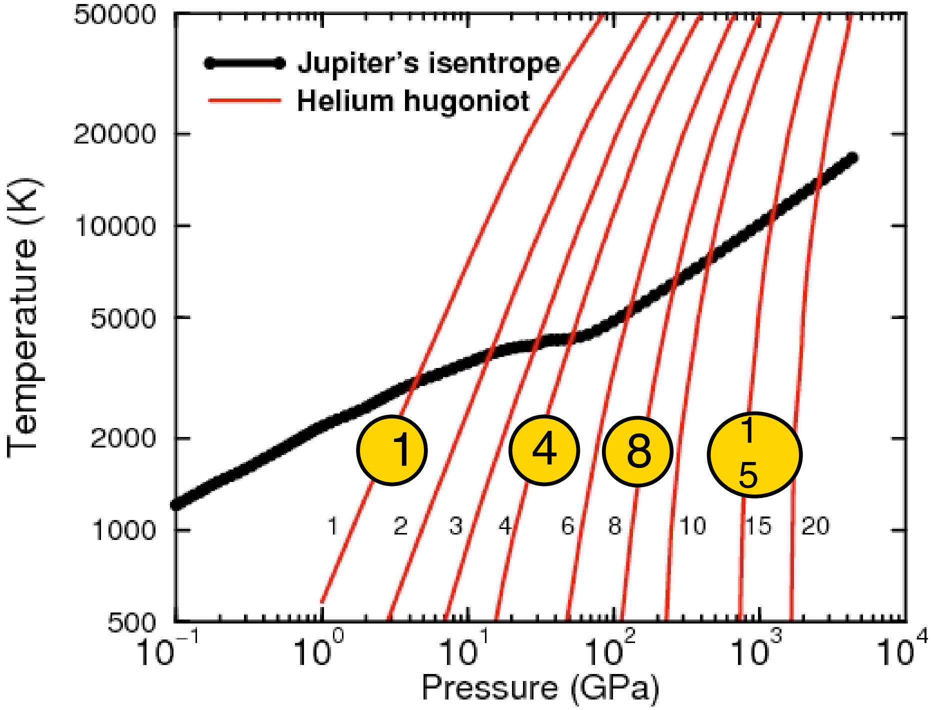


Where does the helium hugoniot intersect with Jupiter's isentrope?



	Precompression	P_0	P_H(GPa)	T_H(K)	Mass fraction	$1-R_H/R_J$
He	1	1 bar	4.4	3000	0.5%	3%

Precompression up to 100 GPa is needed to study Jupter's interior



APS proceedings article (2007)

Militzer, Hubbard, [arXiv:0707.4649]

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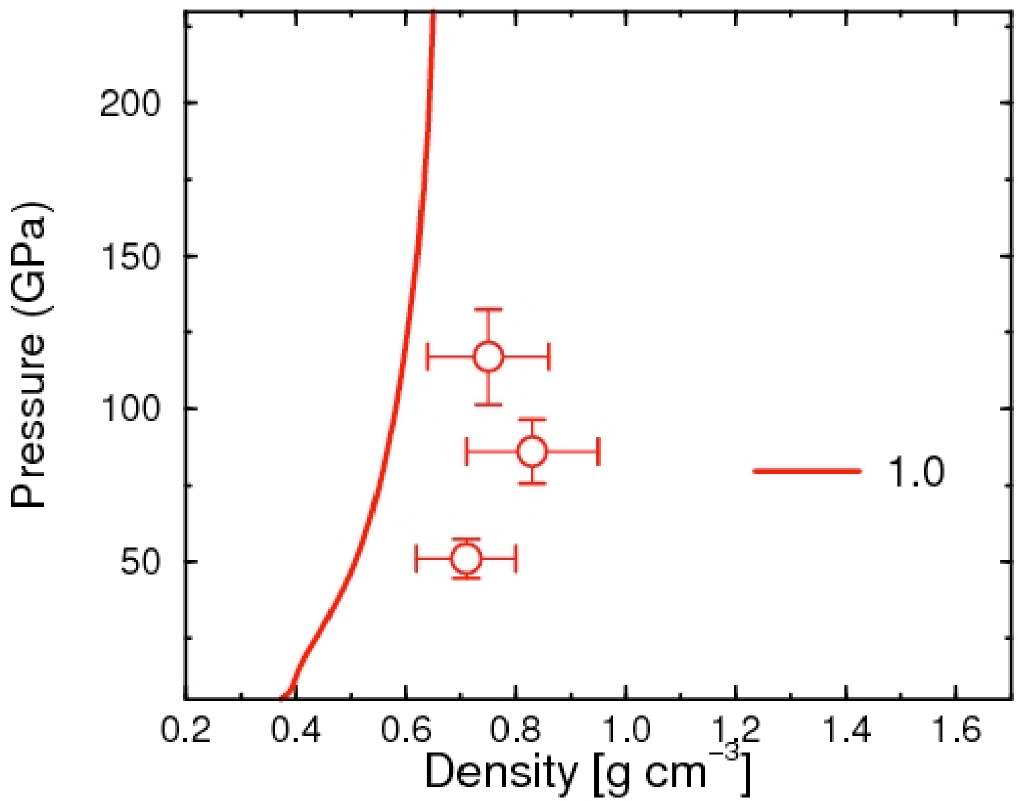
He	1	1 bar	4.4	3000	0.5%	3%
He	4	0.75 GPa	51	4200	5%	10%
He	8	13 GPa	261	6500	21%	
He	15	93 GPa	1200	11000	62%	

Comparison of PIMC Simulations with Laser Shock Experiments on Helium



Principal Hugoniot:

PIMC predicts a lower compressibility.

Theory: Militzer, *Physical Review Letters,* **97** (2006) 175501;
Exp: Eggert *et al. Physical Review Letters*, 100 (2008) 124503.

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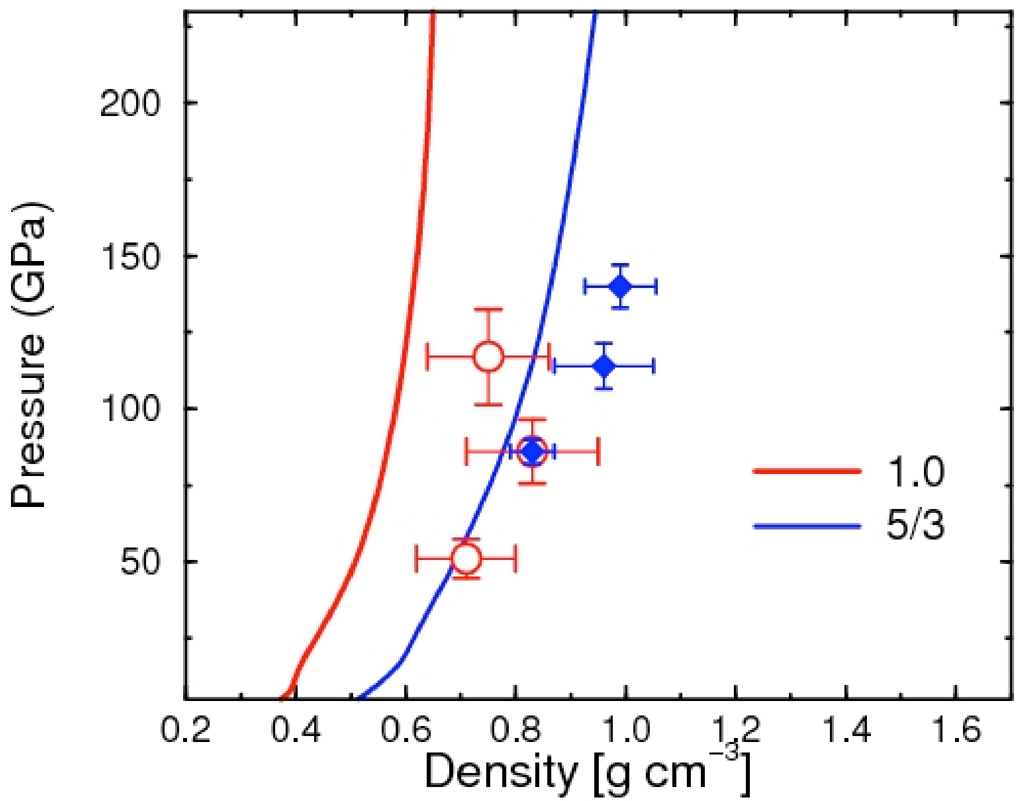

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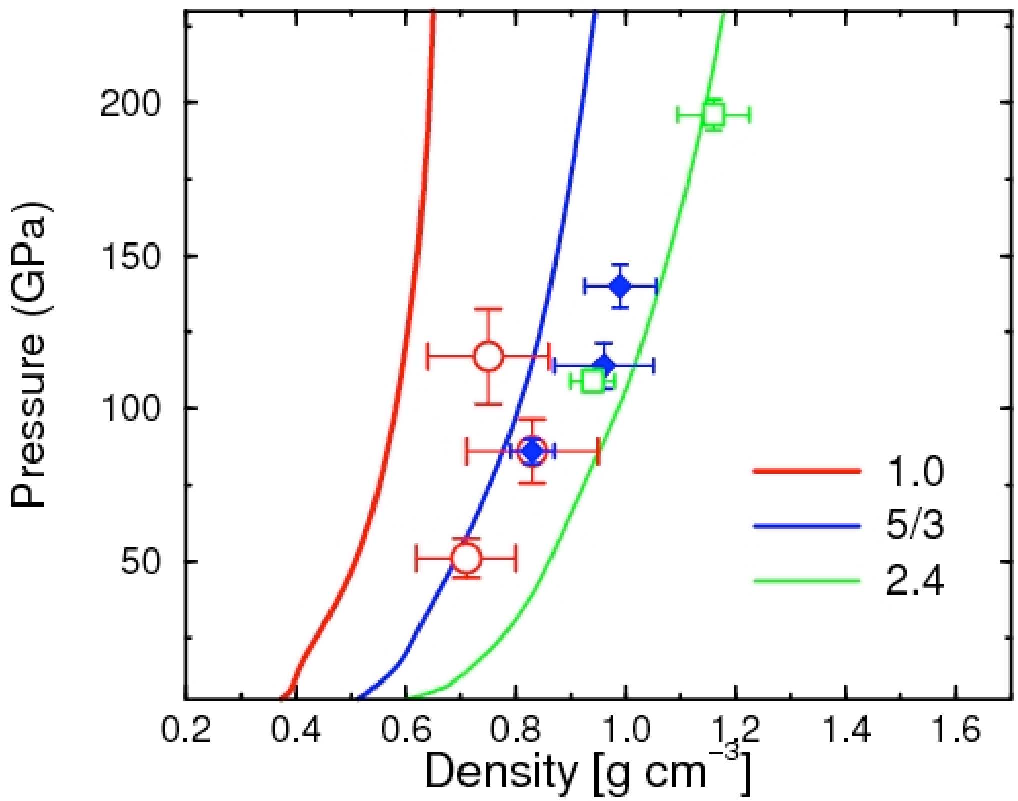

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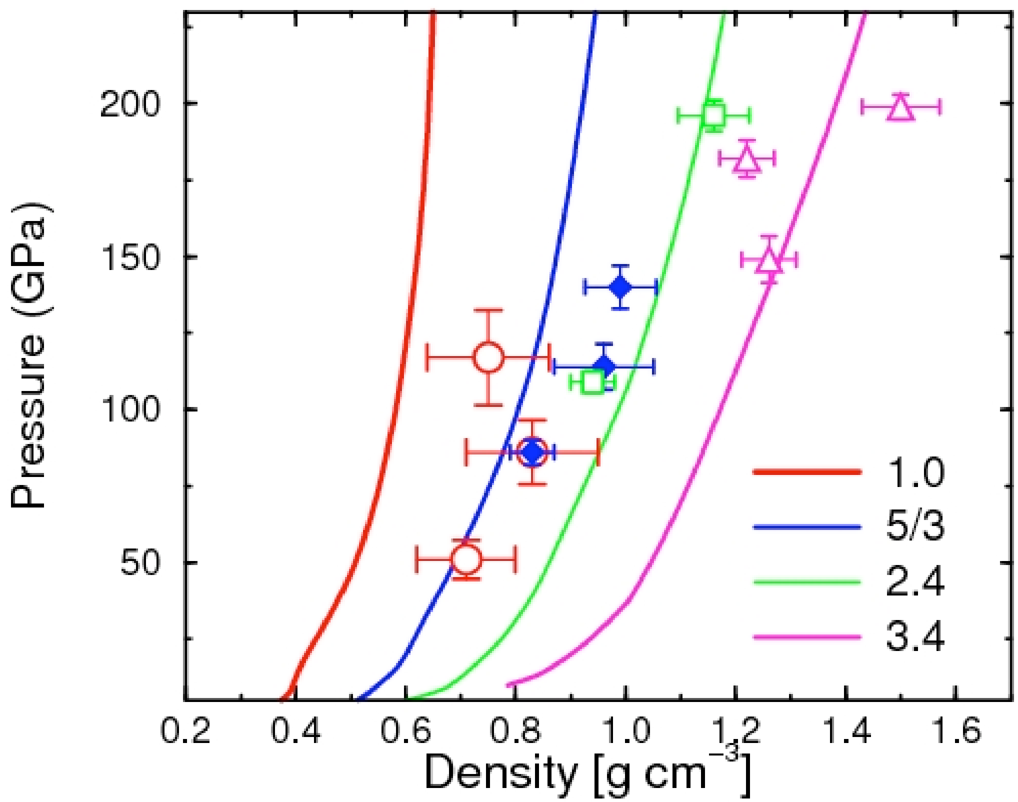

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With 3…4-fold precompression:

PIMC and experiment agree.

Theory: Militzer, *Physical Review Letters,* **97** (2006) 175501;
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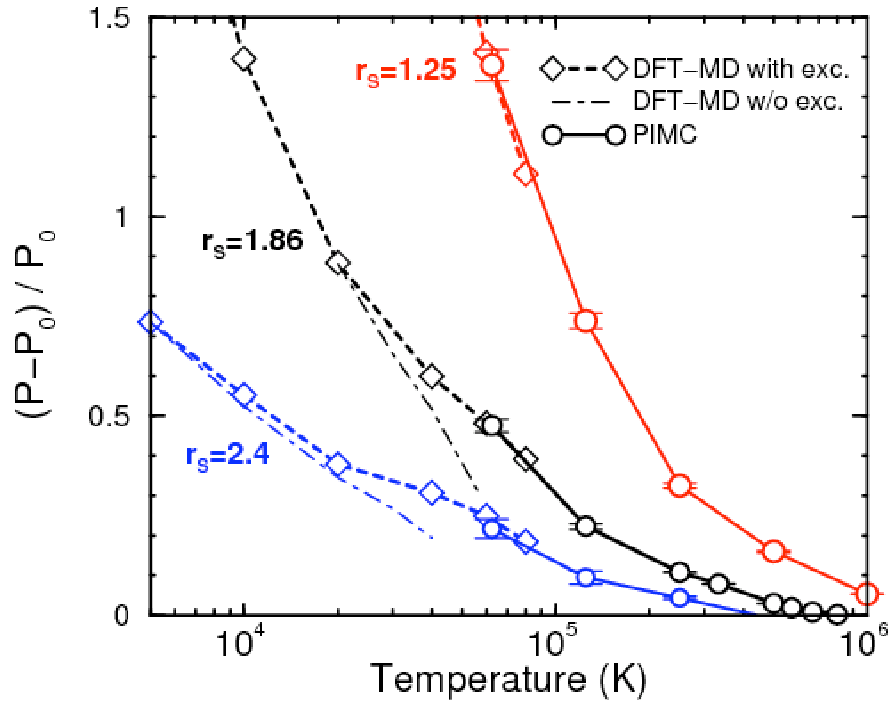
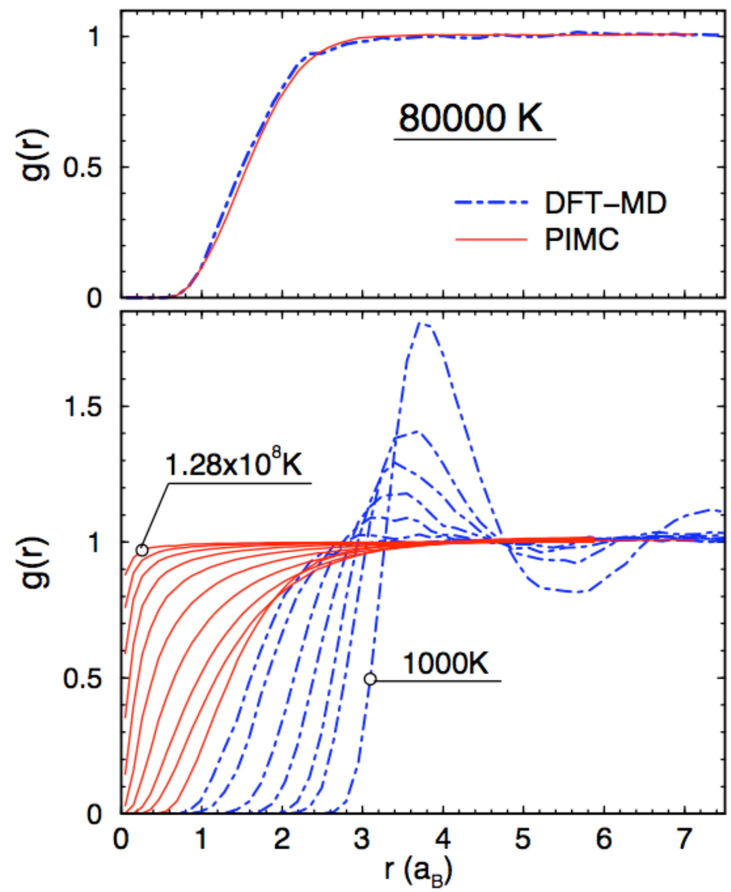
Marry PIMC and DFT-MD EOS Calculations for Dense Fluid Helium

Compare P(T) for a wide range of densities:



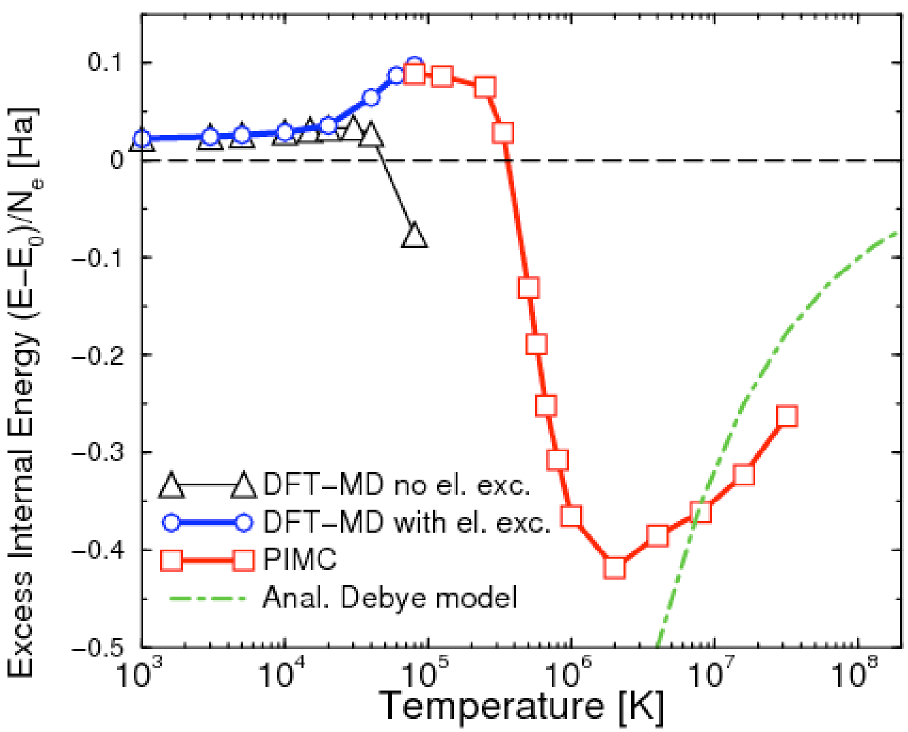


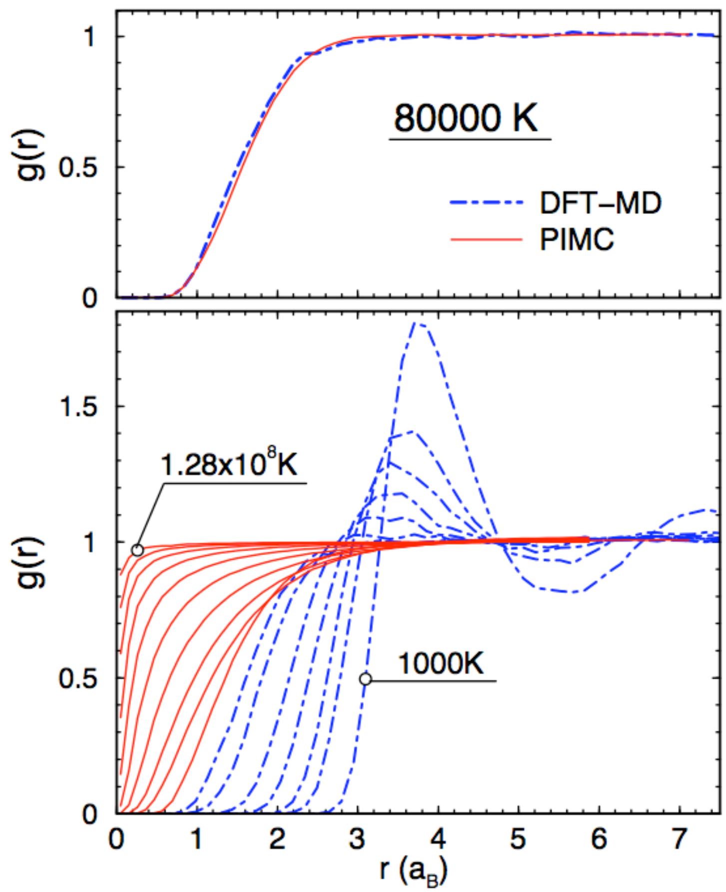
Good agreement found if excited states are included in DFT-MD.

B. Militzer, submitted to *Physical Review B (2008), see* **arXiv:0805.0317**

Marry PIMC and DFT-MD EOS Calculations for Dense Fluid Helium

Compare E(T) for density of r_s=1.86





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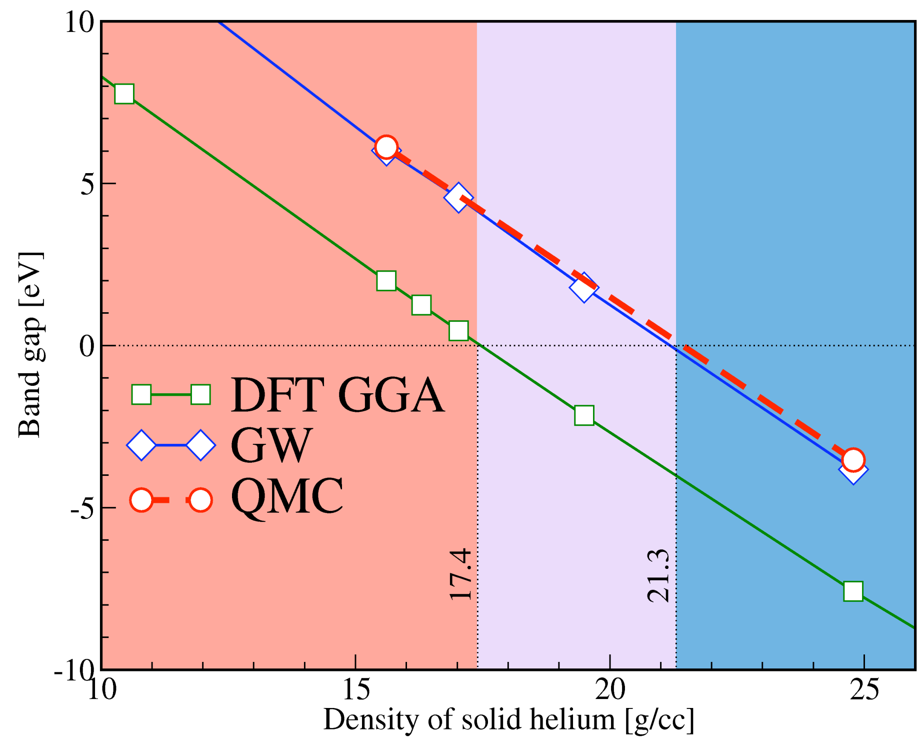
QMC Calculation of the Metallization of Solid Helium under Pressure

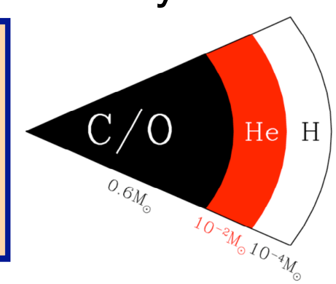
Method comparison

- ◆ QMC and GW: agreement
- ◆ GGA:
  - ×Underestimates gap by 4eV
  - ×40% difference in pressure
  - ×20% difference in density

→QMC done with Casino (Cambridge).



White dwarf layers:



Solid helium metallizes at extreme pressure of 25.7 TPa. This transition is important for the heat transfer in hydrogen poor white dwarfs. Our article: **arXiv:0805.4433**

Summary and Job Advertisement

- **Theory:** First-principles simulations for giant planet interiors
    1) **Massive core of 16 Earth masses predicted**
    2) **Favored formation mechanism: core-accretion**
    3) **To match J_4, we propose differential rotation**
- **Observations:** Rapidly expanding set of known extrasolar planets
- **Experiments:** New laser shock experiments find helium more than 5-fold compressible

- **Possibility to do a PhD in my group**
- **Post-doc position open in Computational Earth and Planetary Science**

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