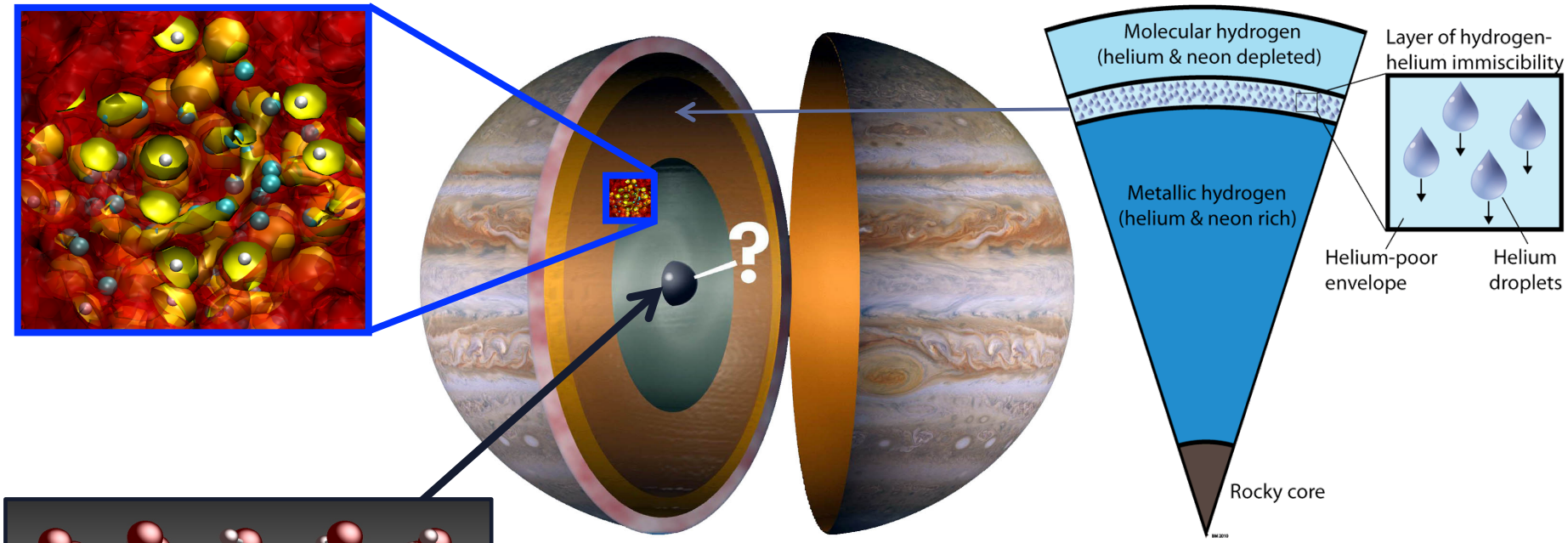
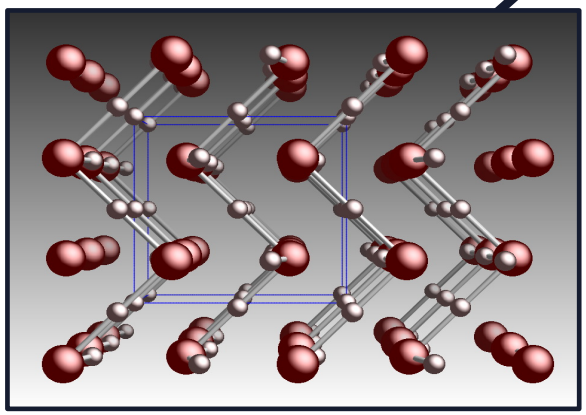
Phase Separation in Giant Planet Interiors and Novel First-Principles Simulation of Plasmas





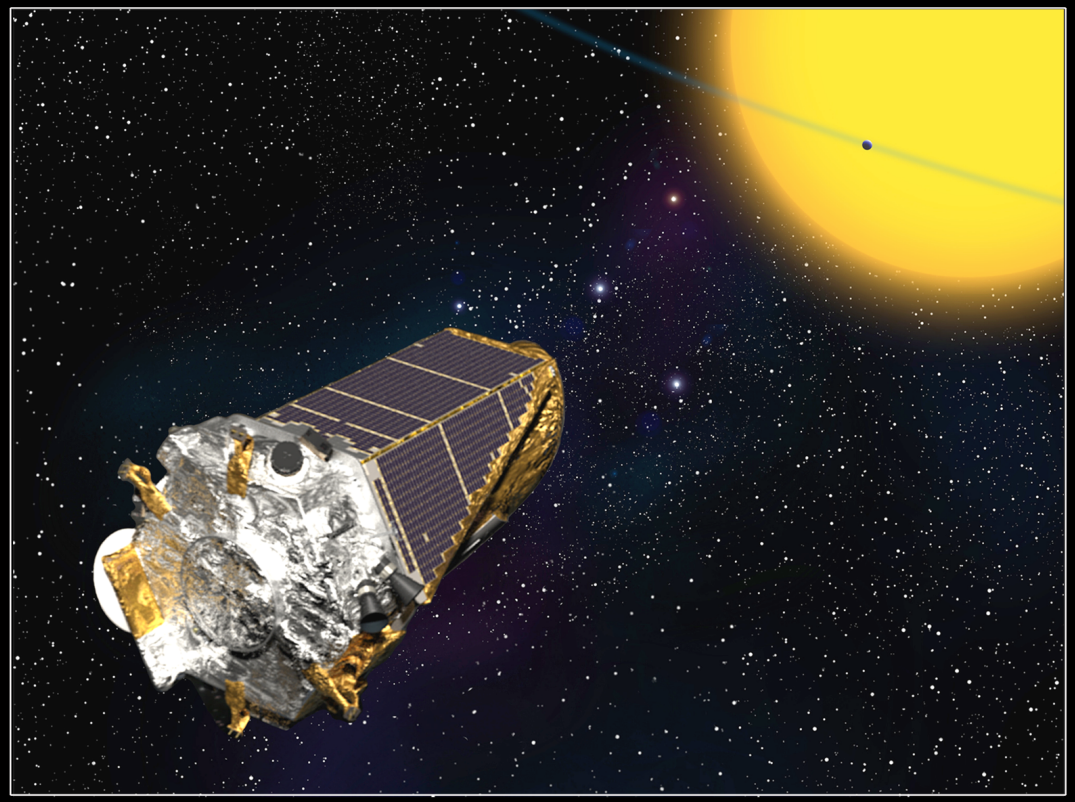
Burkhard Militzer,
Kevin Driver, Hugh Wilson

UC Berkeley

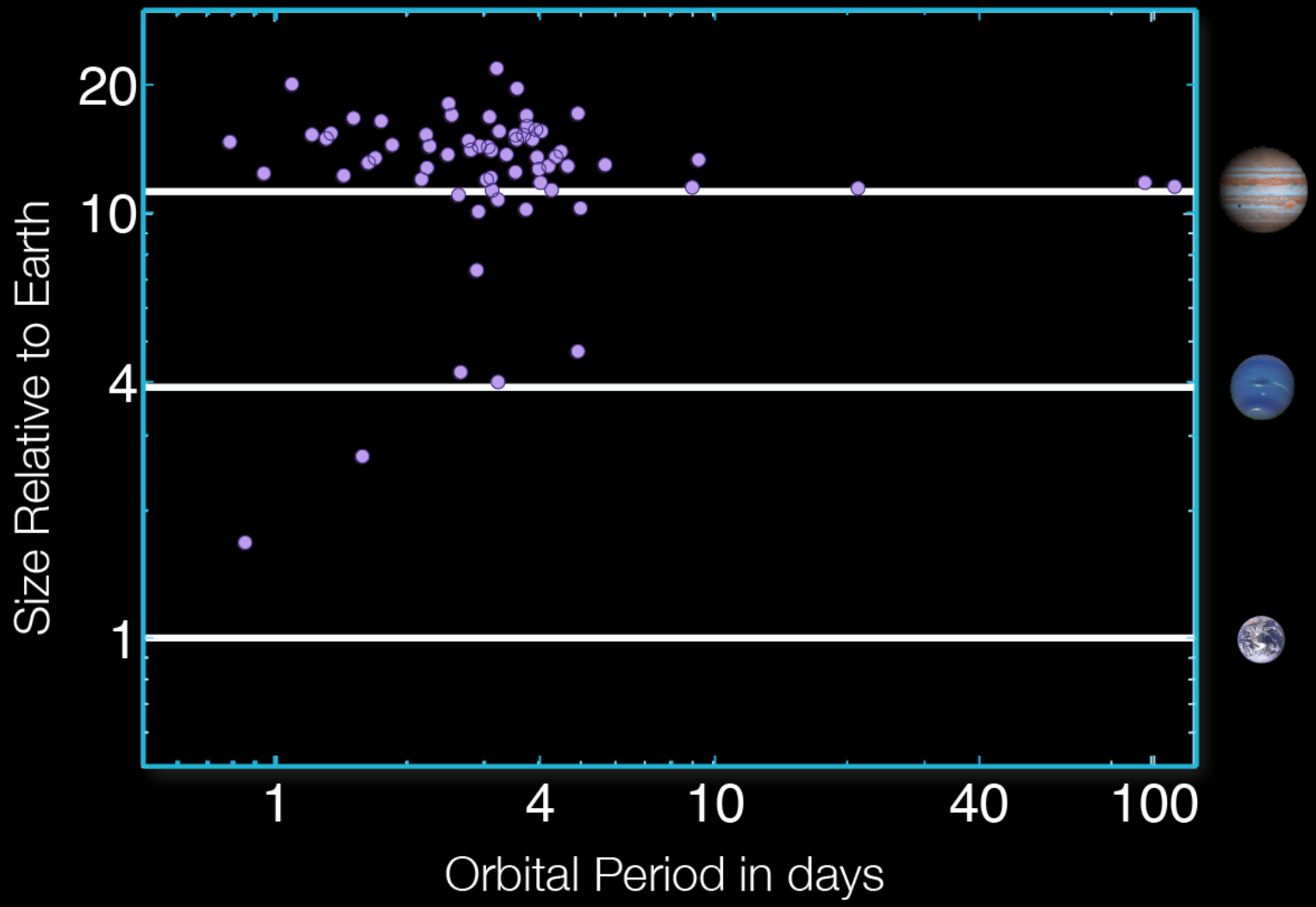
http://militzer.berkeley.edu

NASA's Kepler Mission

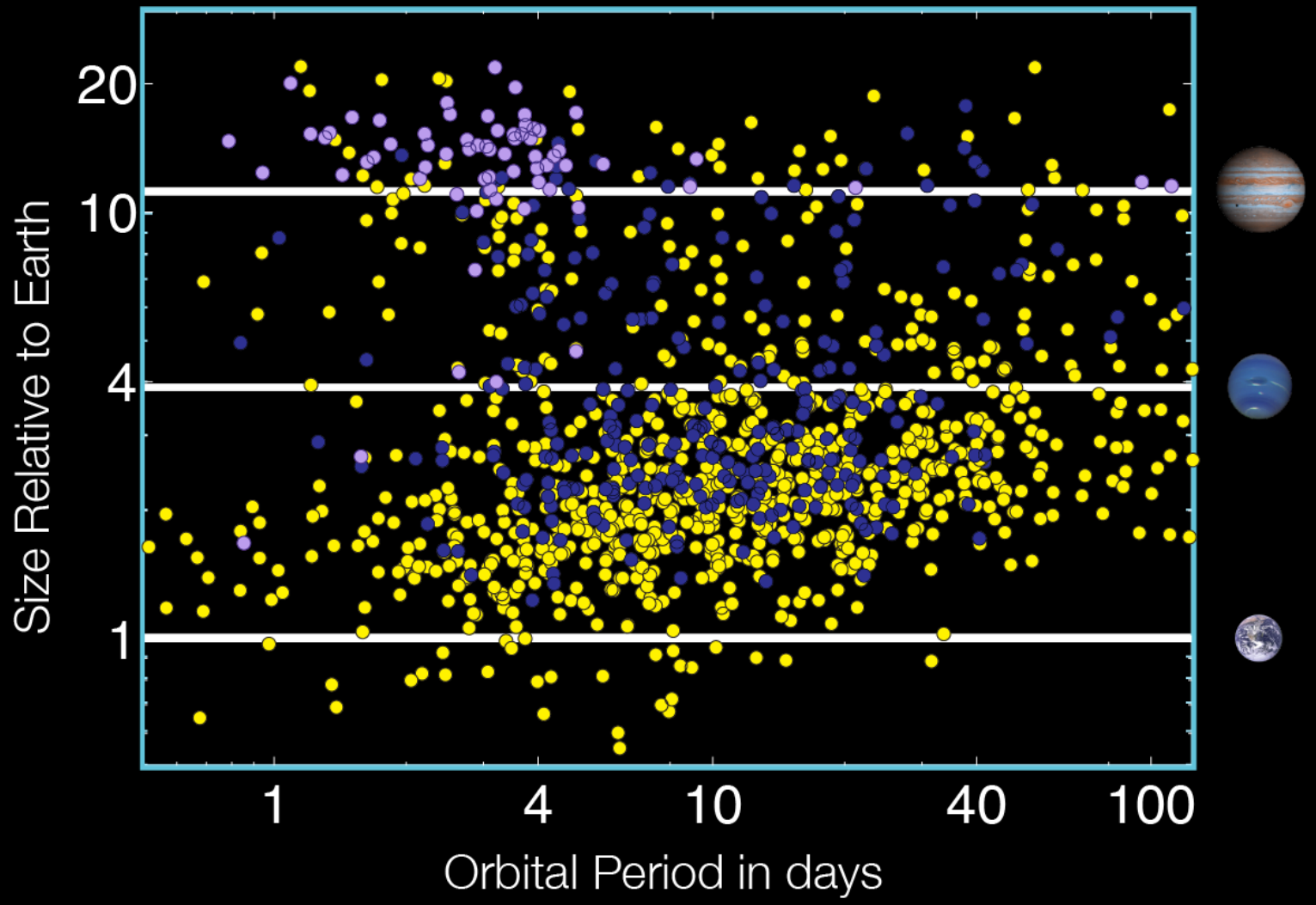
- Determine the frequency of Earth-size and larger planets in the habitable zone of sun-like stars
- Determine the size and orbital period distributions of planets



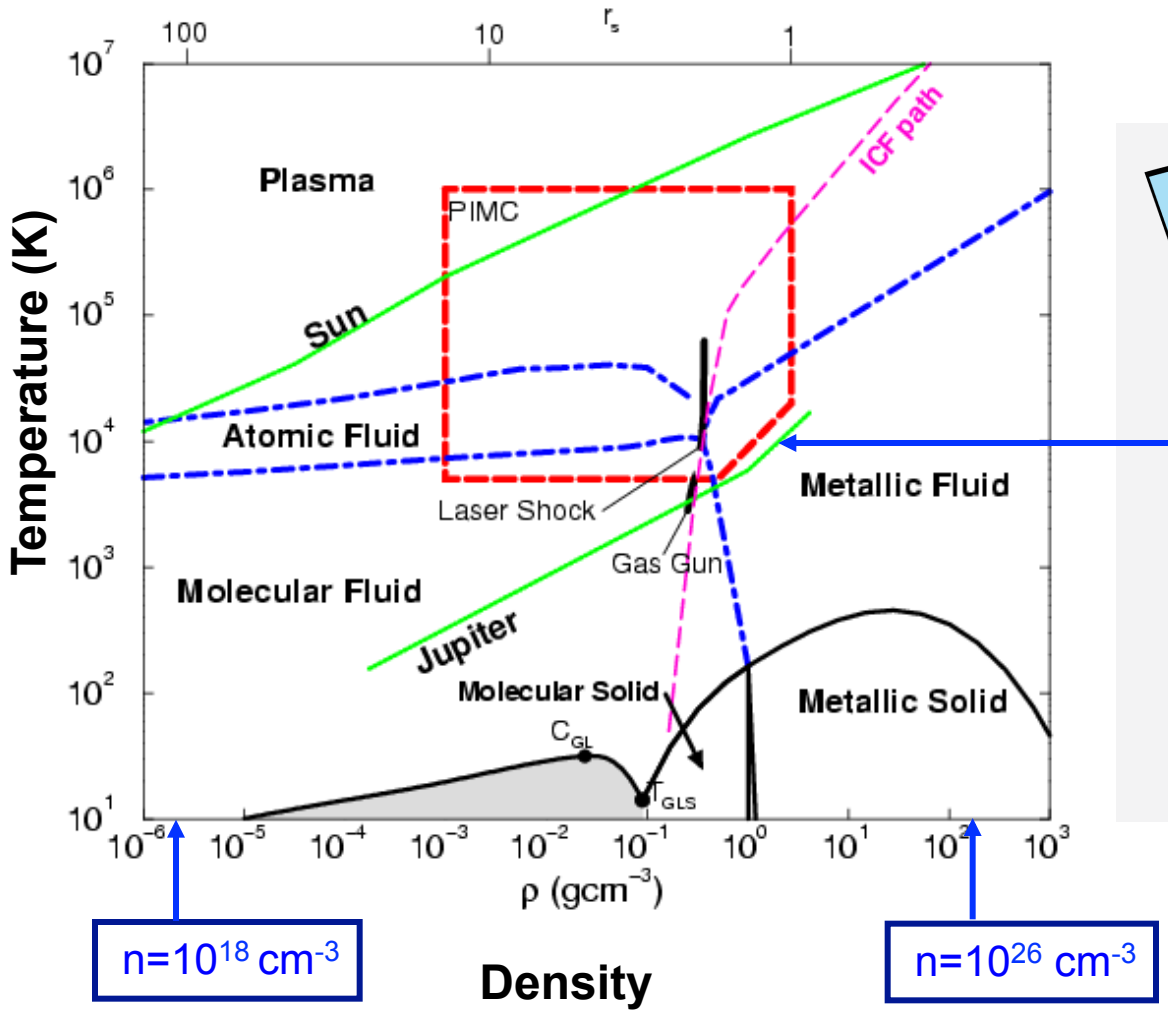
Pre-Kepler Transiting Planets - 2009

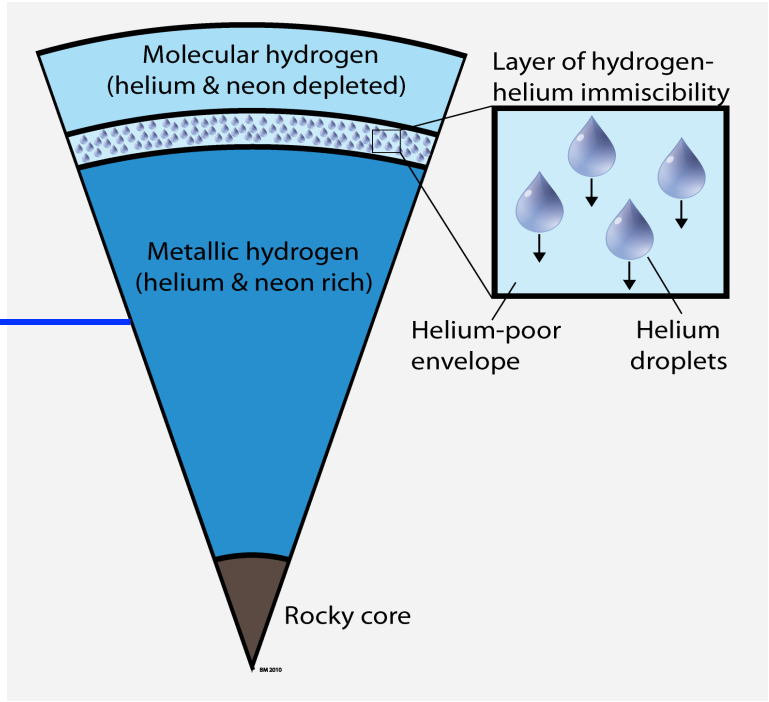


Kepler Candidates as of February 1, 2011

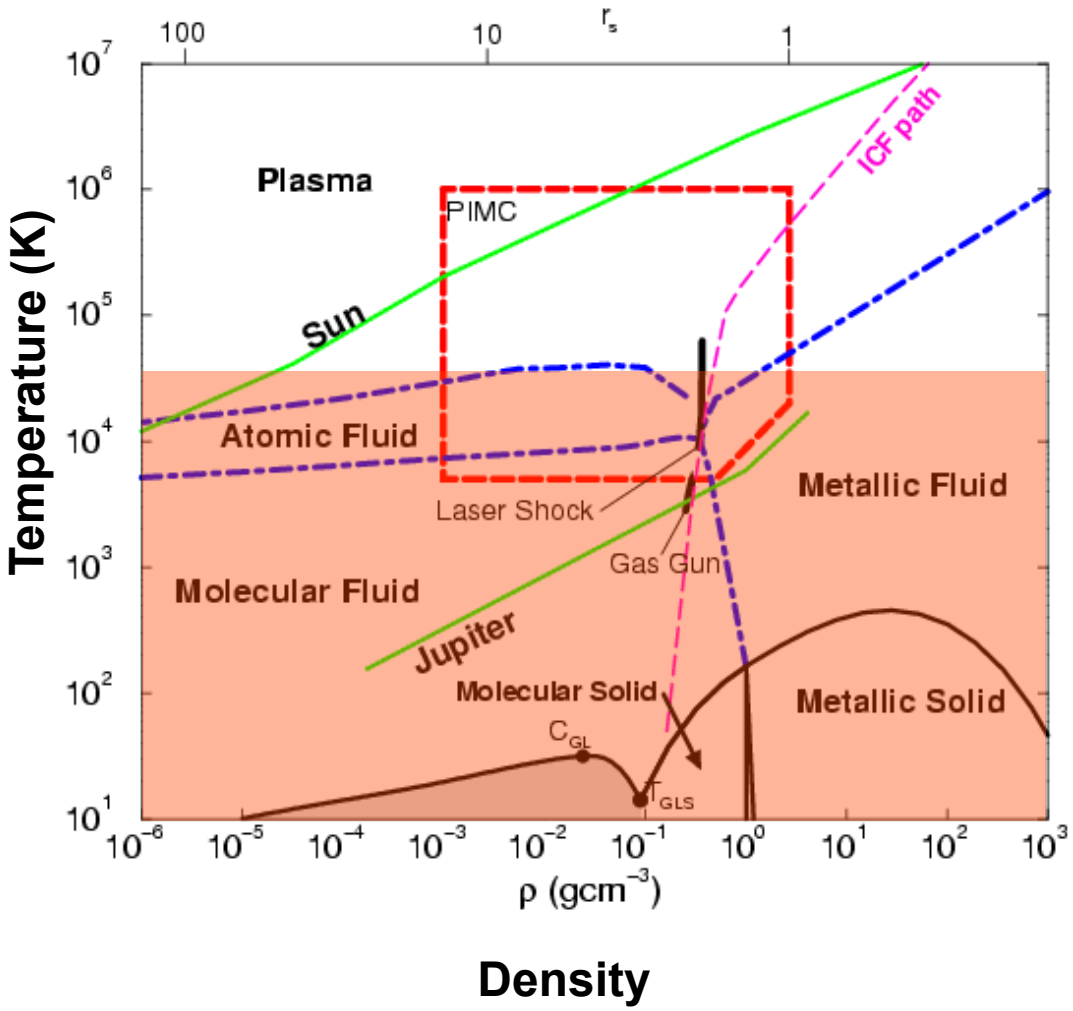


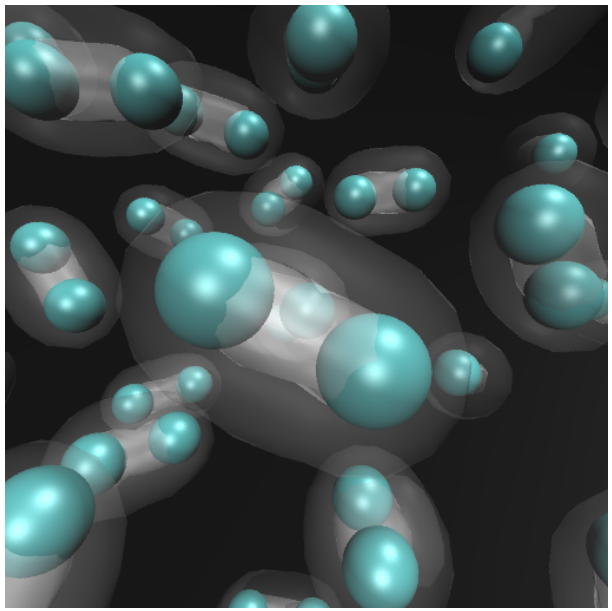
Ab initio Simulations to Characterize of the Interiors of Giant Planets





1) Density functional molecular dynamics



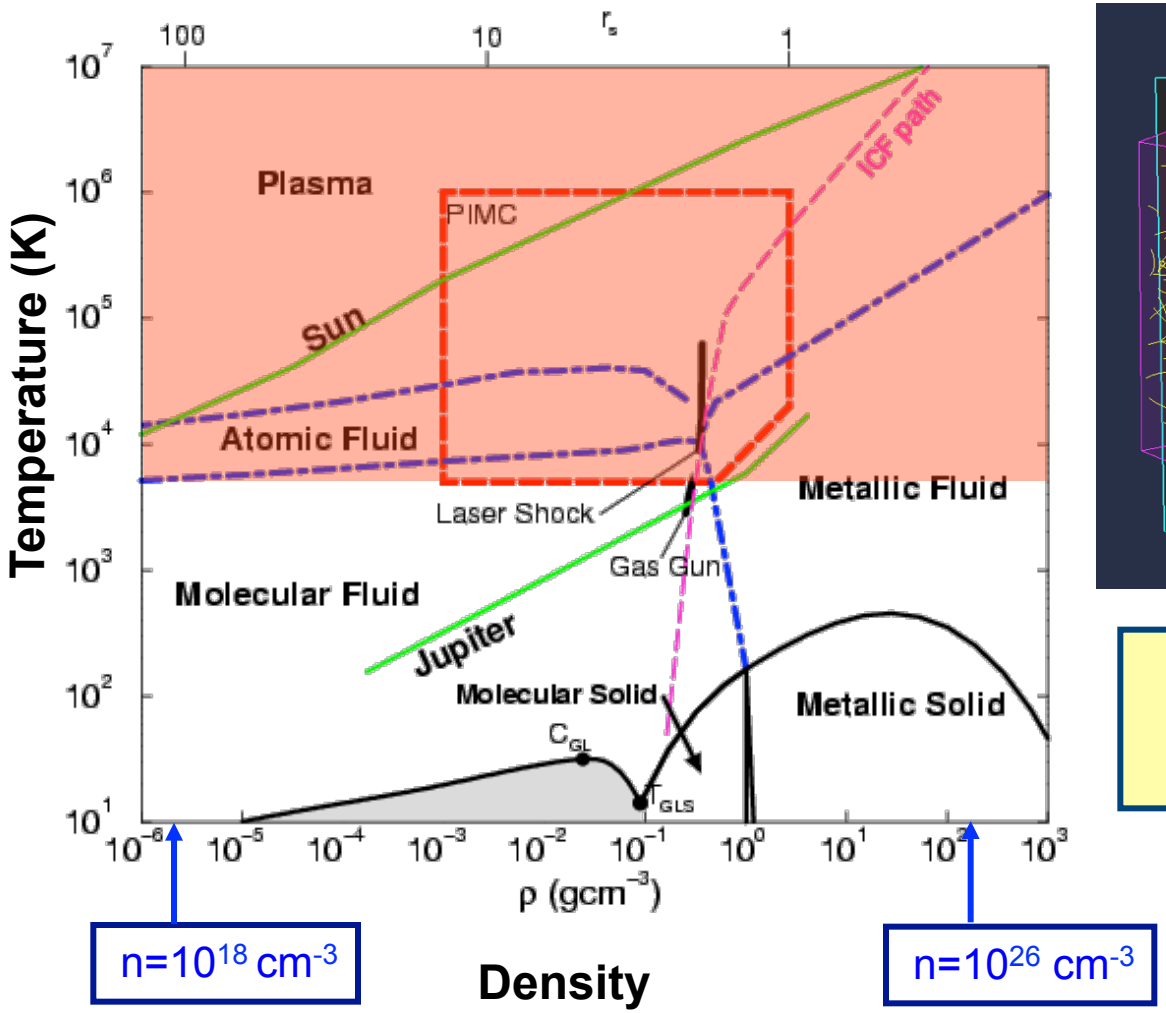


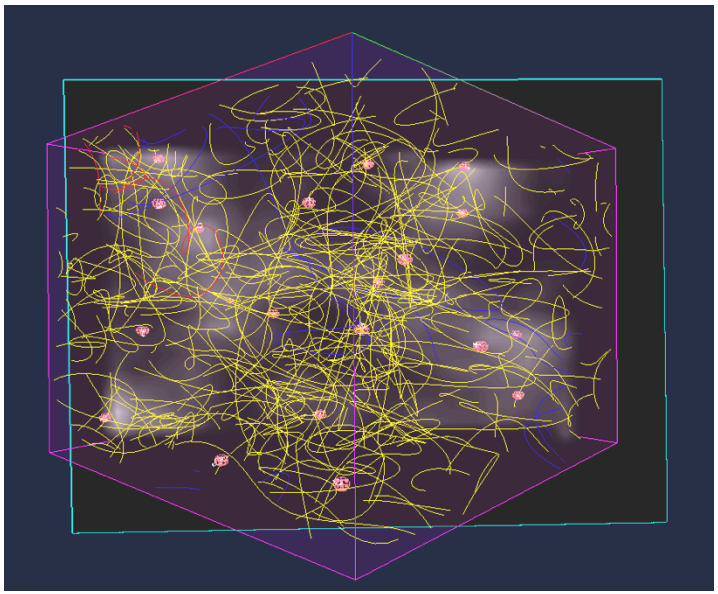
Born-Oppenheimer approx.
MD with classical nuclei:

F = m a

Forces derived DFT with electrons in the instantaneous ground state.

1) Density functional molecular dynamics
2) Path integral Monte Carlo for higher temperatures





PIMC applicable at:
T>5000K

Summer School

2012 Summer School on Computational Materials Science

Quantum Monte Carlo: Theory and Fundamentals

July 23-27, 2012 • University of Illinois at Urbana-Champaign

Topics:

• Introduction to Monte Carlo Methods • Pseudopotential generation • Variational Quantum Monte Carlo • Diffusion Quantum Monte Carlo • Wavefunction optimization methods • Path integral Monte Carlo • QMC applications in geophysics

Details:

Scientists from geophysics, physics, materials science, chemistry and high-performance computing. Includes lectures and labs.
$150 registration fee. Housing provided for non-local participants.

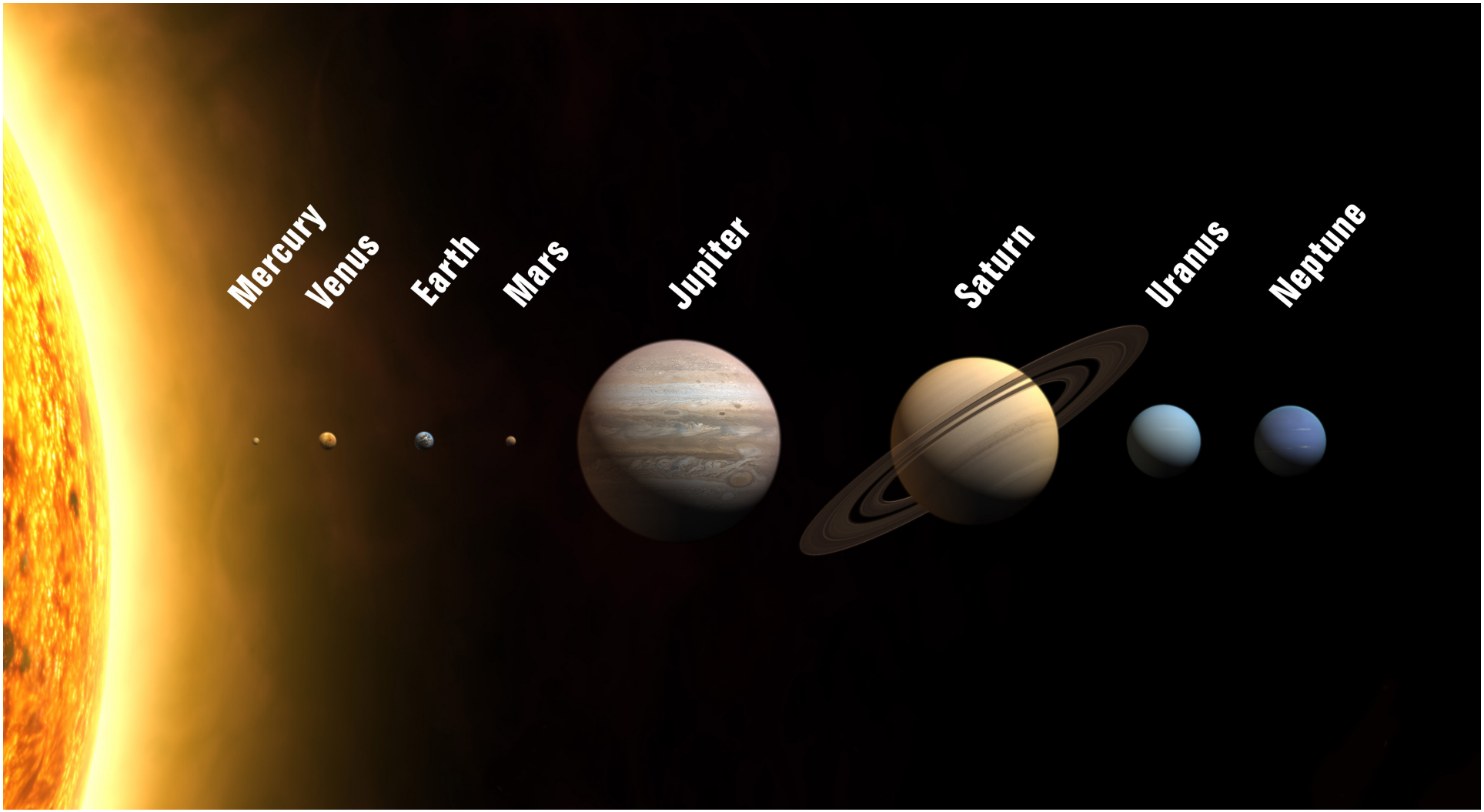
Application deadline: June 11, 2012

Contact: **http://mcc.illinois.edu/summerschool/2012**
Email: **mcc-workshops@illinois.edu**

Organizers:

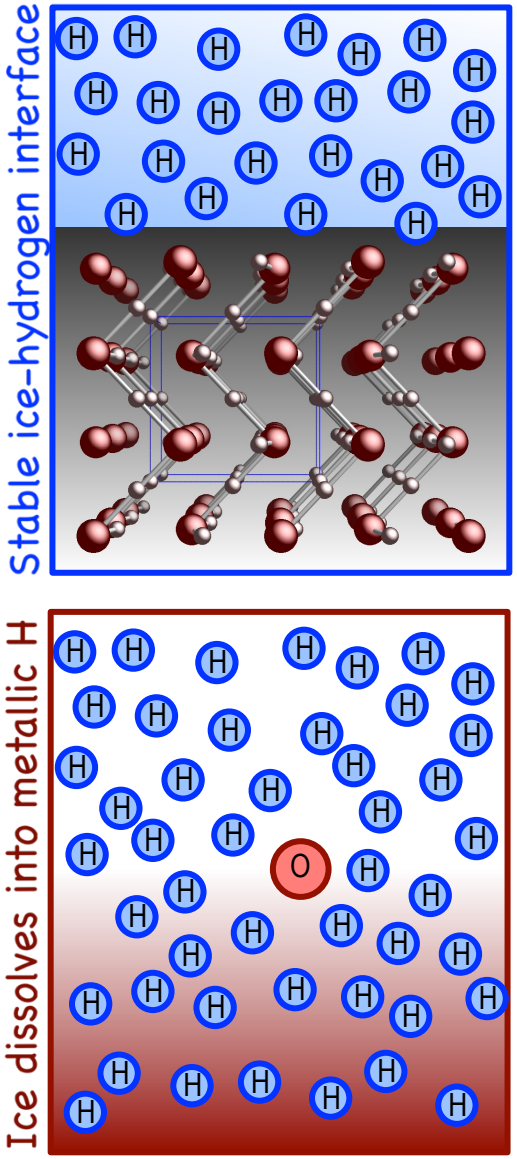
D. Ceperley, R. Cohen, E. de Sturler, J. Kim, B. Militzer, N. Sobh, and U. Ravaioli.

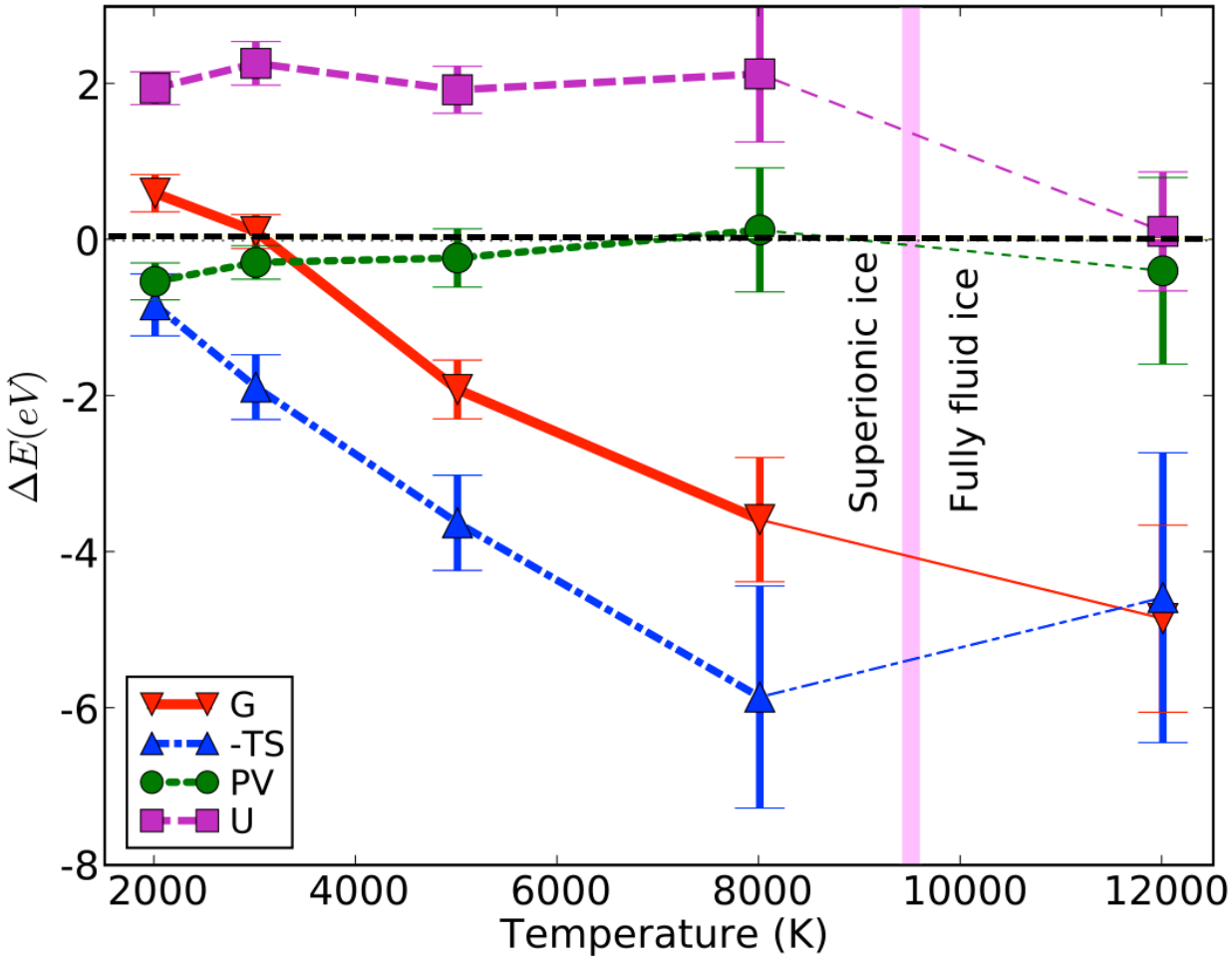
Why grew the giant plants so large while all terrestrial planets stayed small? Because they form beyond the ice line.



I. Are the Cores of Giant Planets Stable?

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

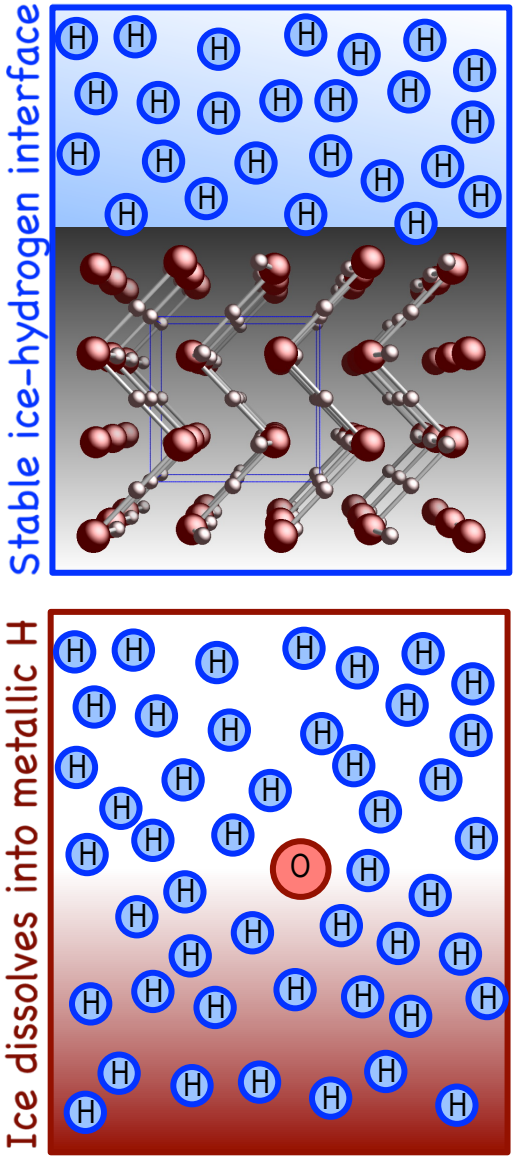


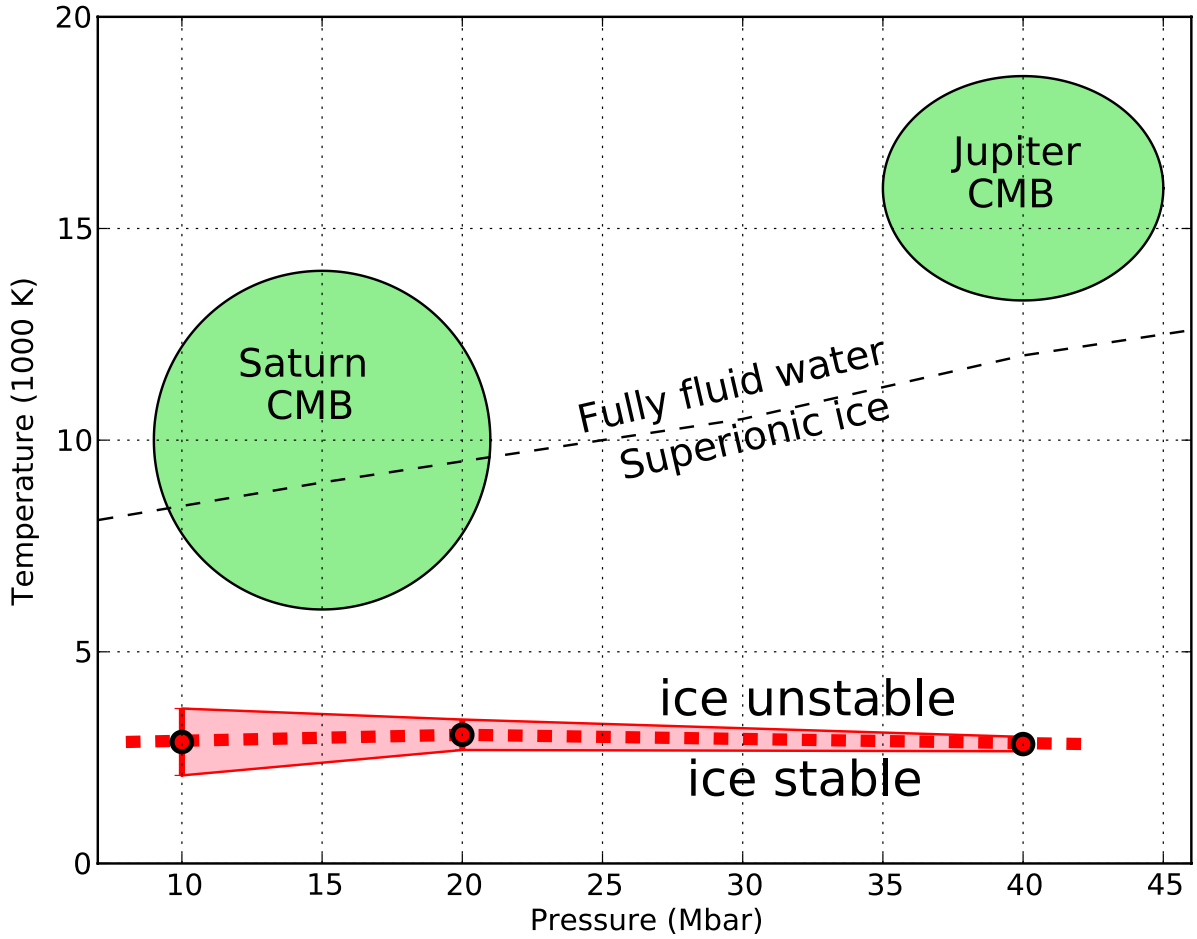


Predict core erosion in both Saturn and Jupiter

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

Computer simulations predict erosion of icy cores in Saturn and Jupiter



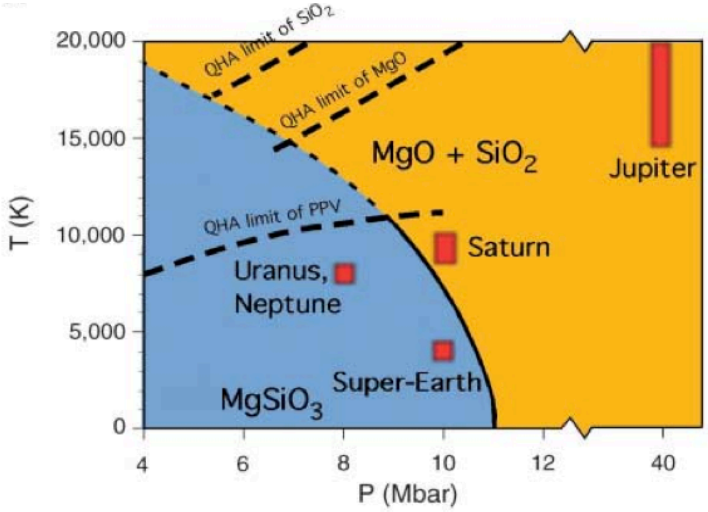


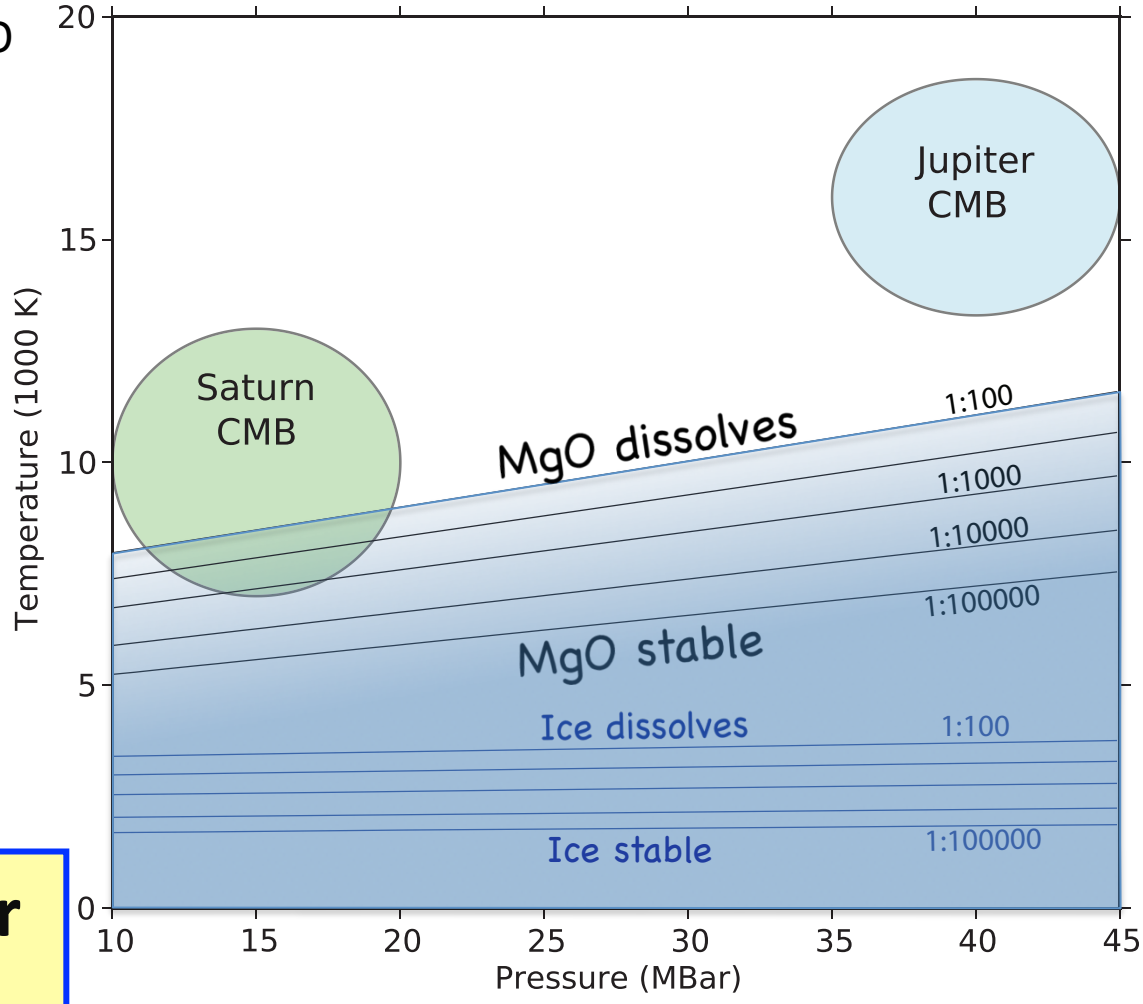
Predict core erosion in both Saturn and Jupiter

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

Erosion of other core materials: silicates and iron

$MgSiO_3$ dissociates into SiO_2 and MgO 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

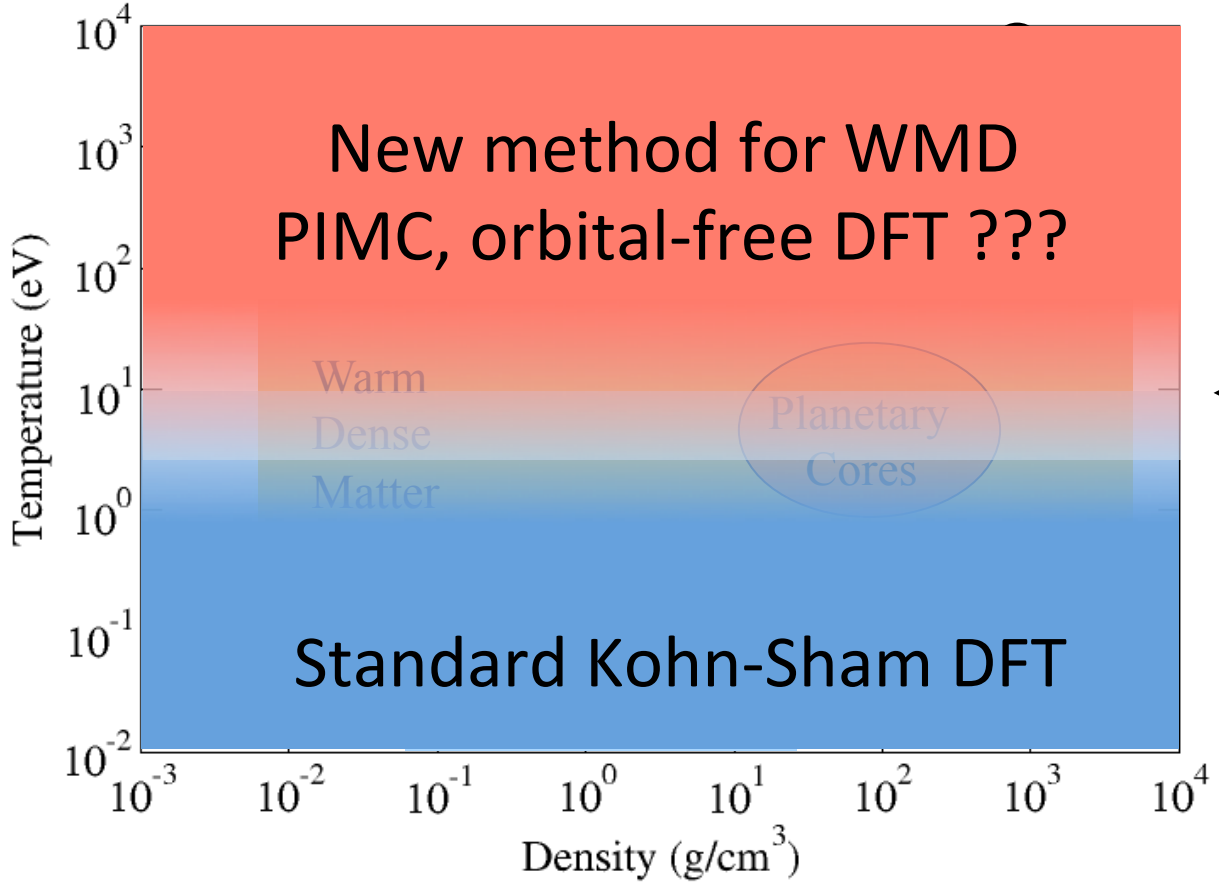
Three core-erosion scenarios:

- **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.**

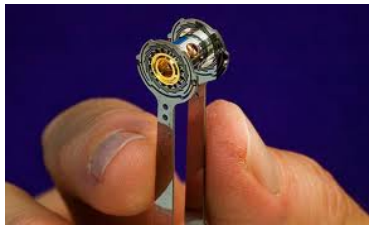
Recent core erosion model using double-diffusive convection:
Leconte and Chabrier, A&A (2012)

II. Warm Dense Matter Simulations

Regime of Warm Dense Matter requires new simulation techniques – Application ICF experiments



ICF Hohlraum

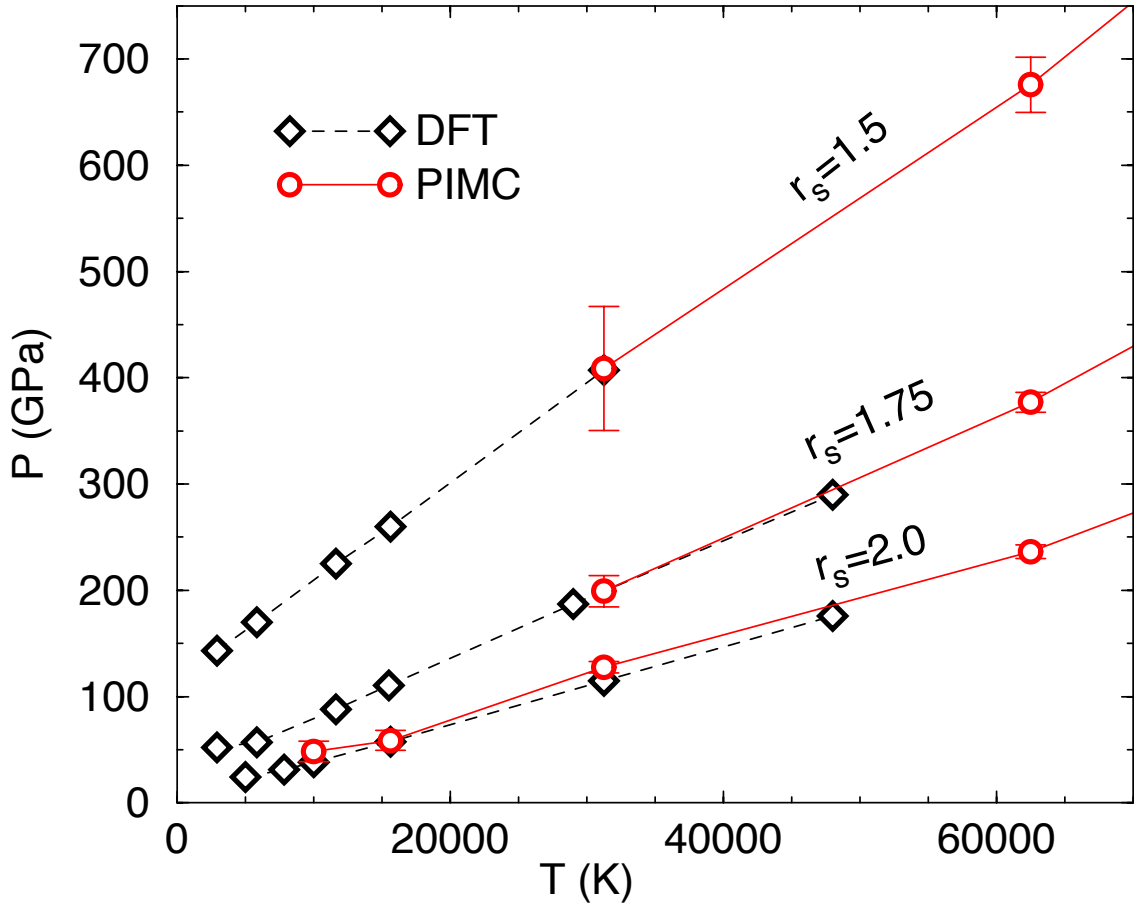


ICF Capsule

← 100000 K

Effects of bonding, ionization, exchange and correlation, and quantum degeneracy all important.
Carbon is a promising ablator for Inertial confinement fusion (ICF).
We are working with LLNL on carbon EOS.

For hydrogen, PIMC and DFT-MD Simulations Predict Consistent Shock Properties



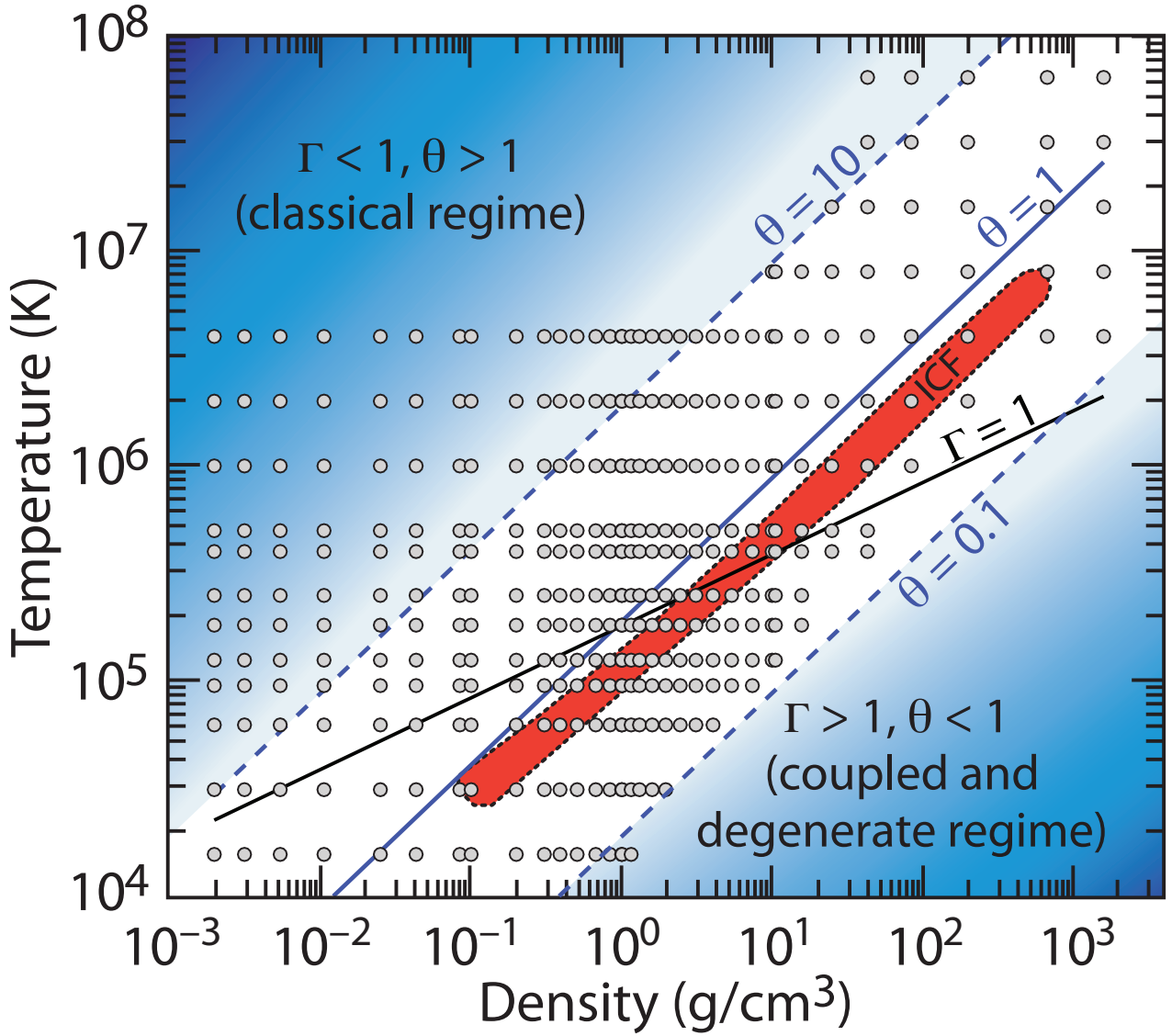
B. Militzer, D. M. Ceperley, J. D. Kress, J. D. Johnson, L. A. Collins, S. Mazevet, *Phys. Rev. Lett.* **87** (2001) 275502

Recent PIMC work provides EOS for ICF conditions (FPEOS table constructed)

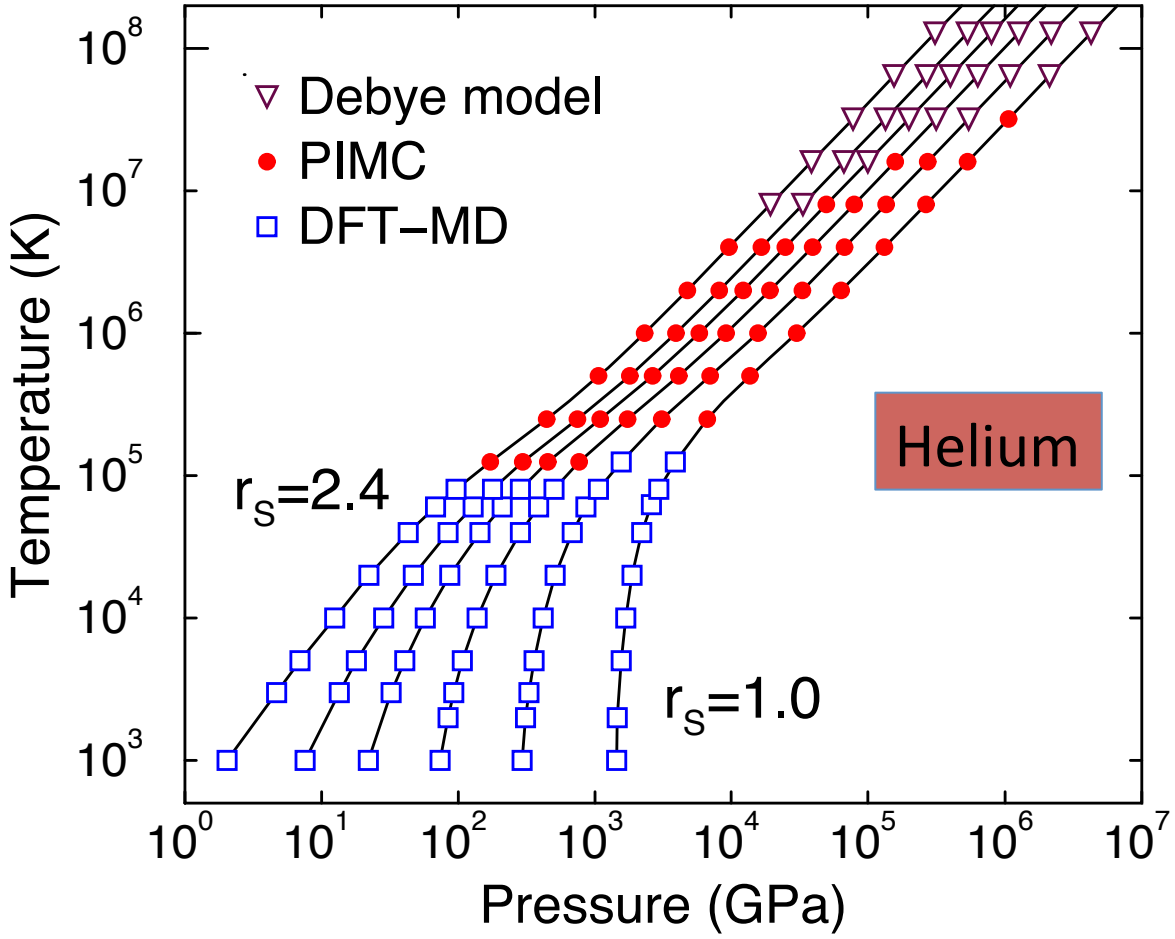
Hydrogen

S. X. Hu, B. Militzer, V. N. Goncharov, S. Skupsky, *Phys. Rev. Lett.*, **104** (2010) 235003

Phys. Rev. B **84** (2011) 224109.

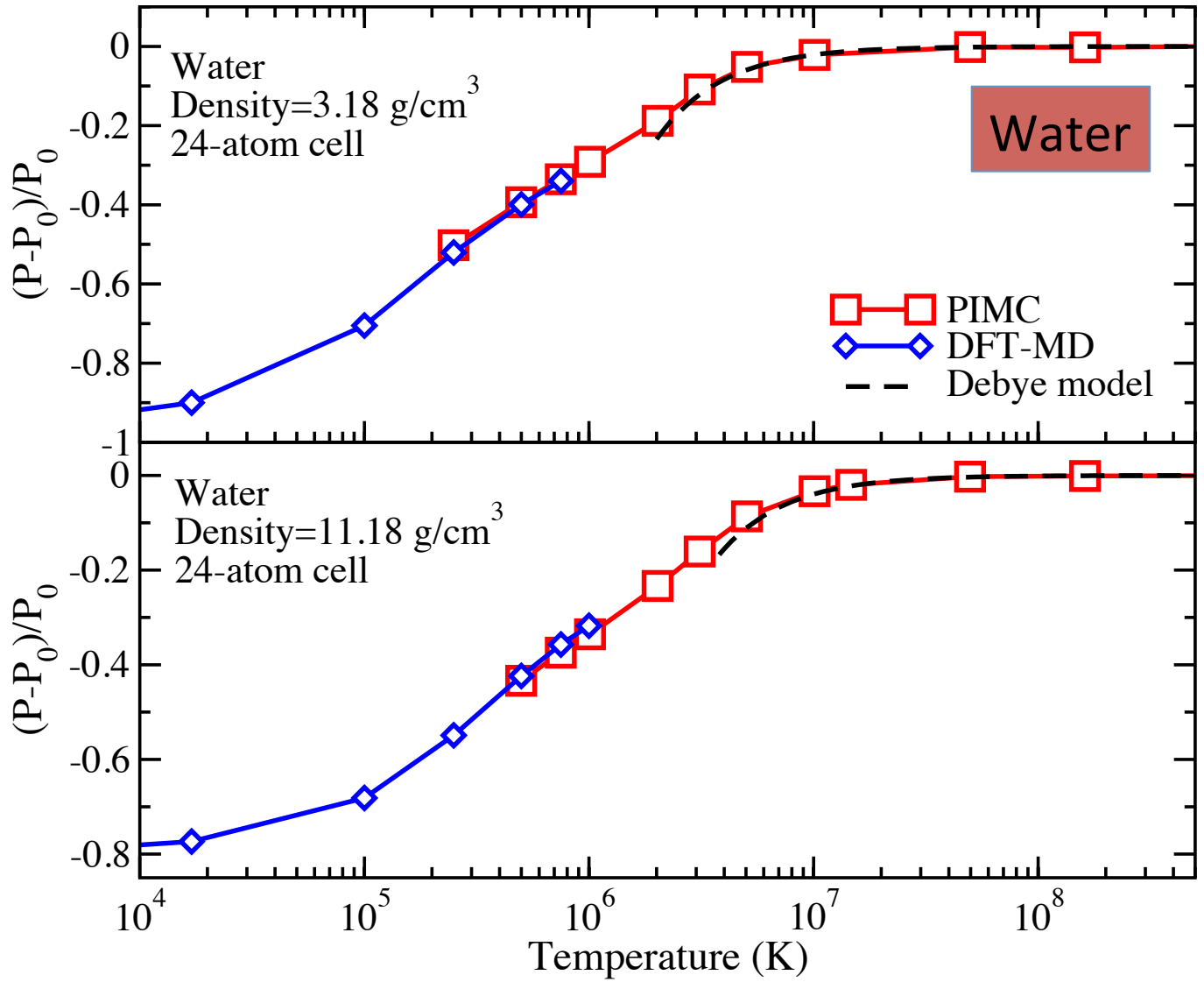


For Helium, PIMC and DFT-MD Simulations have been combined to make one consistent EOS table

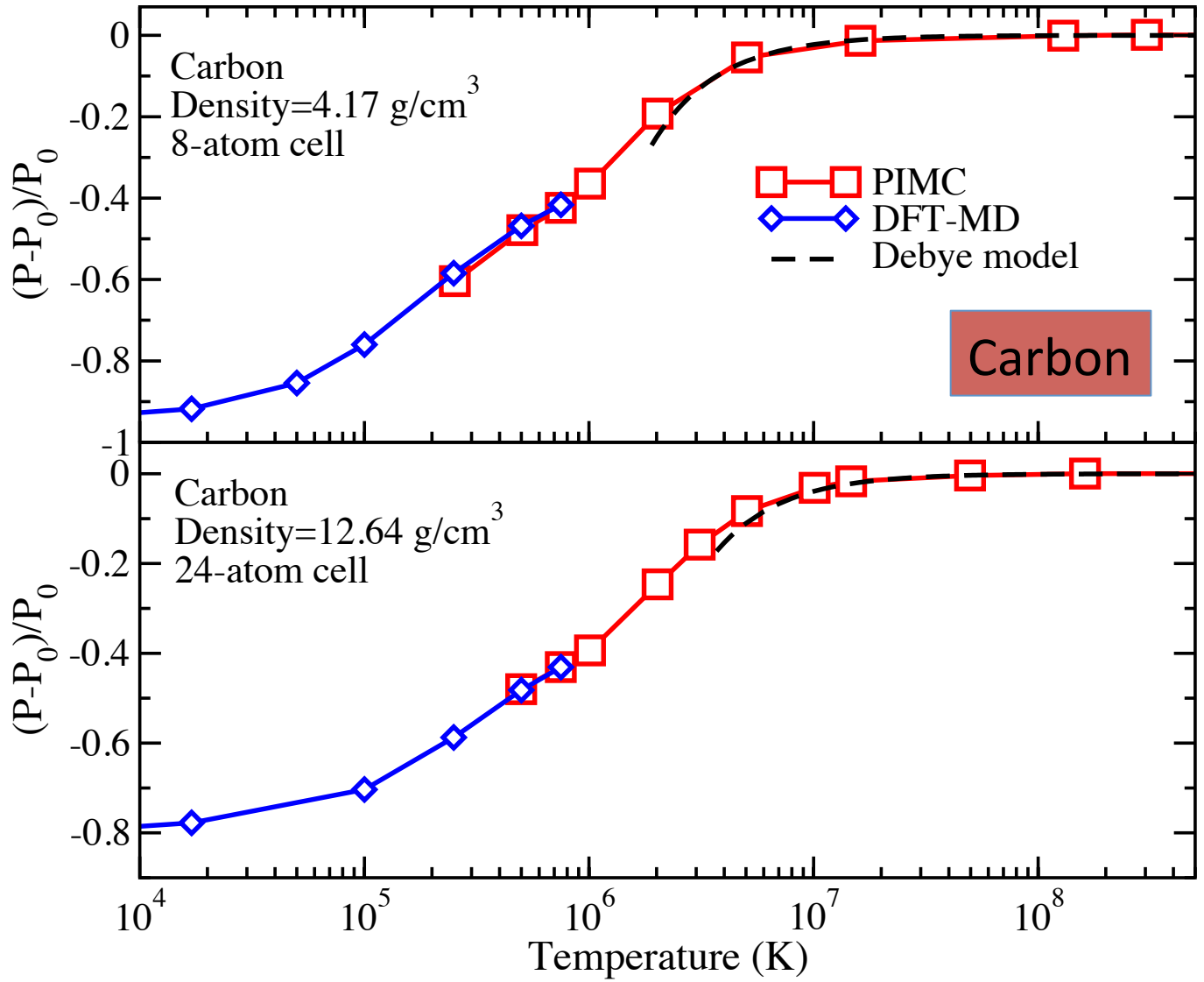


B. Militzer, *Phys. Rev.* B **79** (2009) 155105
B. Militzer, *Phys. Rev. Lett.* **97** (2006) 175501

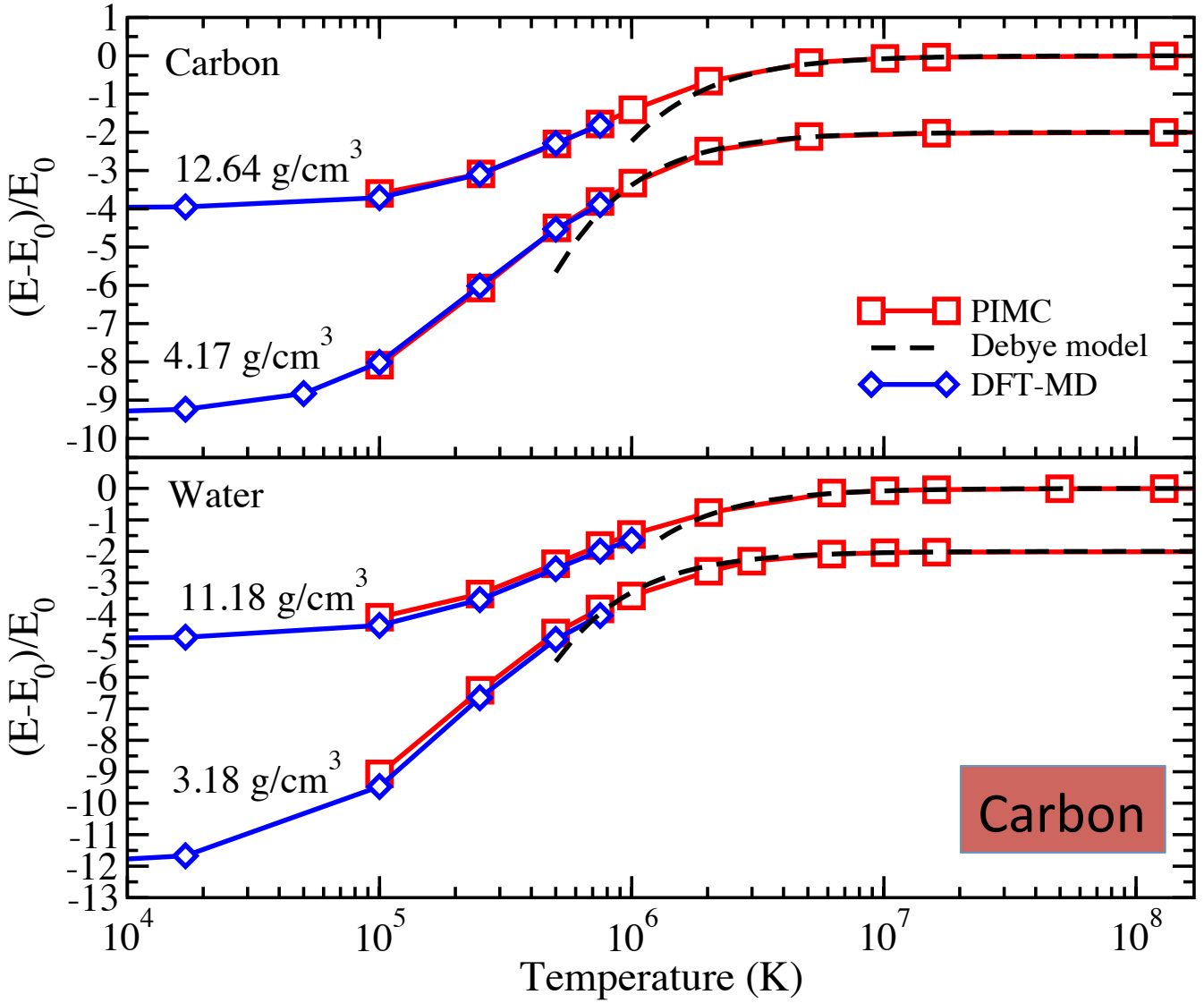
First Path Integral Monte Carlo Simulations for Heavier Elements Fill this Gap in Temperature



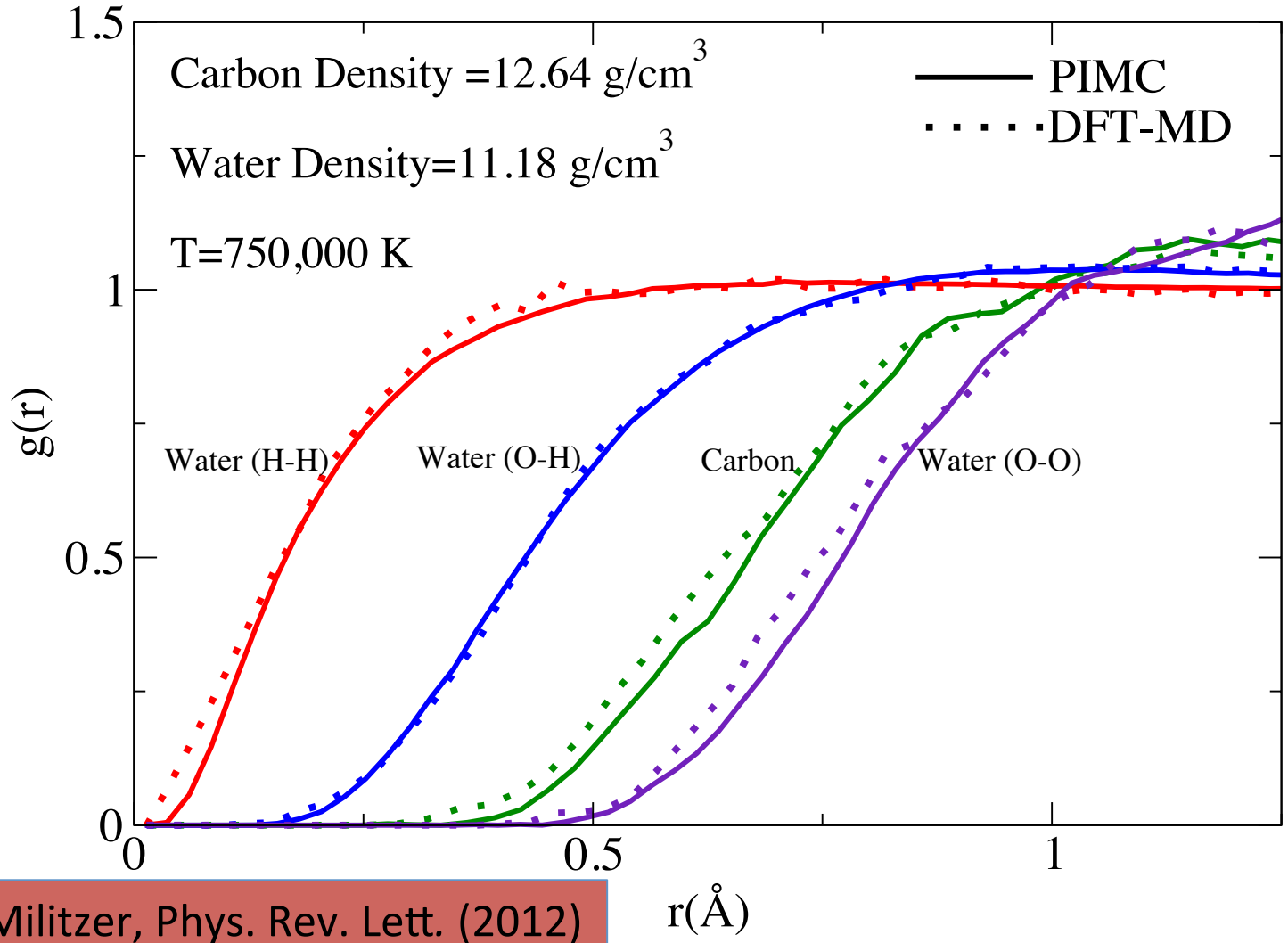
Again Path Integral Monte Carlo bridges the Gap in T between DFT-MD and the Debye Model



Path Integral Monte Carlo bridges the Gap in Internal Energy vs Temperature for Water and Carbon Plasmas



Path Integral Monte Carlo and DFT-MD are in very good agreement



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

Summary

- Presented new path integral Monte Carlo simulations for heavier elements (all-electron simulations, free particles nodes).
- Very good agreement with DFT for carbon and water plasmas.
- No insufficiencies in the ground-state exchange-correlation functionals.
- We constructed again consistent EOS table for C and H_2O.
- More materials to be studied. Please make suggestions!

Driver, Militzer, Phys. Rev. Lett., 108 (2012) 115502.