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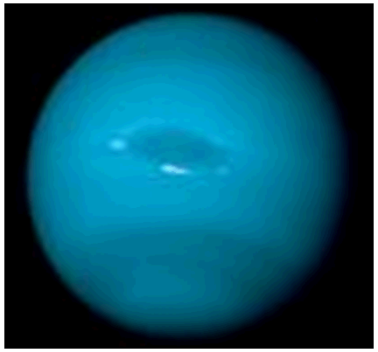

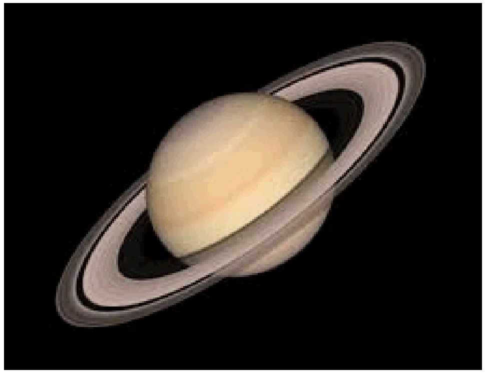
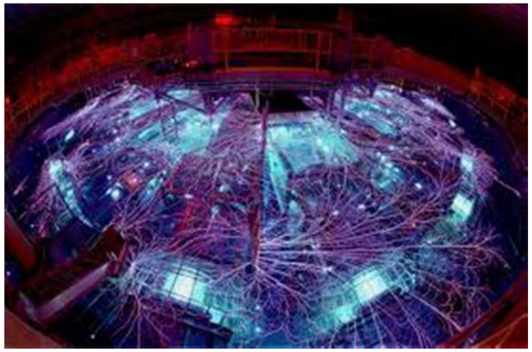

High Energy Density Materials at Sandia: Investigations in Planetary Science

Dawn G. Flicker, Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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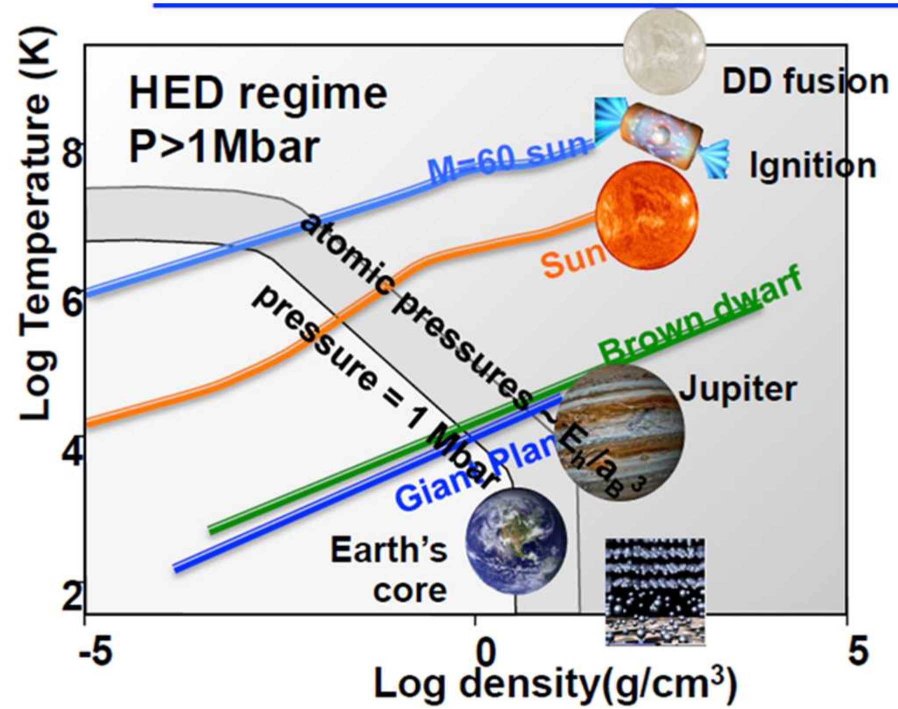
Properties of matter under HED (High Energy Density) conditions are important to many planetary problems

- Gas Giants– Jupiter, Saturn, Uranus, Neptune, and exo planets [e.g. hot Neptunes]
  - H, He, H_2O, C, N & Mixtures
- Earths and super-earths
  - Silicates, MgO, and iron/iron alloys
- Pressures: 100s of GPA
- Temperatures: 10,000K



The relevant phase diagrams are both complex and relevant

Outline

- HED material experiments on Z and the Z Fundamental Science Program
- Hydrogen metallization and the age of Jupiter and Saturn
- The phase diagram of water and the multi-polar magnetic fields of Neptune and Uranus
- Iron vaporization and the earth's moon-forming event

Sandia's Z Machine is a unique platform for multi-mission research on high energy density (HED) environments

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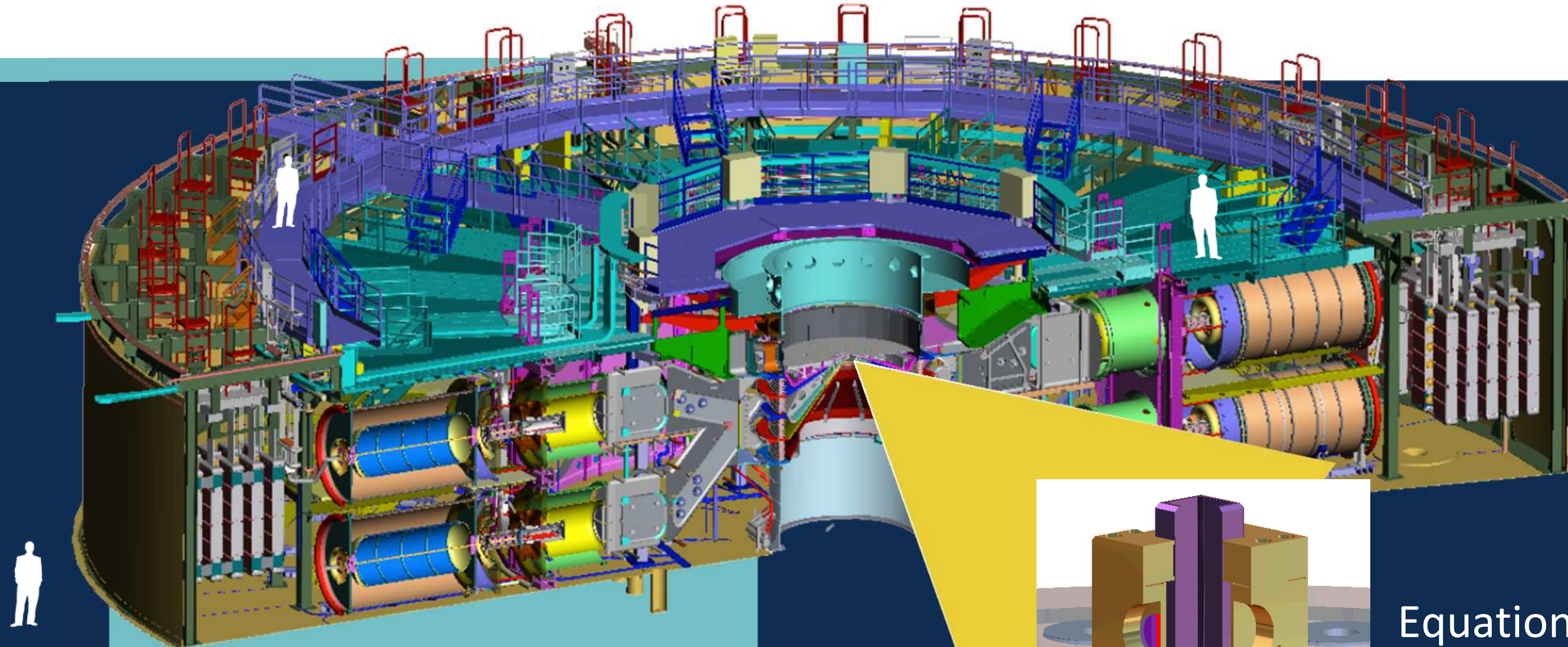
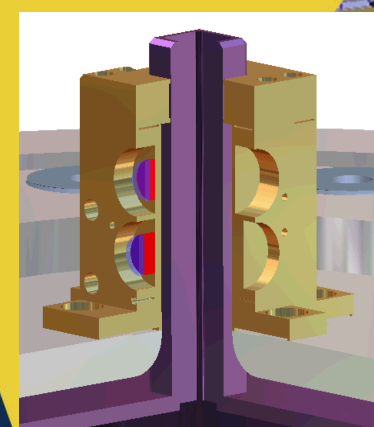


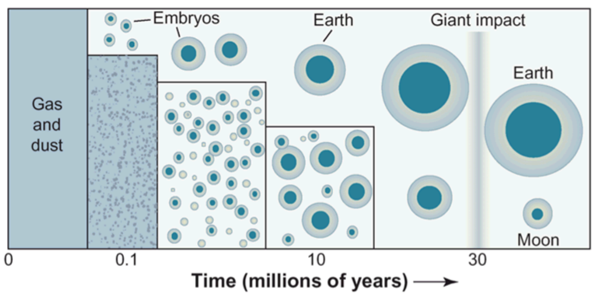
- Pulsed Power Technology
- Magnetically Driven Implosions
- Inertial Confinement Fusion
- Dynamic Materials



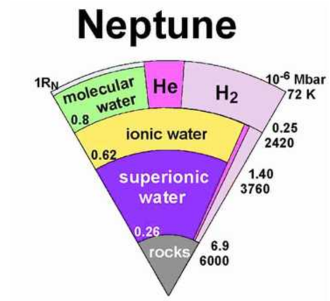
Equation of State

I ~ 26 MA, τ ~100-1000 ns
X-ray power > 250 TW
X-ray energy > 2 MJ

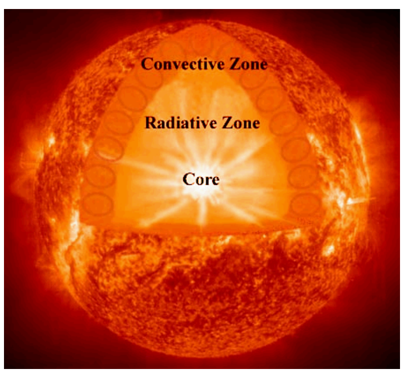
The Z Fundamental Science Program has created strategic partnerships with leading institutions



Earth and super earths
Properties of minerals and metals



Jovian Planets
Water and hydrogen



Stellar physics
Fe opacity and H spectra

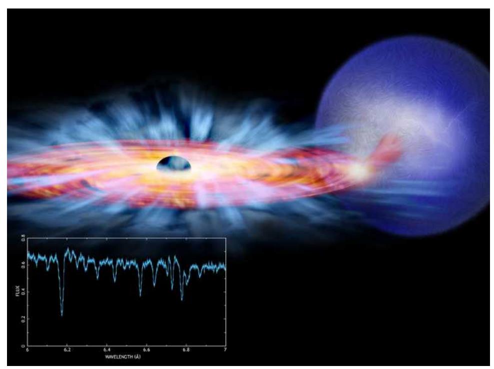


Photo-ionized plasmas
Range of ionization param. ξ

- Opportunities for collaboration and access to Z
- Competitive proposal process
- Science with significant impact
  - Bailey et al, Nature (2015)
  - Kraus et al, Nature Geoscience (2015)
  - Knudson et al, SCIENCE (2015)
  - 1 PRL, 3 PoP, 1 PRA, 1 PRB, and 8 other peer-reviewed publications
- Workshops most years since 2009
  - Next workshop 7/31-8/3 2016

Z Astrophysical Plasma Properties (ZAPP) collaboration uses the same x-ray source to simultaneously address 4 separate astrophysics topics

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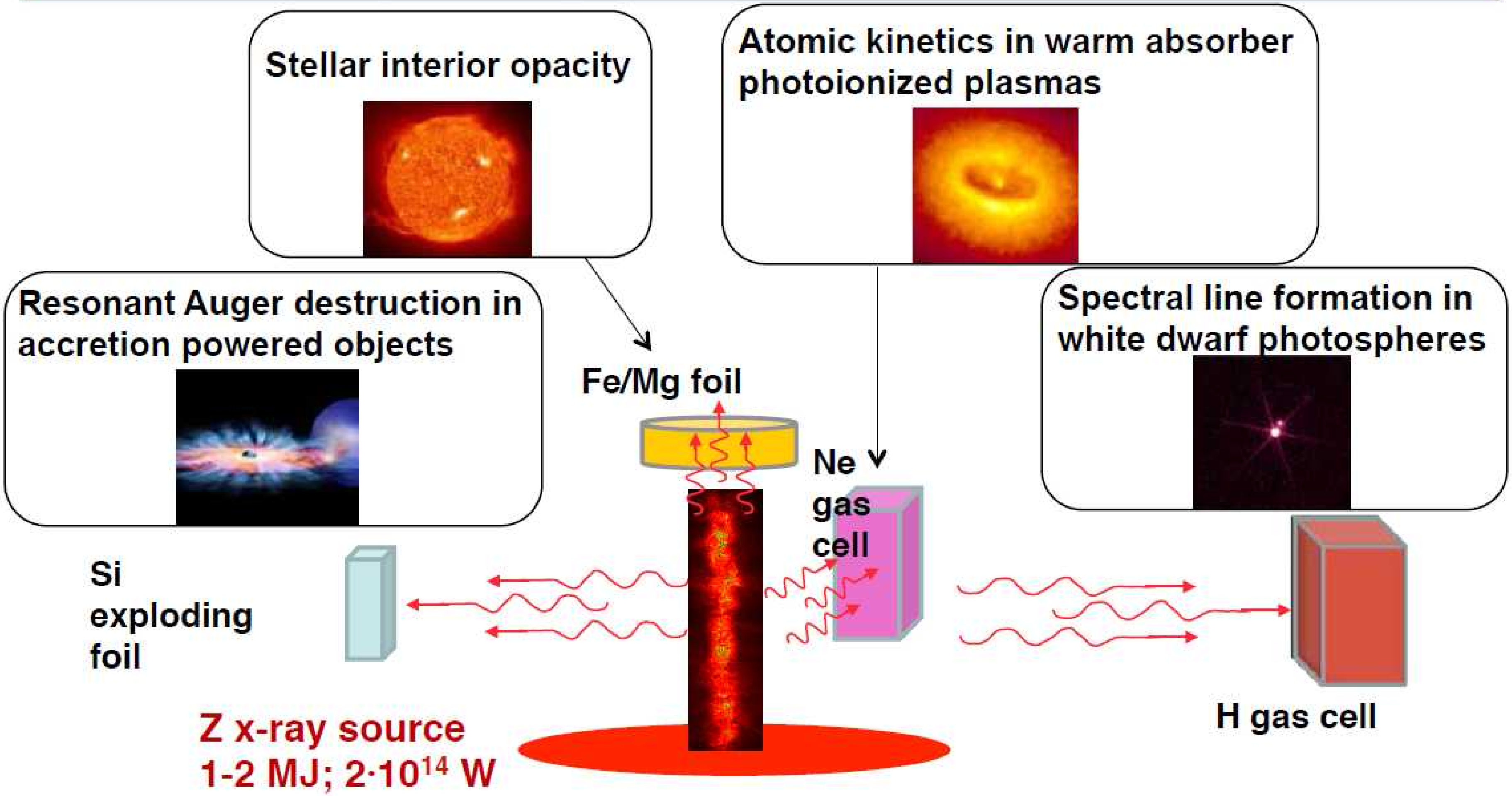
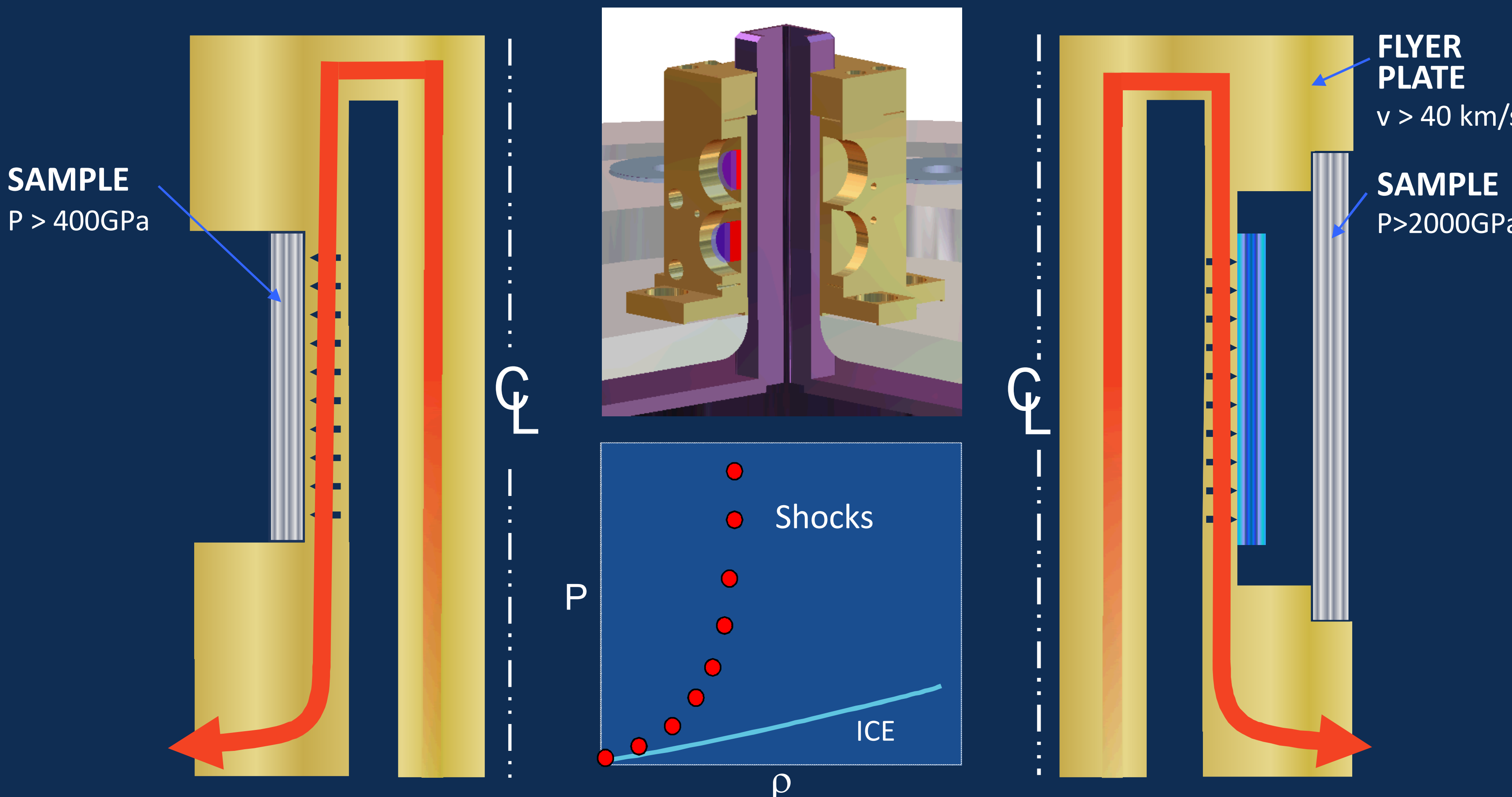


- Multiple samples are exposed to Z x-rays on each shot
- Highly efficient use of the facility

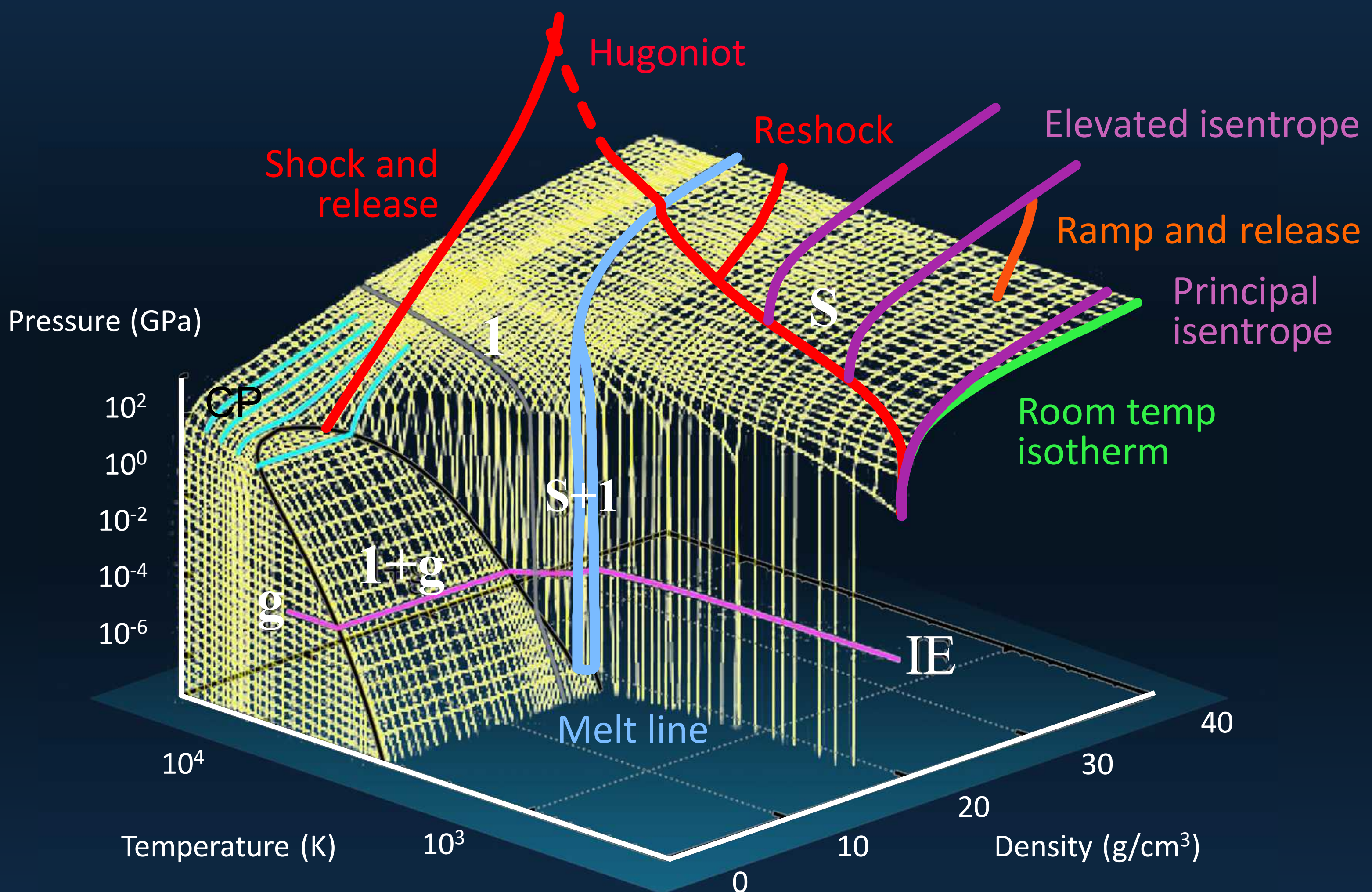
Isentropic compression and shock wave experiments map different regions of phase space



Isentropic Compression Experiments:
Gradual pressure rise in sample

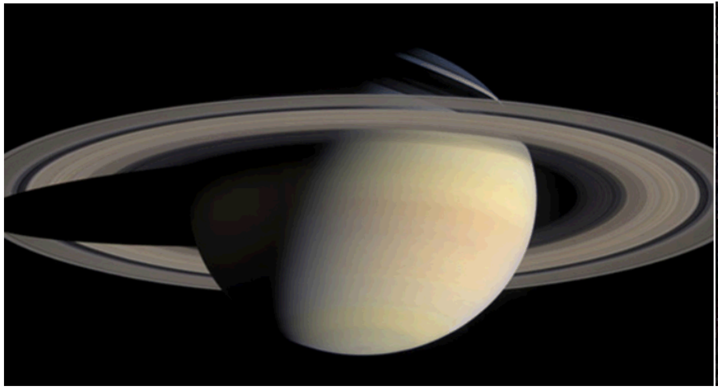
Shock Hugoniot Experiments:
Shock wave in sample on impact

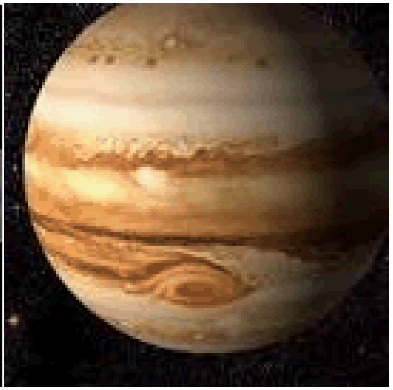
Dynamic compression experiments on Z can probe large regions of a material's equation-of-state surface



Observation of H2 metallization needed to address a planetary mystery

Why is Saturn hot?

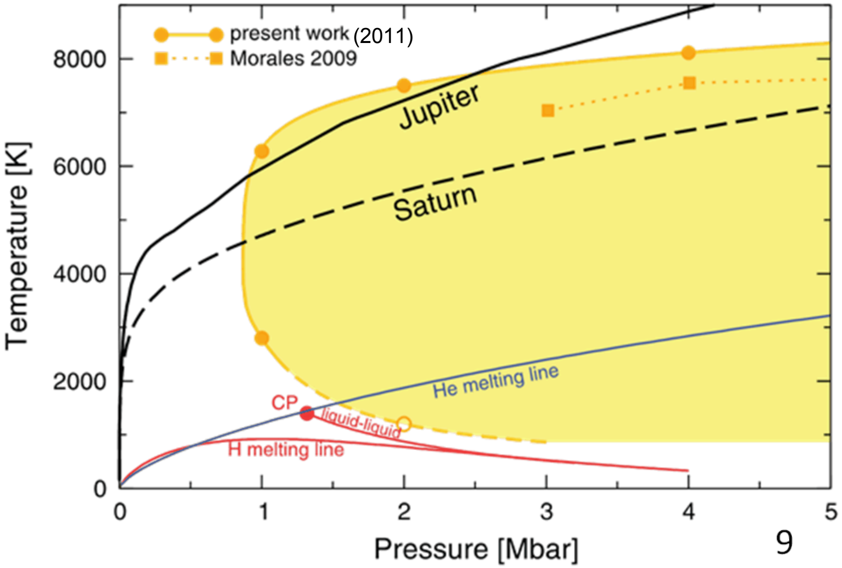




- Hydrogen metallization, as predicted by Wigner(1935) is linked to H-He demixing
- Formation of helium rain would generate heat
- But Jupiter would also have He rain and excess heat according to current models

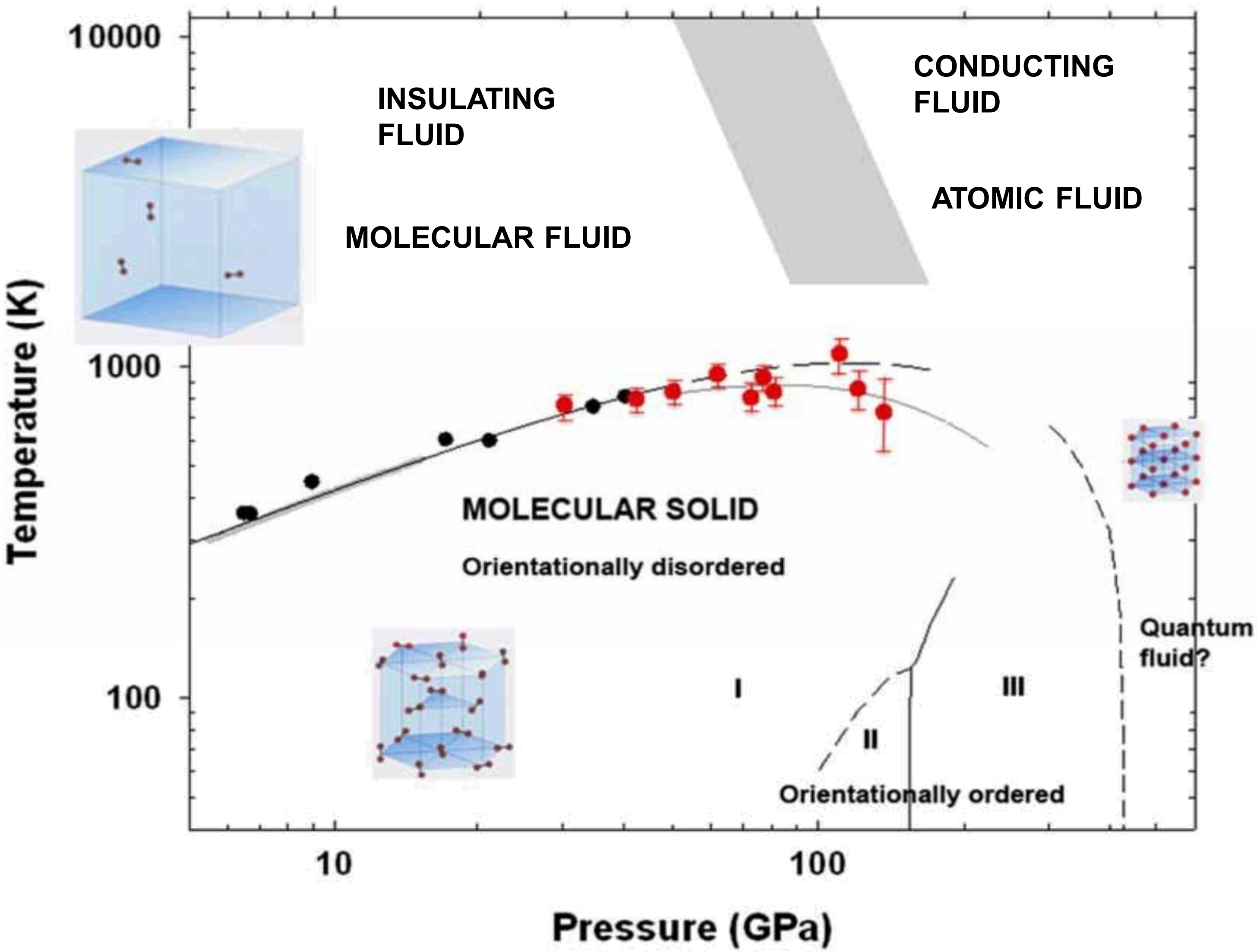
- Planets cool with age,
- Saturn's age is much hotter than would be expected if its age is in line with the rest of the solar system.
- Scientists believe that Saturn is two billion years older than its temperature indicates

Redmer & Knudson explored the D2 insulator to metal transition on Z

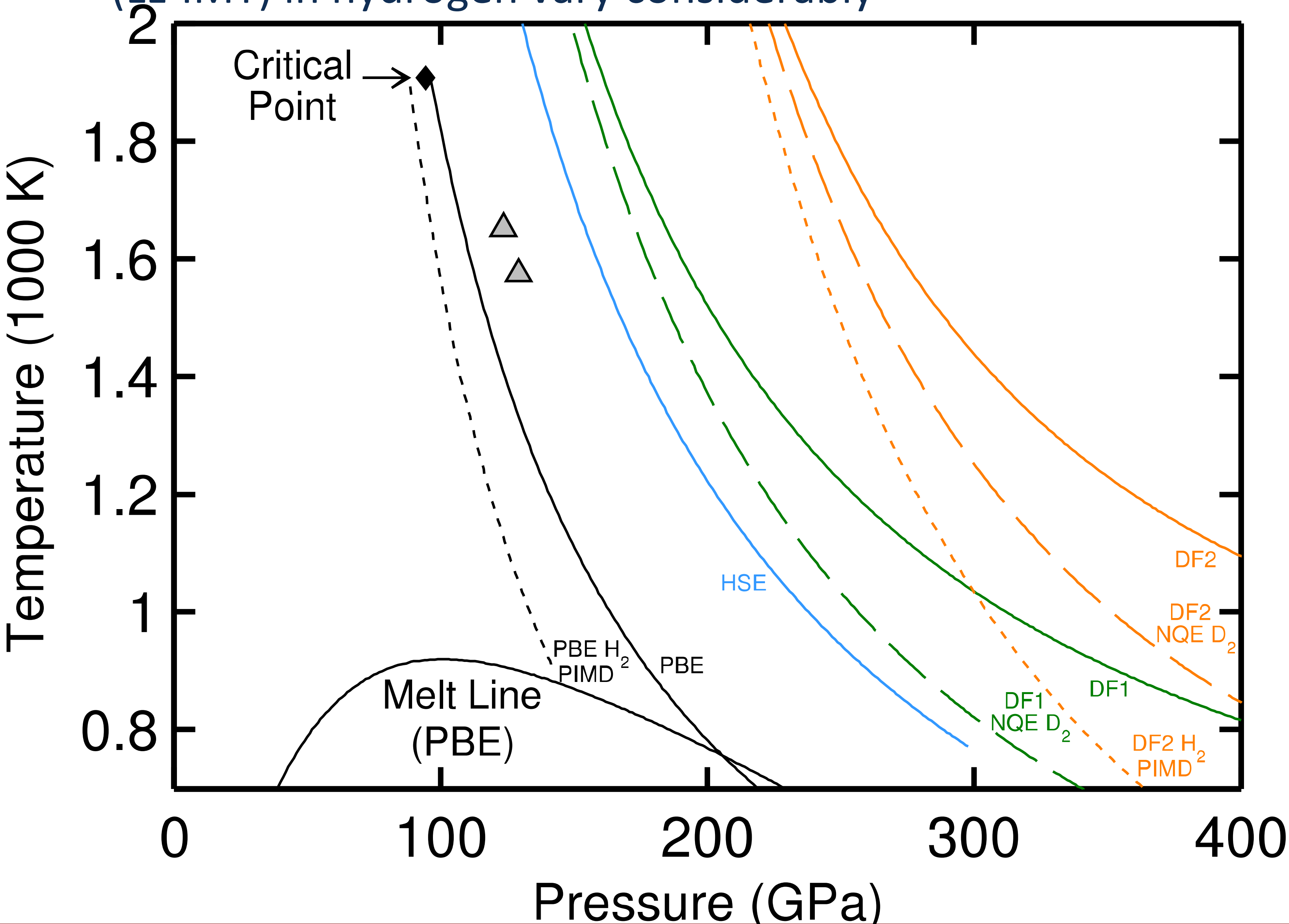


W. Lorenzen, B. Holst, and R. Redmer, Phys. Rev. B 84, 235109 (2011)

Hydrogen has an intriguing phase-diagram at high pressure with several unknown boundaries

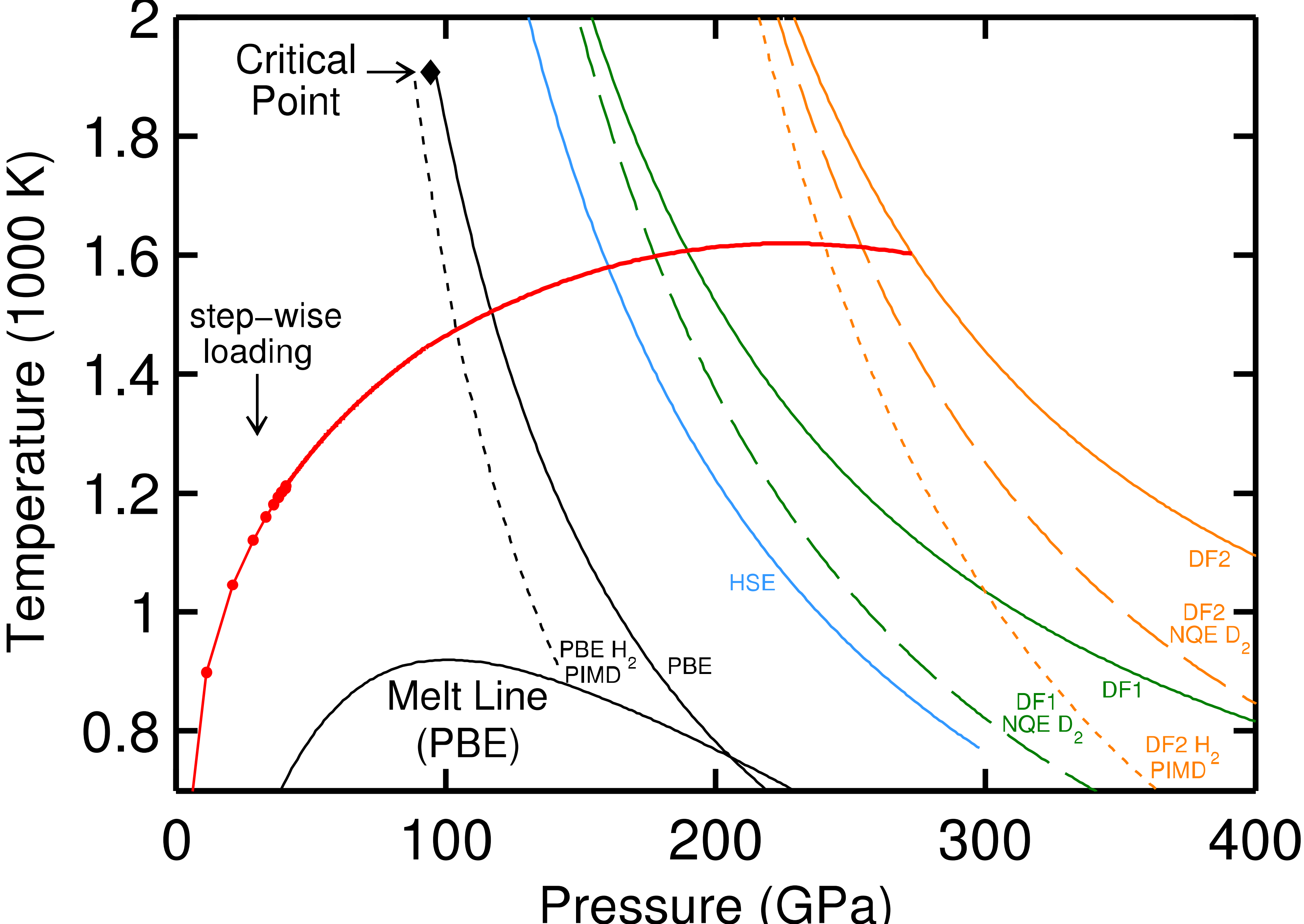


Predictions of the liquid-liquid insulator to metal transition (LL-IMT) in hydrogen vary considerably

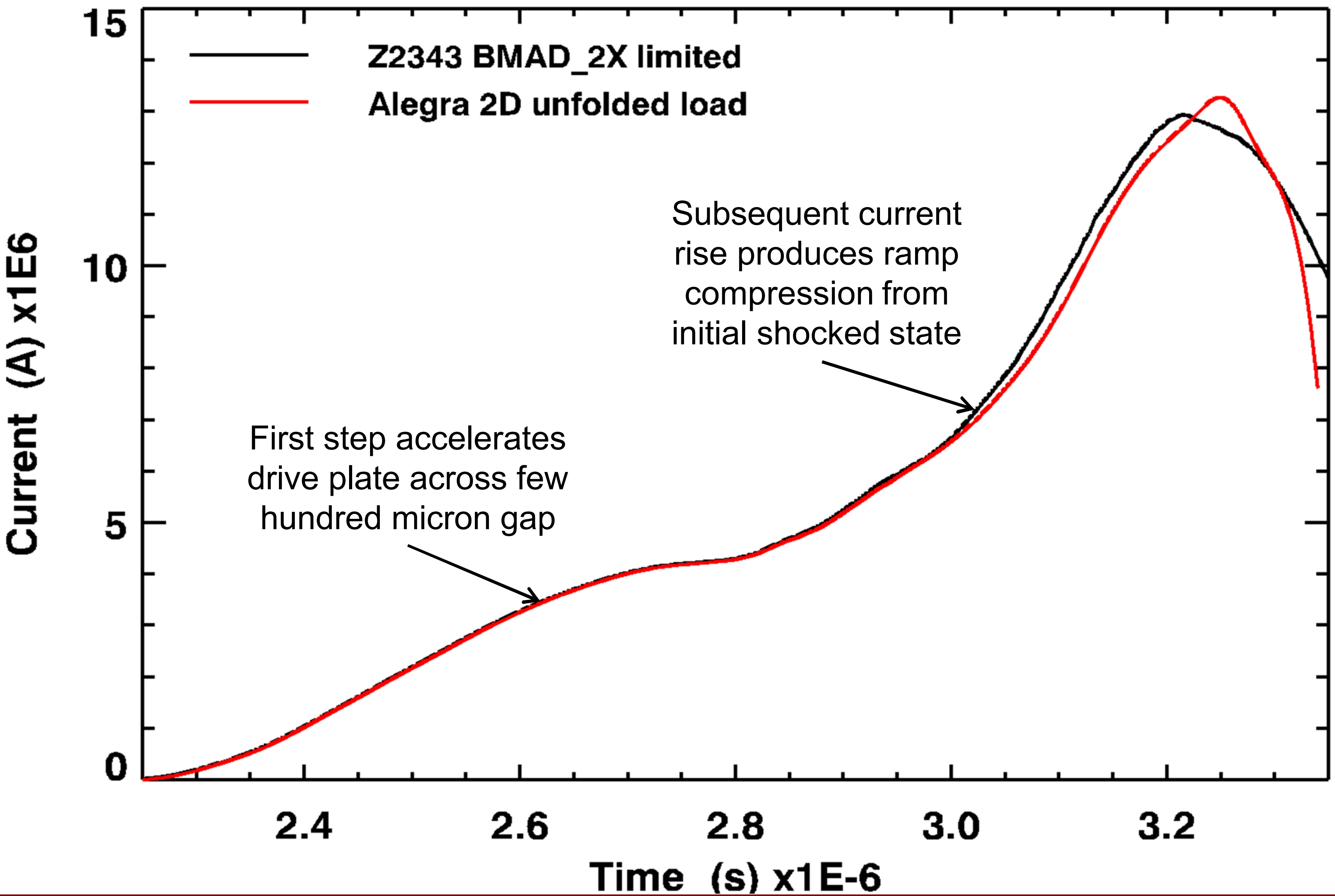


M. Morales, (2010) W. Lorenzen, (2014) M. Morales, (2013) V. Dzyabura (2013)

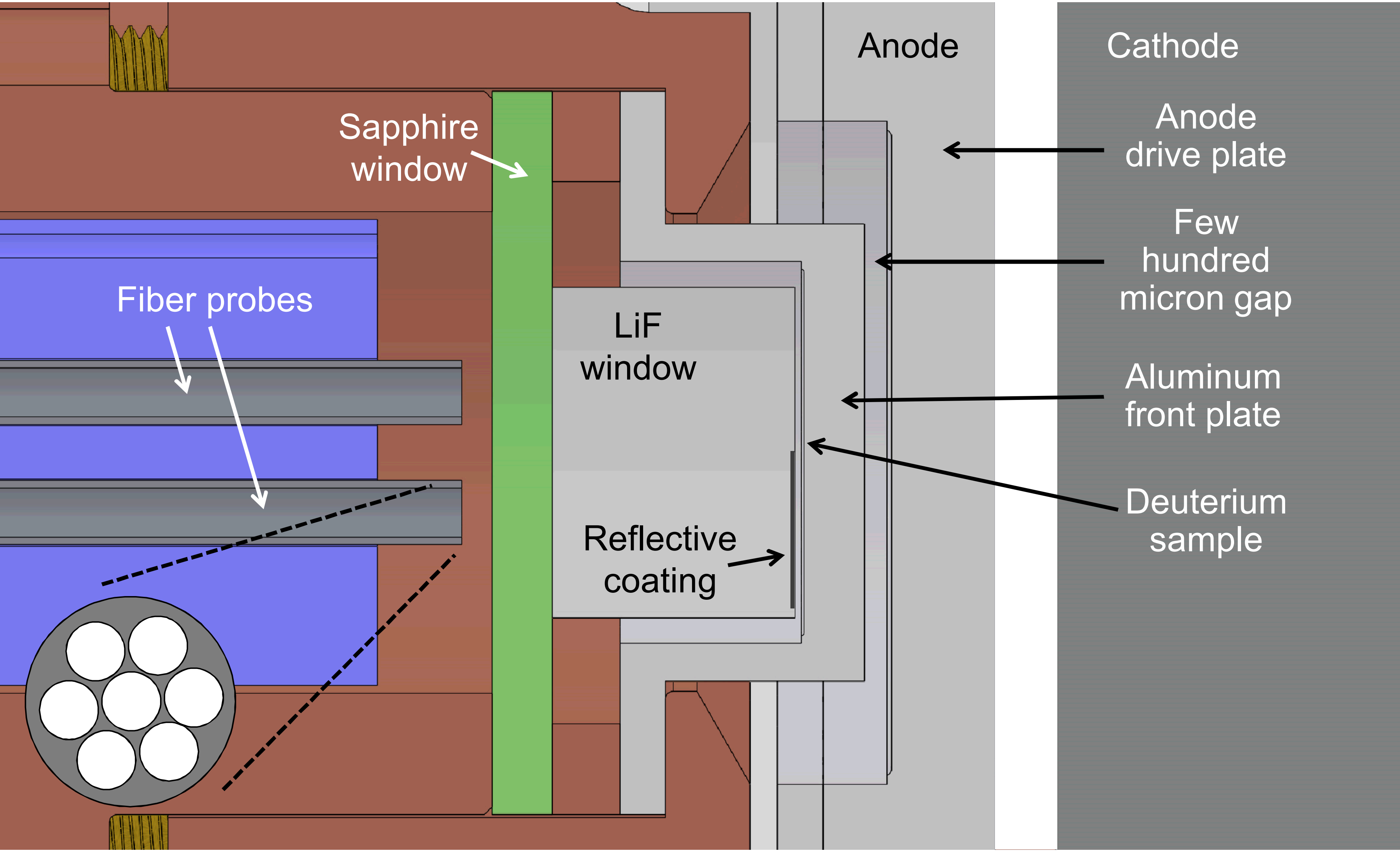
A shock – ramp experiment on Z traverses the proposed LL-IMT boundaries



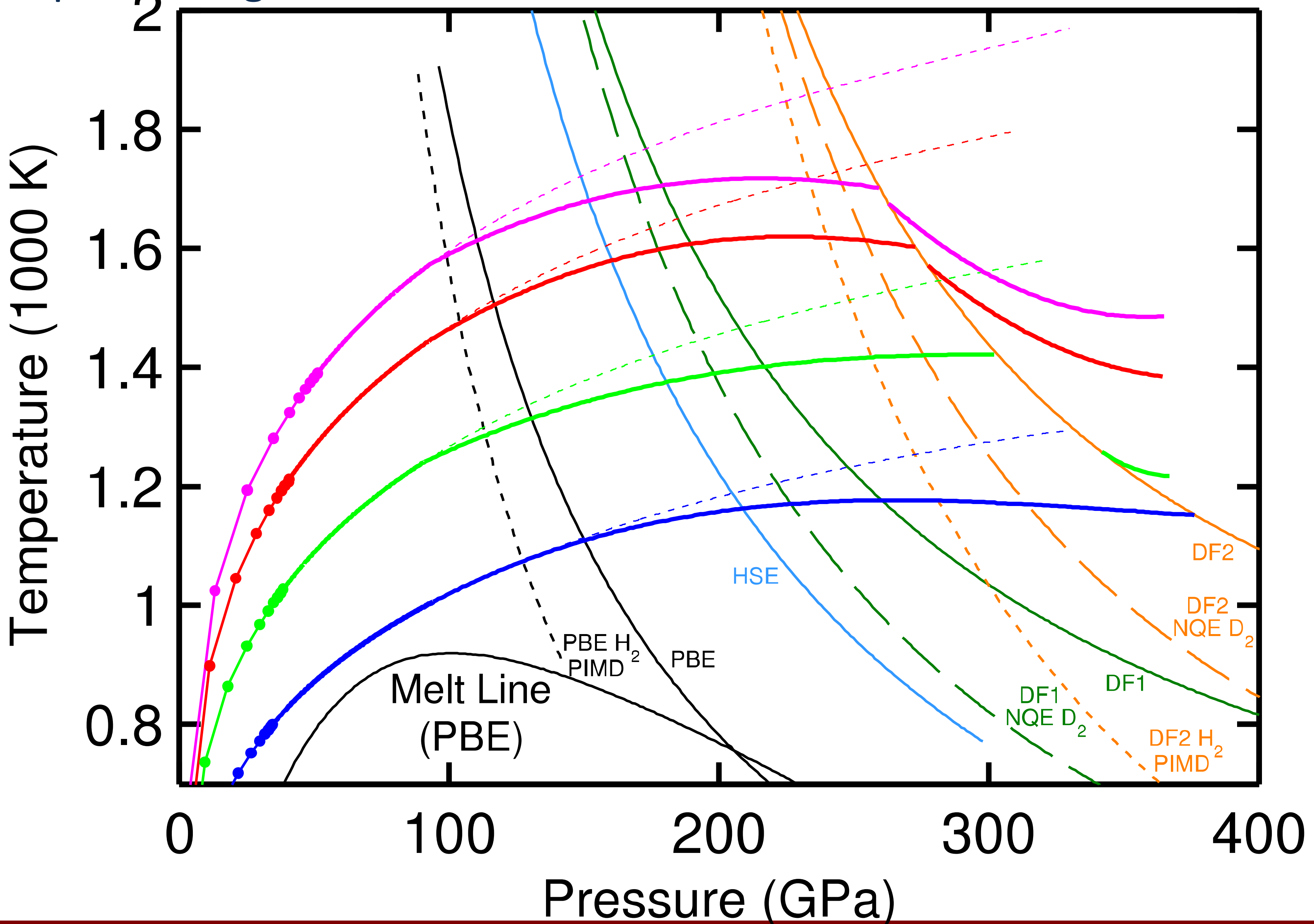
Two-step pulse shape enabled by dual Marx triggers provides the shock-ramp loading of the target



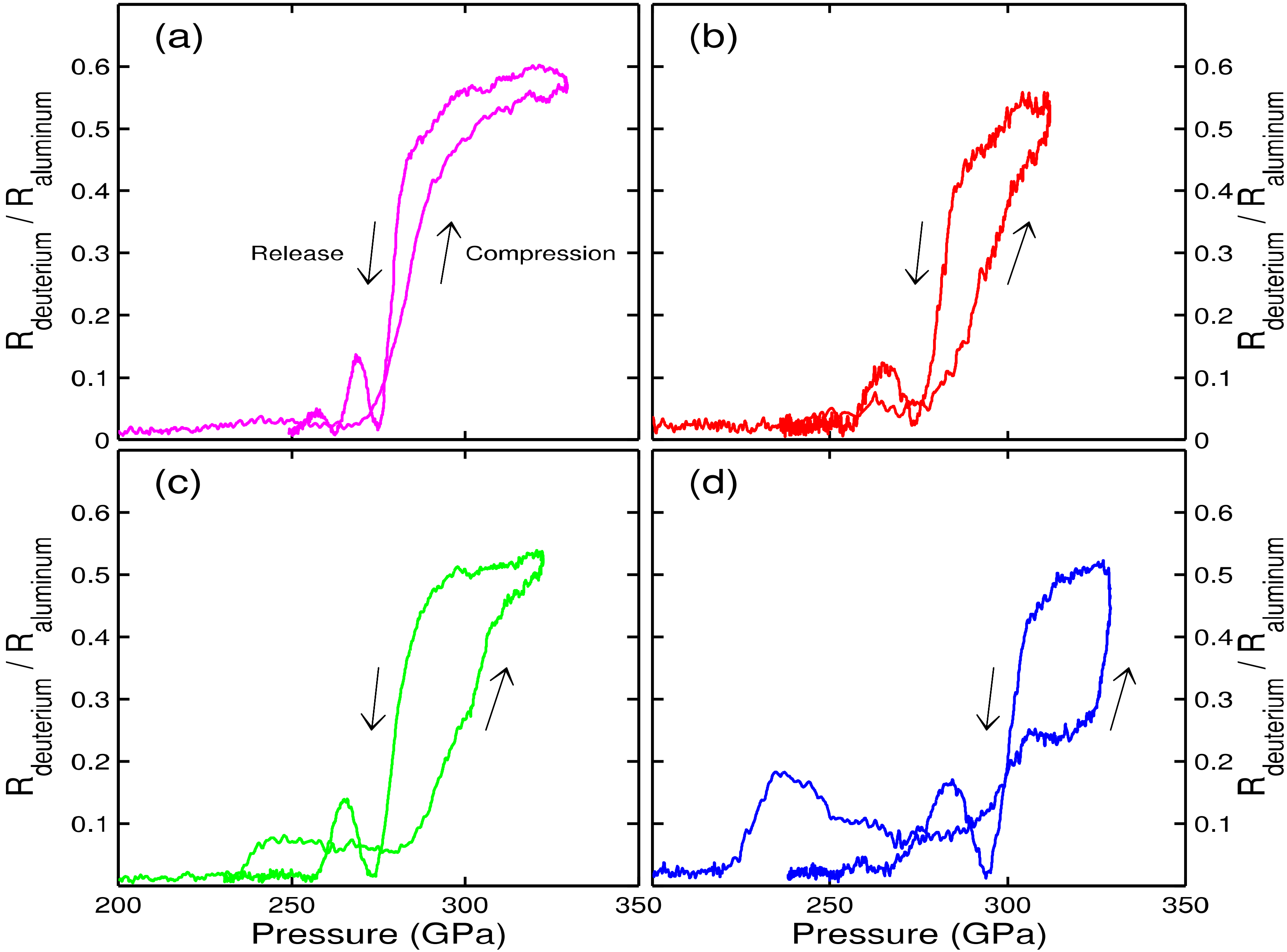
The experimental design allows for multiple diagnostics – tracking the shock-ramp compression of deuterium



The experimental PT Paths span the important region of the phase diagram



The reflectivity is a sensitive diagnostics for metallization



We have located the LL-IMT in deuterium to be at 300 GPa

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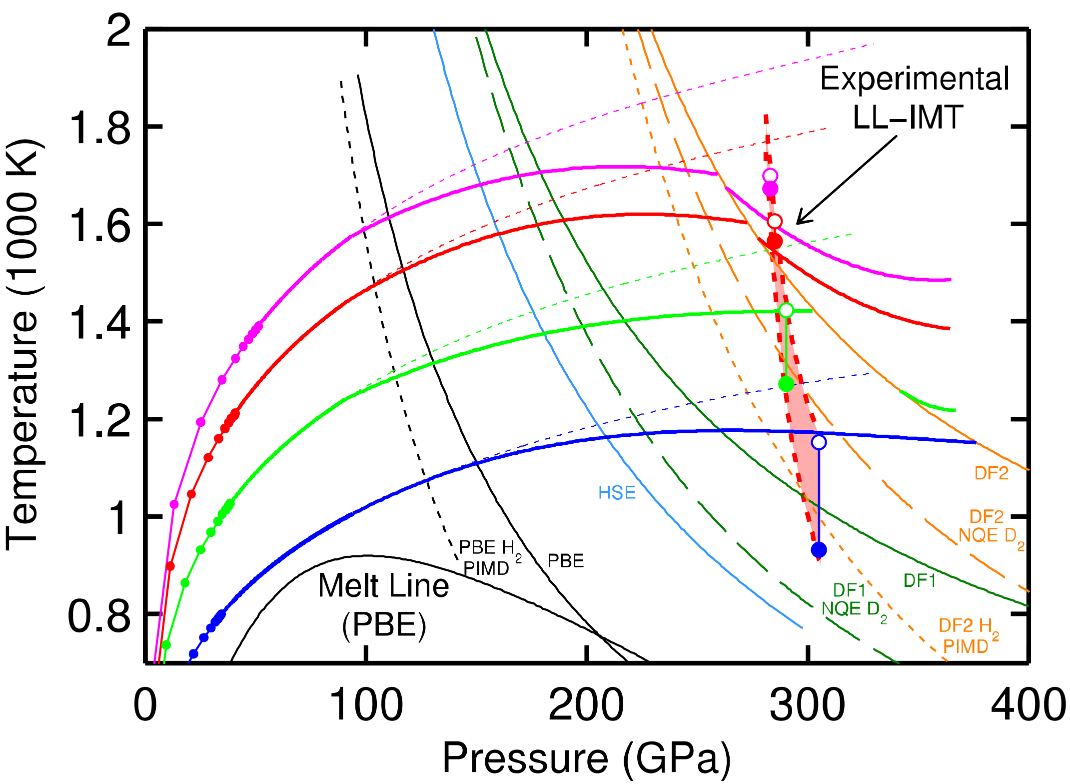

M.D. Knudson, M.P. Desjarlais, A. Becker, R.W. Lemke, K.R. Cochrane, M.E. Savage, D.E. Bliss, T.R. Mattsson, and R. Redmer, SCIENCE **348** 1455, 26 June 2015.

- *Insensitivity to T suggests this is a ρ-driven transition*
  - ρ at the transition is inferred to be ~2-2.1 g/cc in deuterium
  - Qualitatively different transition than in shock experiments (T driven)
- Broad team with expertise in diagnostics, pulse-shaping, experimental design, and first-principles simulations
- A project within the Z Fundamental Science Program
  - Professor Ronald Redmer's group at University of Rostock

We expect the H-He demixing region to be shifted to higher pressure – possibly explaining the Jupiter/Saturn age discrepancy in evolution models

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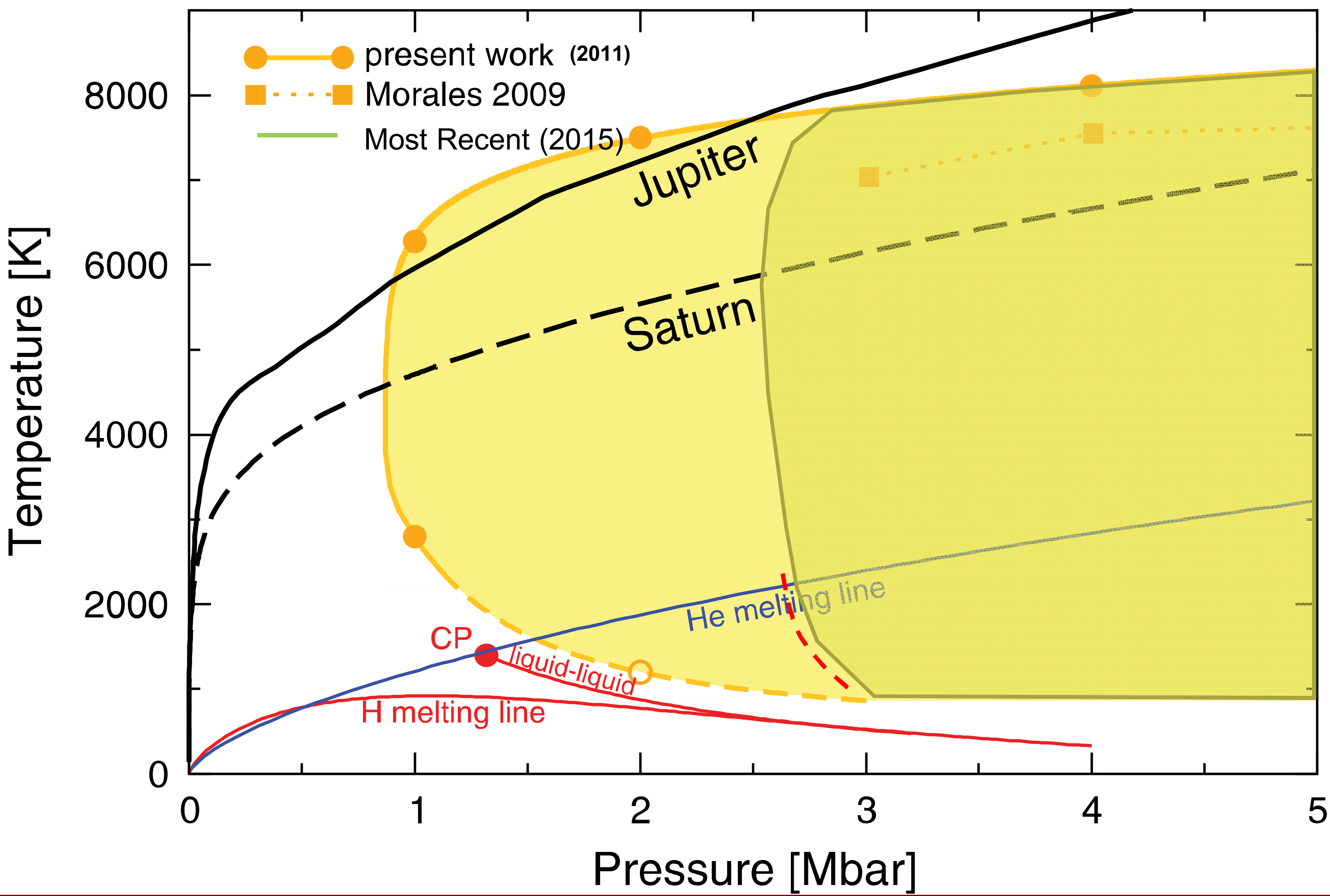
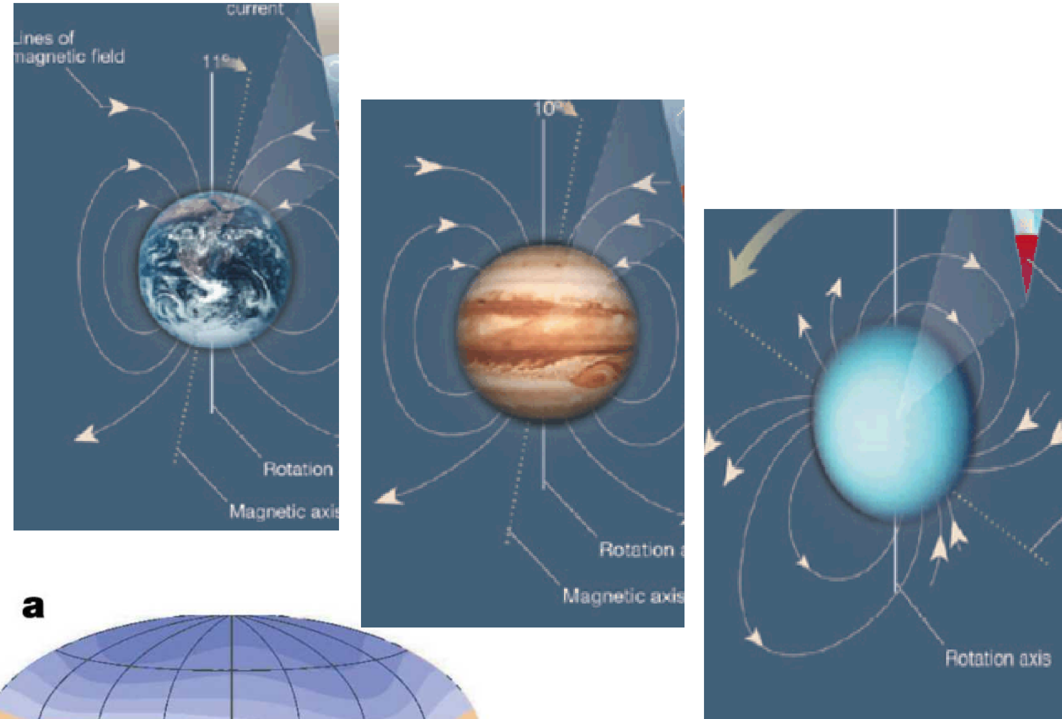


W. Lorenzen, B. Holst, and R. Redmer, Phys. Rev. B 84, 235109 (2011)

The HED properties of water may explain magnetic fields of the gas and ice giants

- Intriguing differences
  - Saturn and Jupiter have bi-polar magnetic fields (like earth)
  - Neptune and Uranus have complex multi-polar magnetic fields
- Magnetic field
  - Magnetic fields are generated by planetary dynamos, which require convection in a conductive medium
  - The differences in field imply different planetary structure



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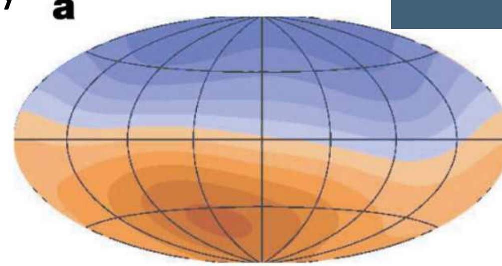
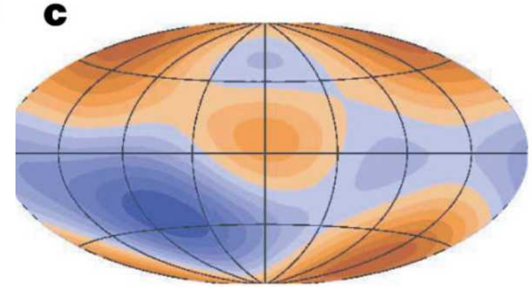


Earth

c

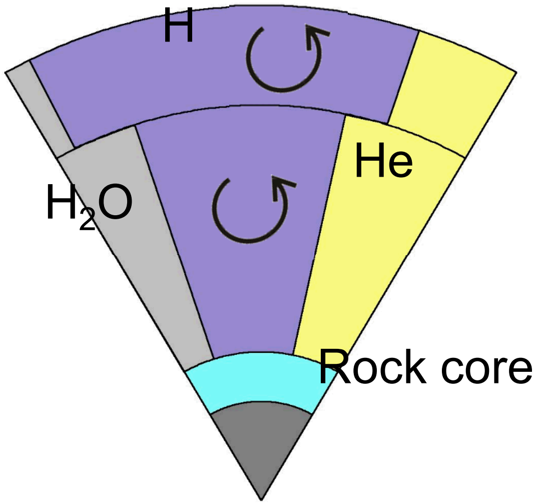


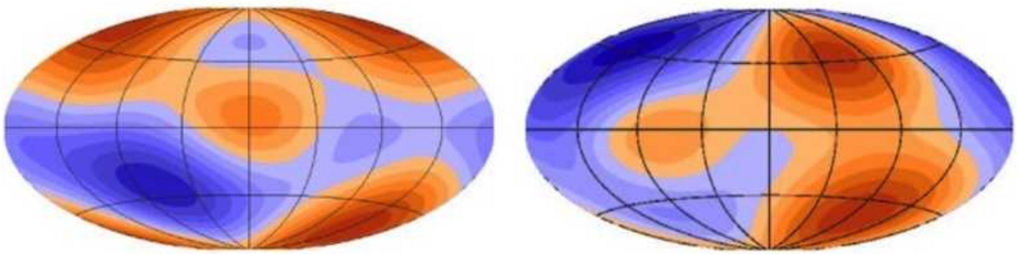
Neptune

Stanley and Bloxham, (Nature 2004, Icarus 2006)

Properties of water control the structure of the ice giants

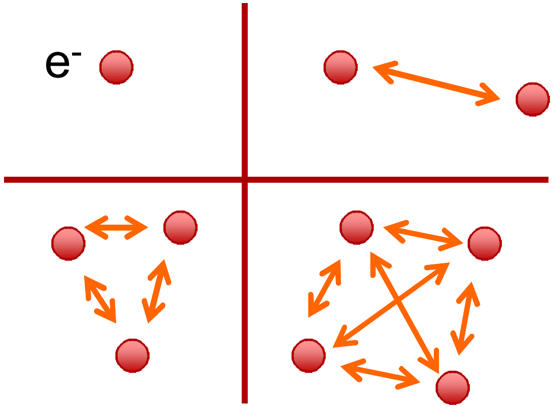
- Inferred structure
  - Layers of different composition while fulfilling observational constraints
  - Solutions are not unique and depends on the equation of state (EOS)
- Magnetic field
  - A thin layer of convective ice near the surface could account for the observations and for high-order terms in the field
- The phase-diagram of water plays a major role
- We explore water with DFT and Z experiments





Stanley and Bloxham, (Nature 2004, Icarus 2006)

Density functional theory (DFT) based MD is an established approach - HEDP sets additional demands



Treating quantum many-body interactions between electrons well is very demanding

Large-scale simulations on the supercomputer cielo

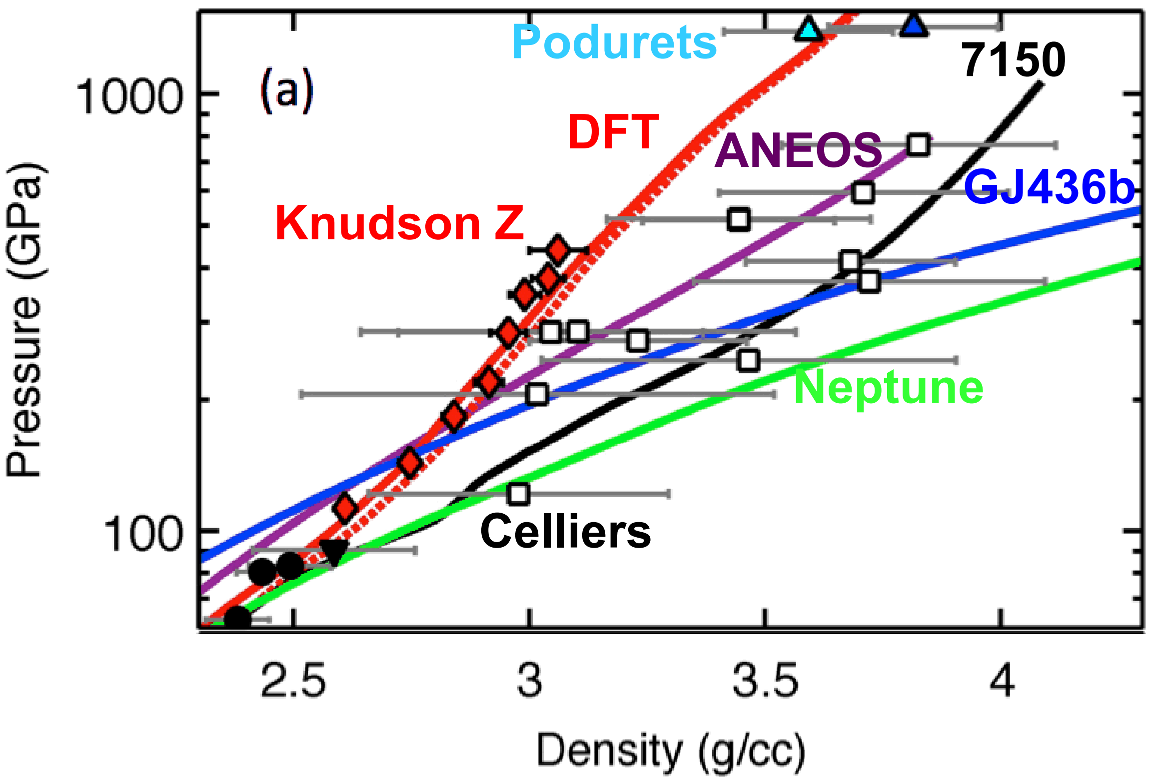
DFT calculations can be predictive

- Based on quantum mechanics – a first-principles method, no empirical parameters/ fits
- Solving the Kohn-Sham equations
- *Accuracy* set by the exchange-correlation (xc) functional
- *Convergence* of simulation parameters to desired precision

VASP code (Georg Kresse, Vienna, Austria)

- Finite-temperature DFT (Mermin)
- Plane-wave basis-set for controlled convergence and free electrons/ionization
- Projector augmented wave core functions (PAW)

Experimental data from Z validates the DFT simulations suggesting water is significantly stiffer than previous models

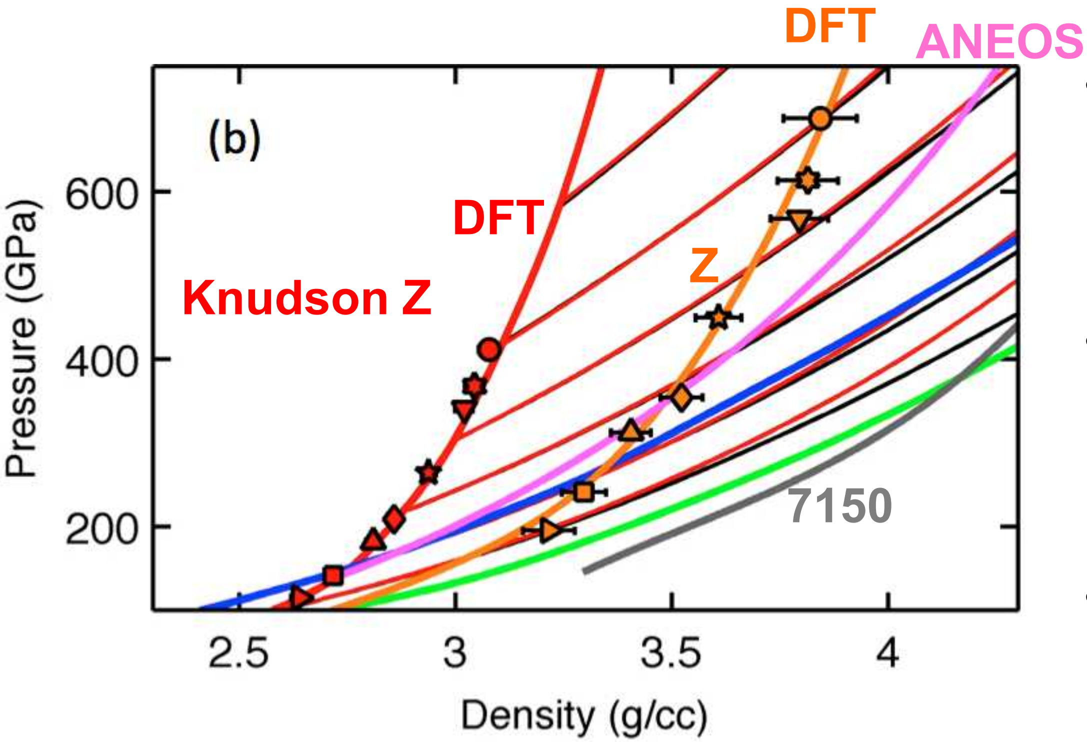


DFT results validated by

- gas-gun data (<100 GPa)
- very high P result from Russia
- high pressure results from Sandia's Z machine

Knudson et. al. (PRL, 2012).

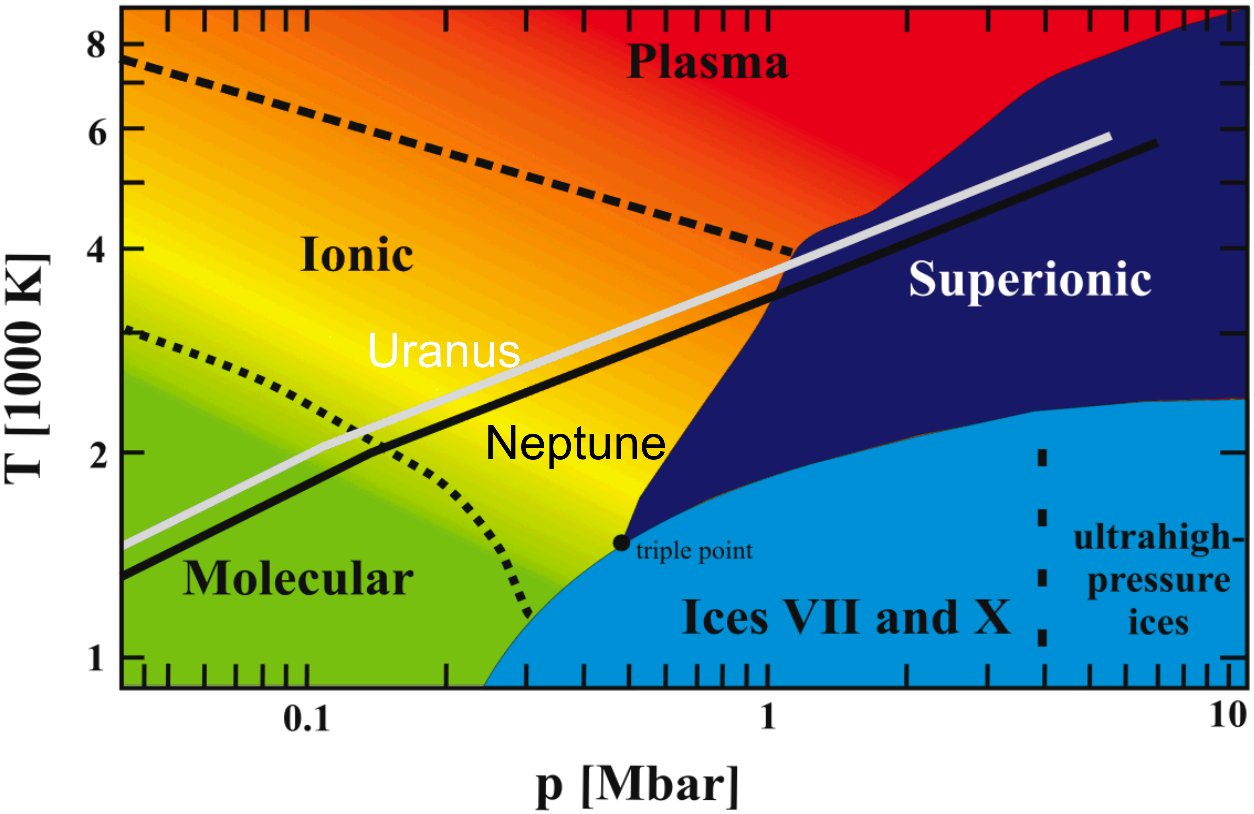
Second shock provides almost isentropic compression from the initial first shock state along the planetary isentropes



- Double-shock results validate isentropic compression results obtained from DFT
- Data along planetary isentropes for Neptune and hot exoplanets like GJ436b
- Note the distinctly different behavior for second shock in ANEOS (pink) and 7150 (gray)

Knudson et. al. (PRL, 2012).

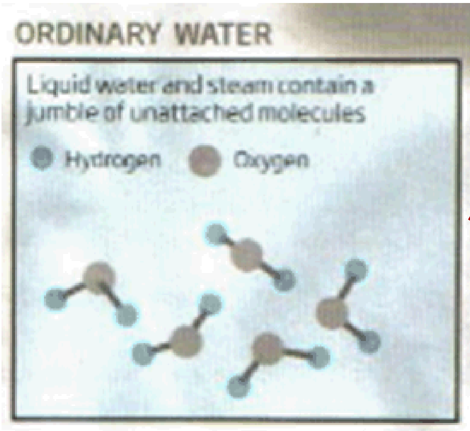
The interiors of Neptune and Uranus transition three phases in the new DFT EOS



- Well-defined traces for isentropes of ice giants
- Implications for several aspects of planetary structure
  - Layering
  - Convection
  - Electrical conductivity

Redmer, et. al (Icarus 2011).

Water phase profoundly affects character of the ice giants



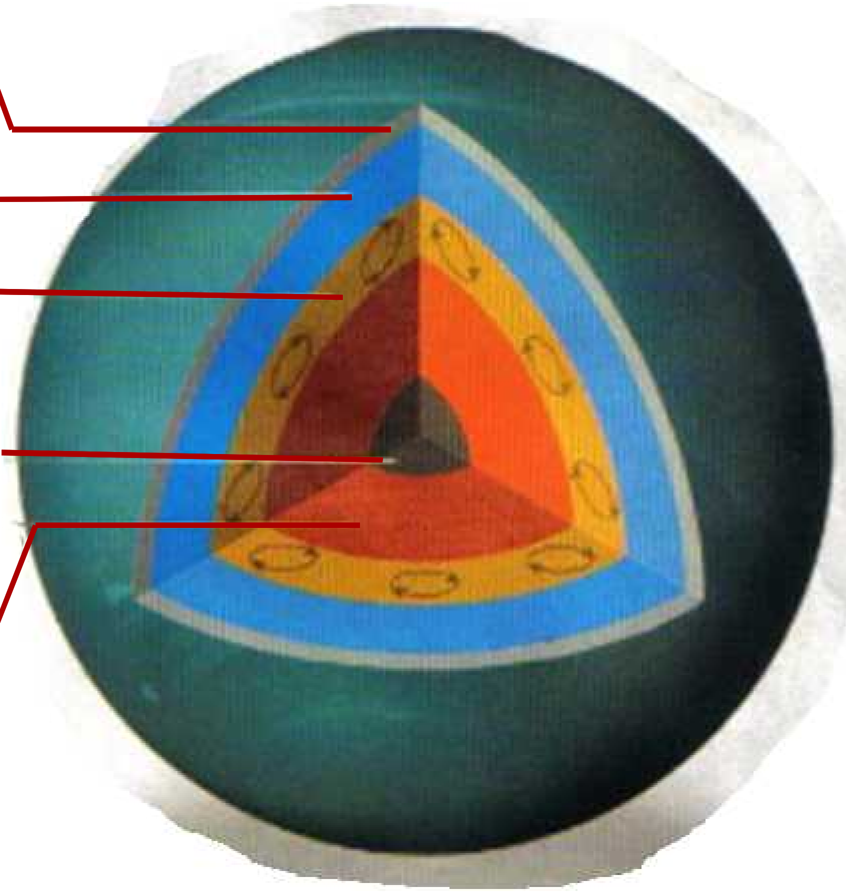
Ice and liquid water

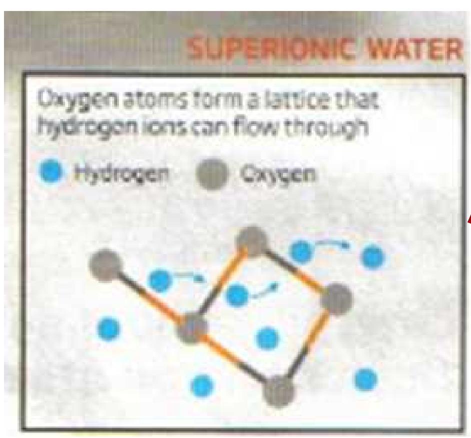
Hydrogen & Helium

Ionic water
Convection creates irregular magnetic field

Rock

Superionic water
No convection: no magnetic field





Shiga (New Scientist 2010)

Z experiments provide material properties in HED conditions to address the moon formation mystery

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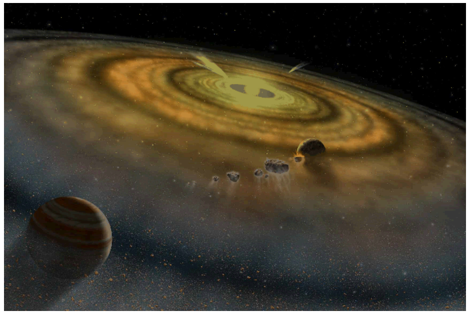
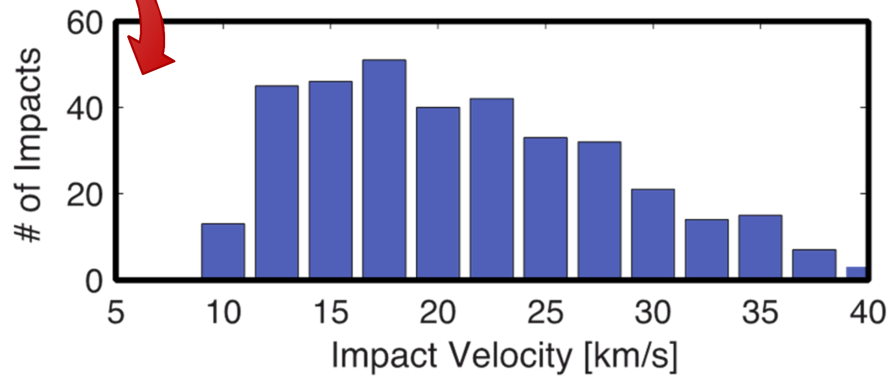
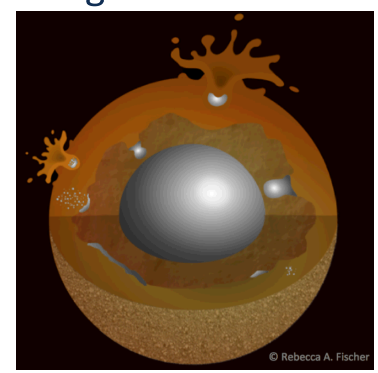


When an iron meteor hits the earth,(in the future or during the formation of the solar system) does it plow into the ground as a bullet, splatter as a drop of rain, or vaporize into a cloud of iron to return to earth as iron rain?



Planetary dynamics suggests high impact velocities

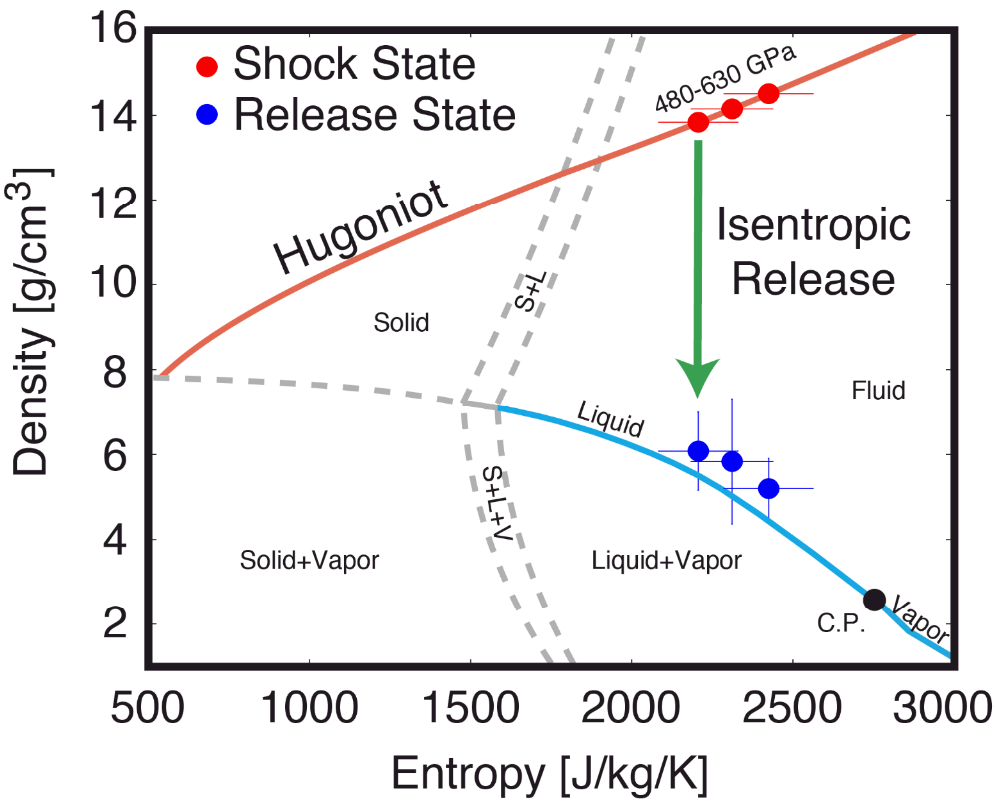


The models depend on the HED properties of iron (particularly vaporization)!

Geophysicists have shown fluid instabilities CAN NOT sufficiently mix the incoming iron cores to explain observed iron content in the mantle or the similarity in isotopics between the earth and the moon

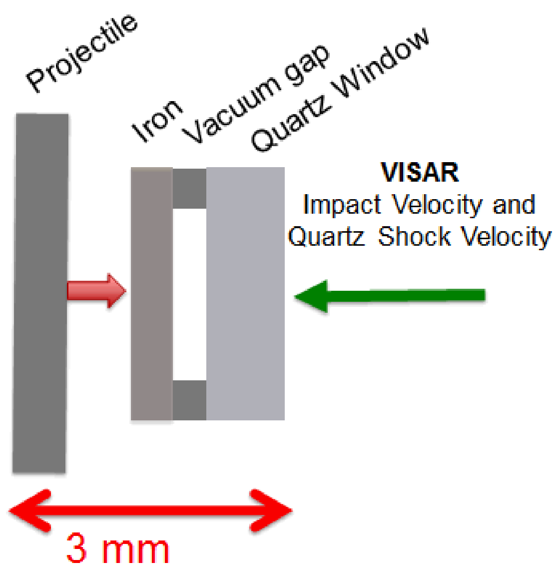
N-body simulations from Raymond et al. 2009

Z can study vaporization for states produced by planet forming impacts

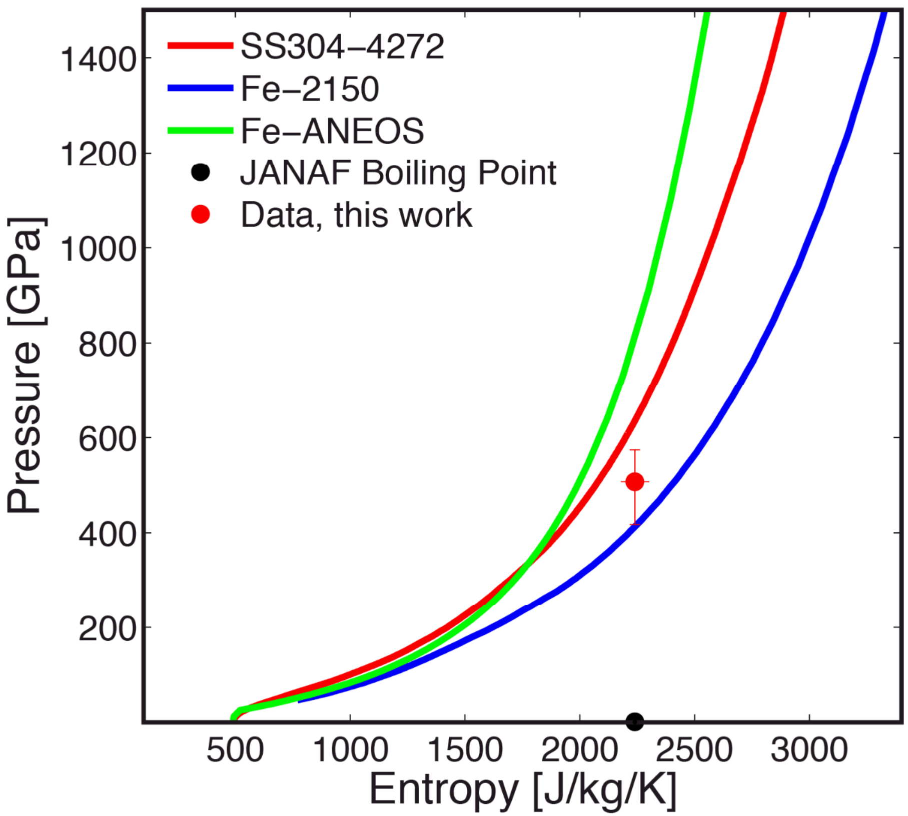


Iron Shock and Release Data

- Sandia Z facility can launch flyer plates at > 40 km/s
- We can directly simulate all impact conditions
- A shock-release approach was used to evaluate the liquid-vapor dome as a function of entropy



HED experiments: Iron vaporization occurs at lower pressures than previously assumed



- Vaporization is significantly easier than ANEOS , the most broadly used model for geophysics, suggests
- Iron cores will vaporize at 13 km/s impacts – The state of the earth and moon are now much easier to explain
- A project within the Z Fundamental Science Program
  - Stein Jacobsen, Harvard
  - Sarah Stewart at UC Davis
  - Rick Kraus, LLNL

Impact vaporization of planetesimal cores in the late stages of planet formation, R.G. Kraus, S. Root, R.W. Lemke, S.T. Stewart, S.B. Jacobsen, and T.R. Mattsson, Nature Geoscience 2015 DOI: 10.1038/NGEO2369

Summary

- HED materials are central to many interesting planetary science problems
- The Z facility can provide high precision relevant data to address
- The Z fundamental science collaborations have shed light on several long-standing questions

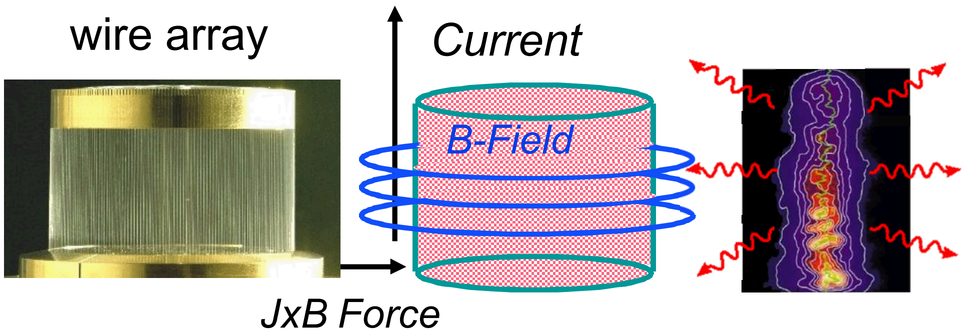
Acknowledgements:

- Z operations and diagnostic teams
- Dynamic material properties and HEDP theory teams
- The Rostock team
- The Harvard/Davis/LLNL team

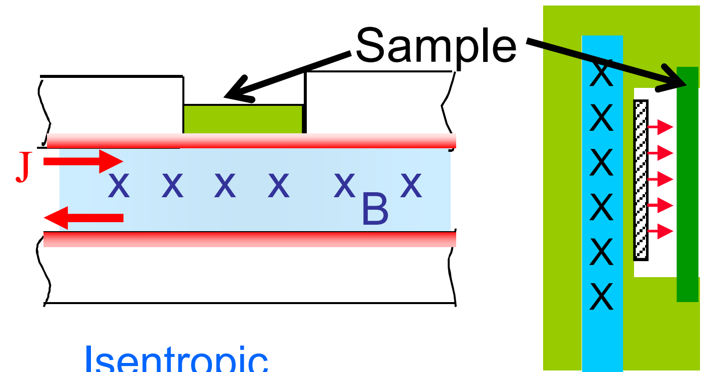
Backups

We use magnetic fields to create HED matter in different ways for different applications

Radiation physics using Z-Pinch X-ray Sources



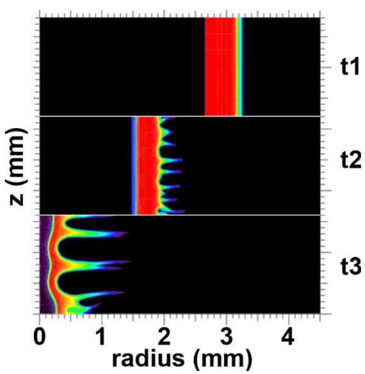
Materials Properties: EOS



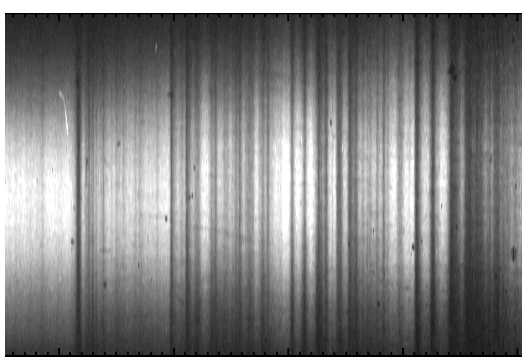
Isentropic Compression

Flyer Plate

Atomic- and plasma physics

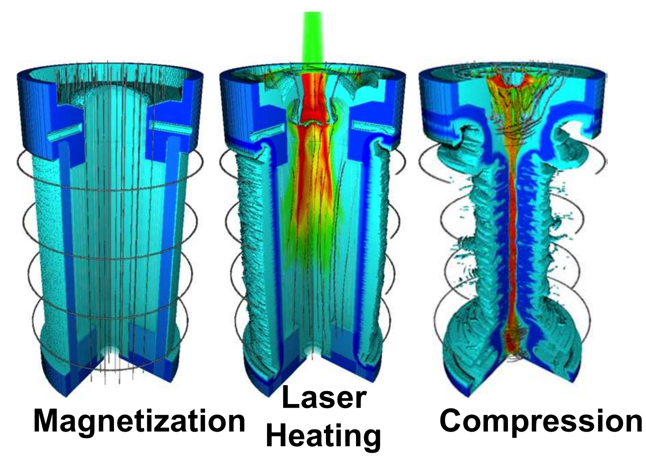


MRT instabilities



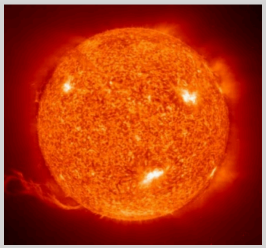
Iron spectrum

Inertial confinement fusion



ZAPP campaigns simultaneously study multiple issues spanning 200x in temperature and 10^6x in density

Solar Opacity



Question:
Why can't we predict the location of the convection zone boundary in the Sun?

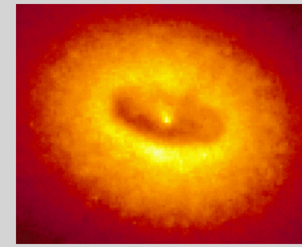
Achieved Conditions:
$T_e \sim 200$ eV, $n_e \sim 10^{23}$ cm^{-3}

White Dwarf Line-Shapes

Question:
Why doesn't spectral fitting provide the correct properties for White Dwarfs?

Acheived Conditions:
$T_e \sim 1$ eV, $n_e \sim 10^{17}$ cm^{-3}

Photoionized Plasmas



Question:
How does ionization and line formation occur in accreting objects?

Achieved Conditions:
$T_e \sim 20$ eV, $n_e \sim 10^{18}$ cm^{-3}

Does opacity uncertainty cause the disagreement between solar interior models and helioseismology?

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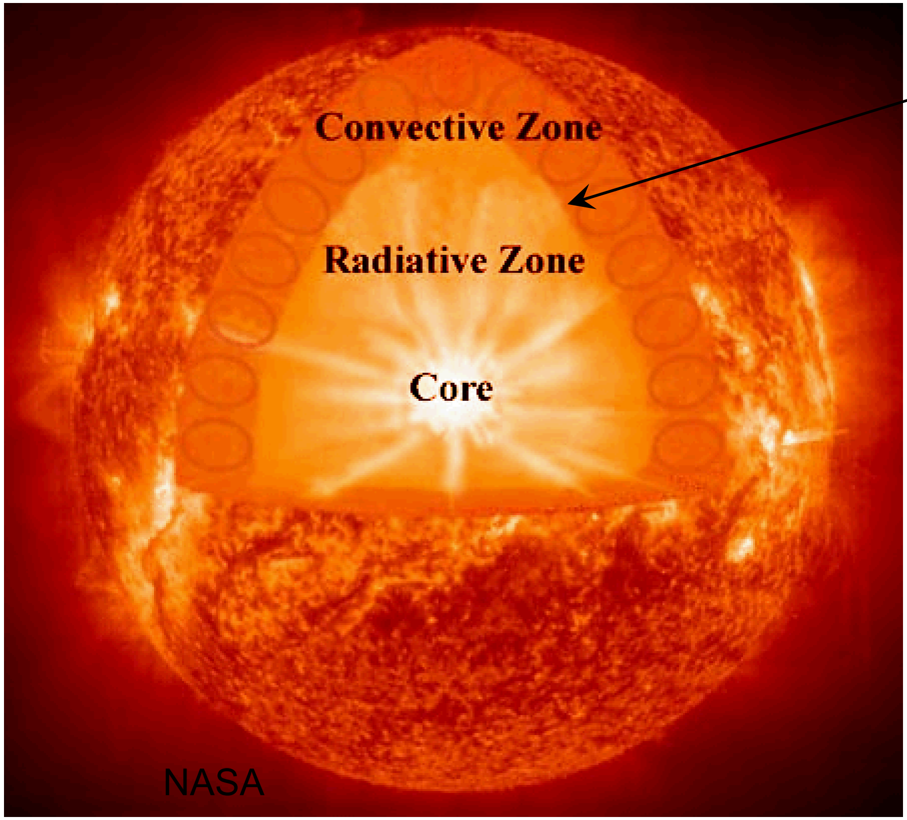


Discrepancies in CZ boundary location, C_s (r), and ρ(r)

Models depend on:
- element abundances
- EOS
- opacity

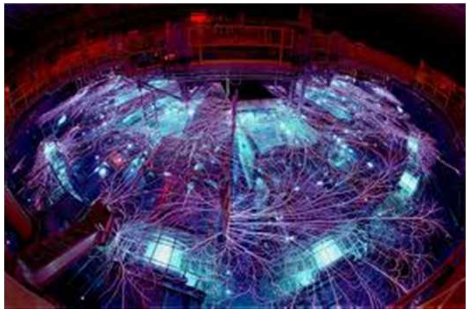
focus: iron at convection zone base {187 eV, 9e22 e/cc}

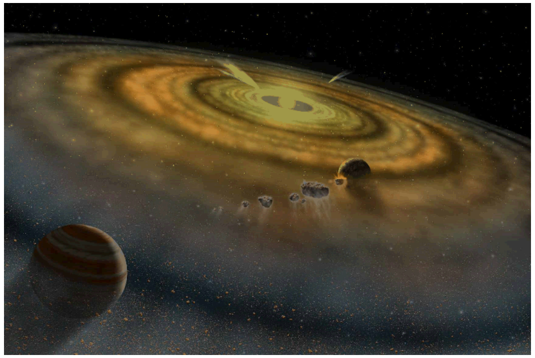
Disagreement could be resolved if the true mean opacity for solar matter is 10-20% higher than predicted

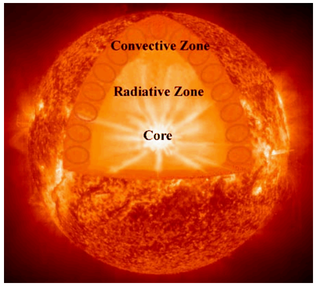
S. Basu *et al*, Physics Reports (2008). M. Asplund *et al*, Annu. Rev. Astro. Astrophys (2005)

Pulsed power is exquisitely suited for HED science

- **Sandia's Z machine is ideal for Mbar material experiments**
  - Compression of solids and liquids
  - Obtain conditions of the interiors of gas giants and the Earth/ super earths, other exoplanets
- **The Z machine produces MJs of x-rays**
  - Radiation effects on materials
  - Fundamental properties of matter
- **Fundamental plasma physics**
  - Spectroscopy and plasma conditions: line broadening and opacity
- **Promising fusion concept**
  - Direct cylindrical drive
  - Pre-magnetized and –heated fuel
  - *Systematic studies of the underlying physics*
- **Strong integration between experiments, theory, and simulations**
  - From quantum mechanics to MHD and beyond
- ***Well-defined path for the future – decades of exciting HED Science research lies ahead***

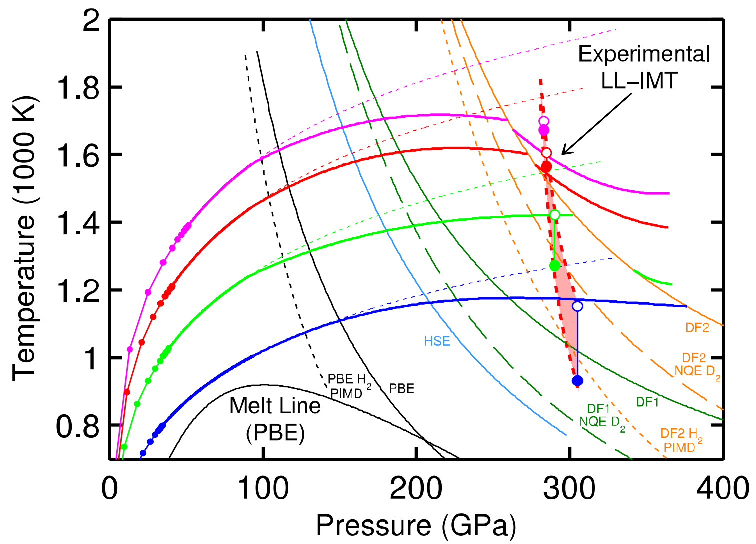


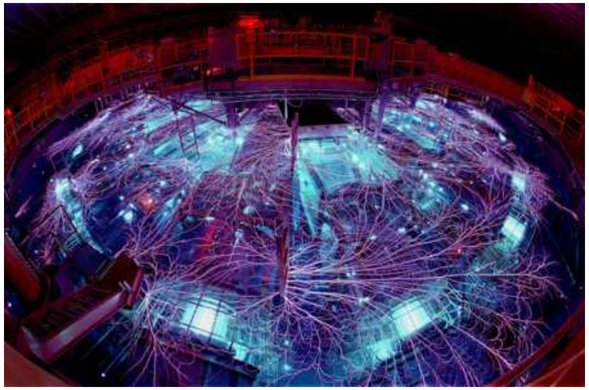




We have determined the location of the density-driven LL-IMT phase transition in hydrogen

- Shock-ramp technique enables experimental access to the liquid-liquid, insulator-metal transition (LL-IMT) for hydrogen
  - The temperature is set by the initial shock
- Experiments above ~250 GPa show clear evidence of metallization of deuterium
  - Very abrupt increase in reflectivity to ~40-50%
  - Pressure is well above numerous first principles predictions
  - Implications for understanding Jupiter, Saturn, and thousands of exoplanets
- Insensitivity to *T* suggests this is a ρ-driven transition
  - ρ at the transition is inferred to be ~2-2.1 g/cc in deuterium
  - Qualitatively different transition than in shock experiments (T driven)



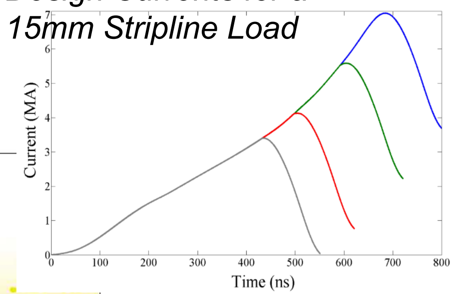


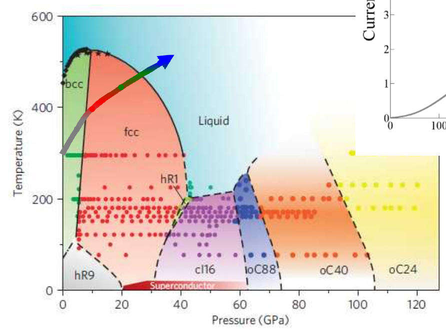
A high throughput megabar-class accelerator is under construction

- Improved repetition rate allows systematic study of rate dependent phenomena
  - Phase transitions
  - Kinetics of melt and re-freeze under ramp compression
  - Strength, including phase transitions
- We have developed experimental designs for phase-transition and strength experiments
- Systematic studies of materials, grain size and texture for phase-kinetics and strength
- Targeting late 2017 completion
  - Interesting possibility for DCS

Peak Ramp Compression States in Li

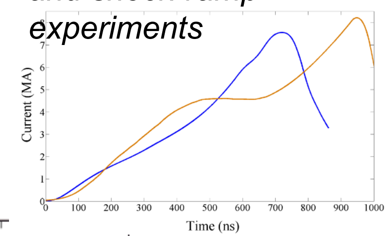
Design Currents for a 15mm Stripline Load



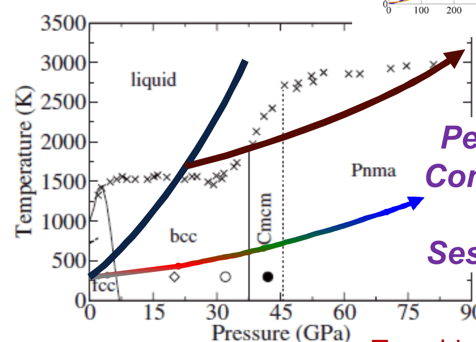


Guillaume, et al. , Nature Physics, 2011

Design Currents for ramp and shock-ramp experiments



Phase space accessible in Ca

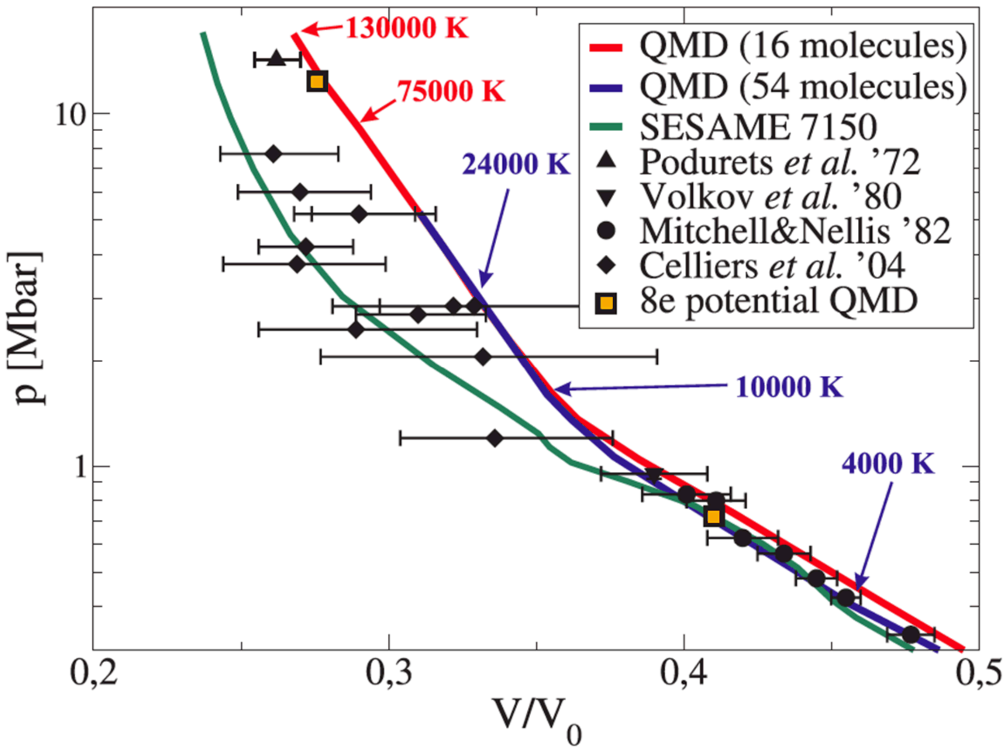


Shock-Ramp Example

Peak Ramp Compression States Sesame 2030 EOS

Teweldeberhan and Bonev, PRB, 2008

DFT calculation of principal Hugoniot of water



Equation of state and phase diagram of water at ultrahigh pressures as in planetary interiors
French, Mattsson, Nettelman, and Redmer
PRB **79**, 054107 (2009).

- DFT results agree with gas-gun data (<1 Mbar)
- DFT results agree with very high P result from Russia

- DFT results disagree with SESAME 7150
- DFT results disagree with laser data (Celliers 2004)

- Technical detail: all-electron calculations (8 e O potential)
- Careful calculations but disagreement with data is a point of concern

Density functional theory (DFT) based MD is an established approach - HEDP sets additional demands

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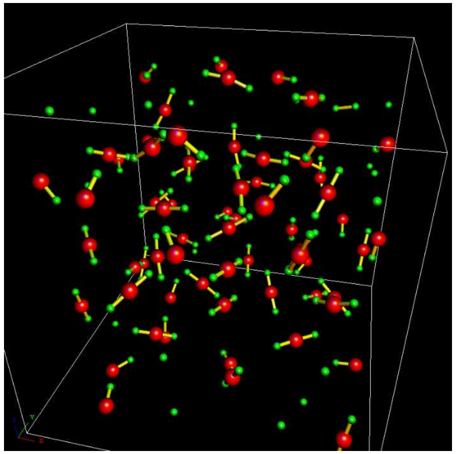
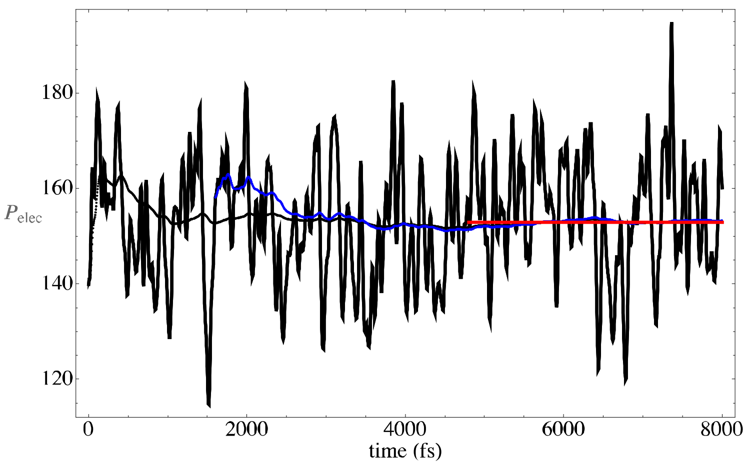




Time-averaging of pressure during a molecular dynamics (MD) simulation.

DFT calculations can be predictive

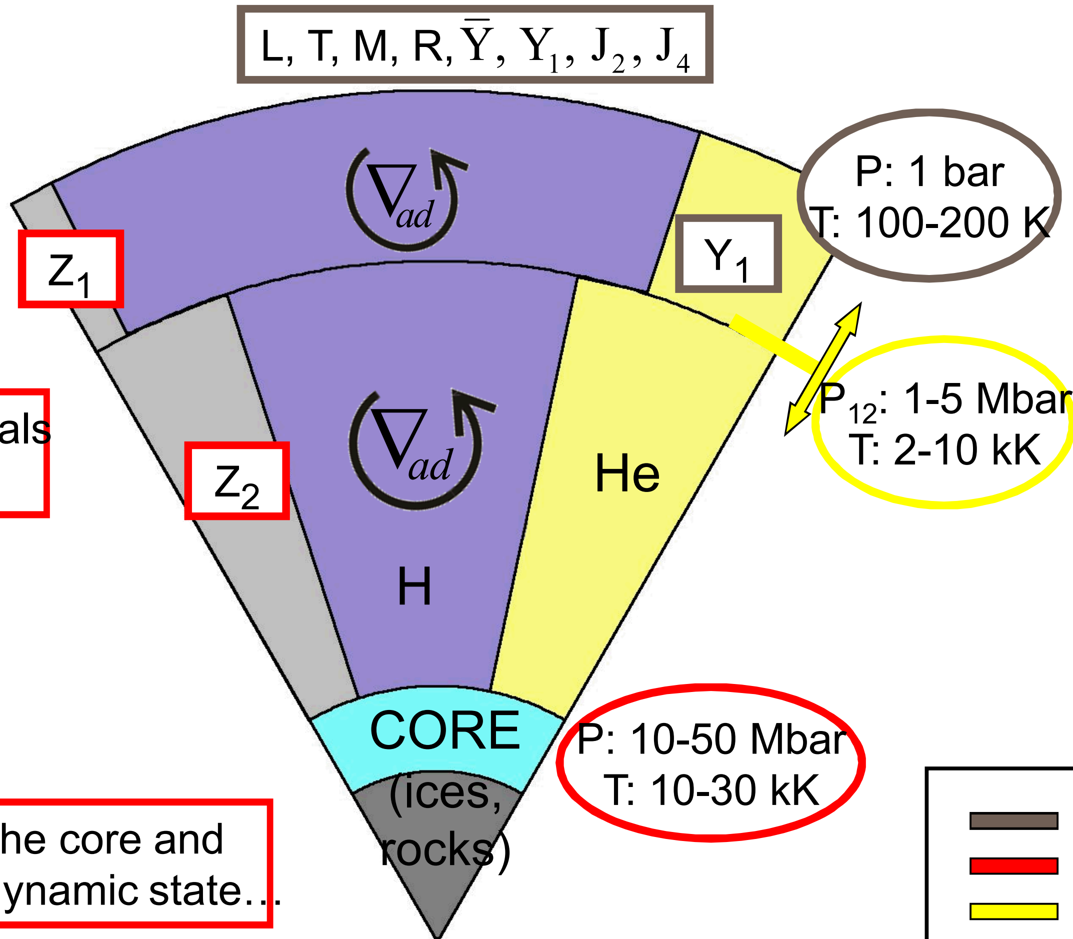
- Based on quantum mechanics – a first-principles method, no empirical parameters/ fits
- Solving the Kohn-Sham equations
- *Accuracy* set by the exchange-correlation (xc) functional
- *Convergence* of simulation parameters to desired precision

VASP code (Georg Kresse, Vienna, Austria)

- Finite-temperature DFT (Mermin)
- Plane-wave basis-set for controlled convergence and free electrons/ionization
- Projector augmented wave core functions (PAW)

First-principles thermodynamics simulations yield $P(\rho,T)$, $E(\rho,T)$, structure, diffusivity, etc.

Standard three-layer structure model for GPs



Fraction of metals in the layers…

Size of the core and thermodynamic state…

Y: fraction of He

Z: fraction of metals

J_2, J_4: gravitational moments

Physical origin and location of the layer boundary…
→ MIT (PPT)
→ H-He demixing

- constraints
- results from modeling
- free parameter

Interior structure models of this type are uniquely defined by the observables, except P_{12}

Interior of Neptune and Uranus using EOS from DFT and layering due to phase-transitions in water

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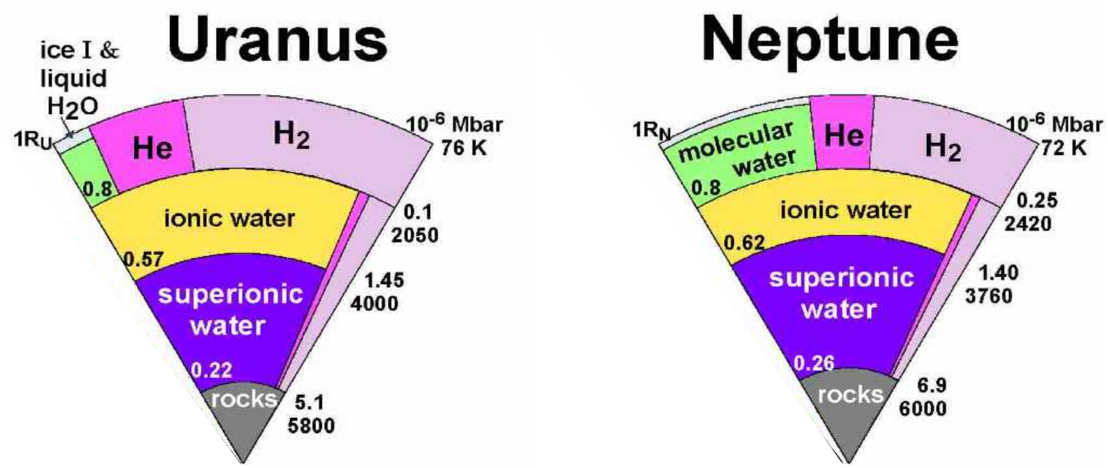

The phase diagram of water and the unusual magnetic field of Uranus and Neptune
R. Redmer, N. Nettelmann, T.R. Mattsson, and M. French, Icarus **211**, 798 (2011).

Convective-region geometry as the cause of Uranus' and Neptune's unusual magnetic field
Stanley and Bloxham, Nature 428, 151 (2004).
Numerical dynamo models of Uranus' and Neptune's magnetic fields
Stanley and Bloxham, Icarus 184, 556 (2006).

- Planetary structure
    - Molecular
    - Ionic
    - Superionic
    - Core
- Corresponds well to the model of Stanley/Bloxham for magnetic field
- The phase-diagram of water provides a distinct physical reason for the layering