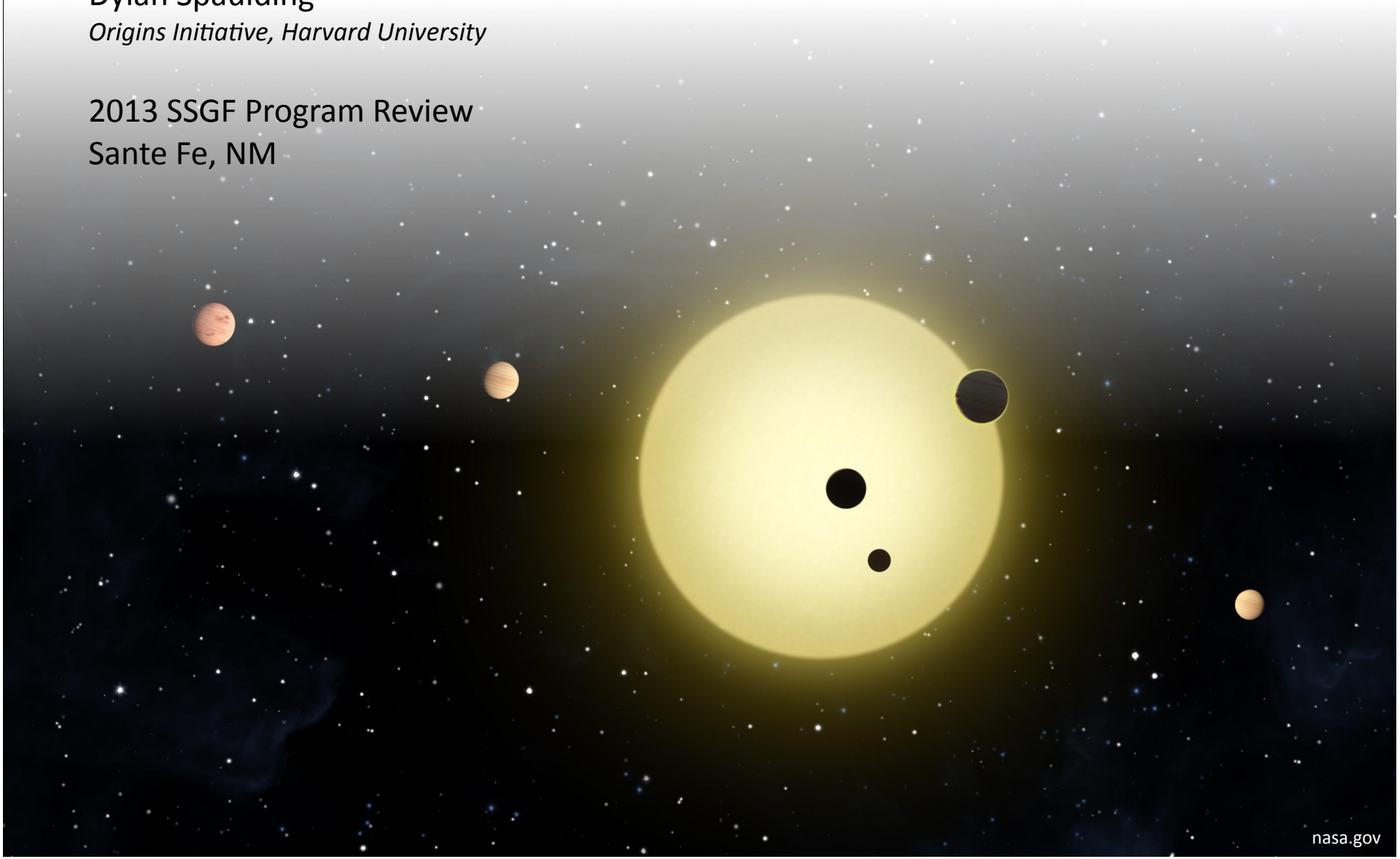
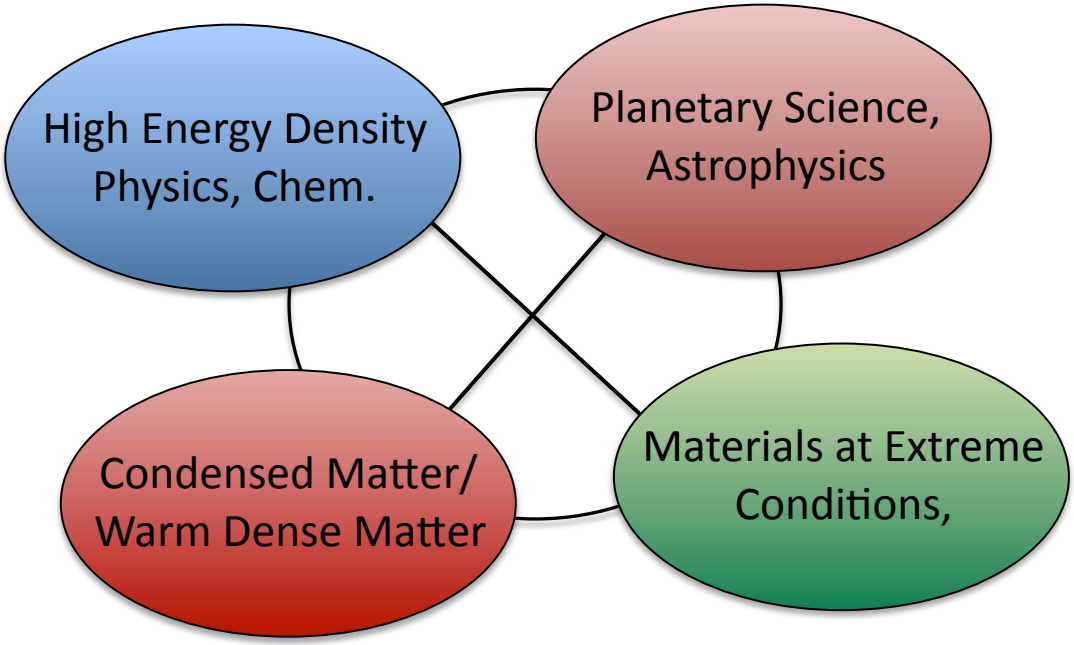
Stewardship Science ‘Outside the Box’

Dylan Spaulding
Origins Initiative, Harvard University

2013 SSGF Program Review
Sante Fe, NM



Stewardship Science Tools and Interdisciplinary Possibilities



•Finding cross-overs between disciplines and *dual-purpose* problems

• How to apply tools to do something completely new?

Tools

• Accessing High P/T States in Increasingly Controlled Ways

• Diagnosing those states

• Computation

Properties

• Compressibility

• Melting, Phase Relations

• Transport Properties

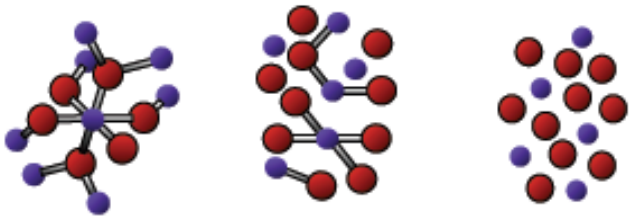
• Opacities

• Mesoscale Physics/Chemistry

The Physics and Chemistry of High Pressure – 'Terra Incognita'

"Ultrahigh" Pressures

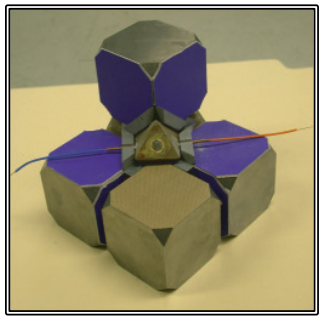
~ 100 GPa = 1 Million Atmospheres (1 Mbar)

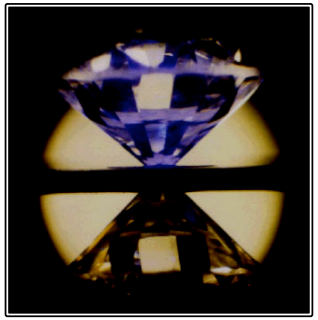


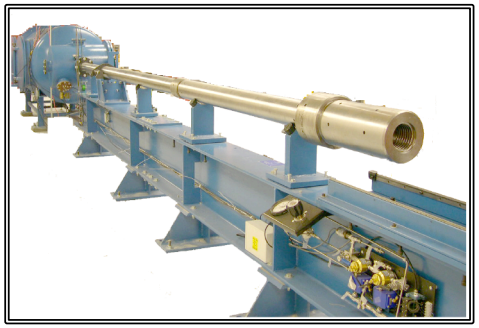
Compression Work ≈ **Chemical Bonding Energies**

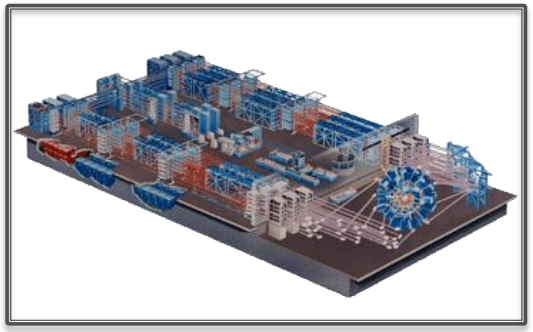
$P\Delta V$ ≅ 1 eV ≅ 100 kJ/mol of atoms

(Valence electron energies)









Multi-Anvil — Few GPa

DAC — ~100 GPa

D" — *135 GPa*

Gas Gun — ~250 GPa

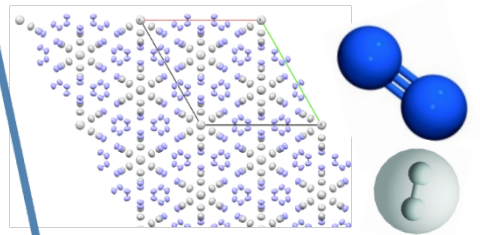
Earth's Core — *360 GPa*

Lasers — >>10^3 GPa

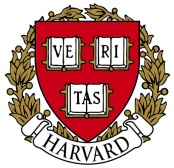
Increasing Pressure

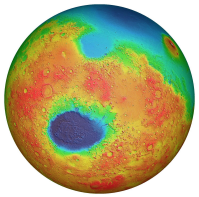
My Path Through High-Pressure Science

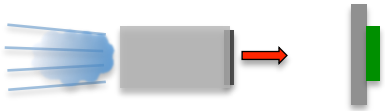
CEA, France
Molecular Fluids
Spectroscopy, Synchrotron Techniques



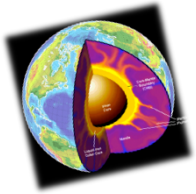
Harvard
Planetary surfaces, impacts
Prebiotic Chemistry



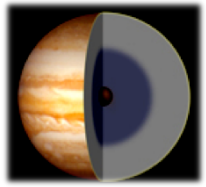


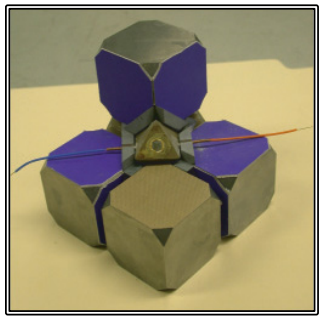


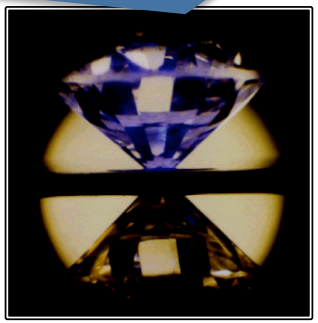
UC Berkeley, LLNL
Mineral Equations of State
Laser-Driven Shocks

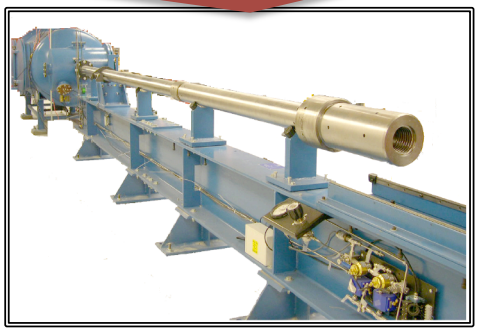


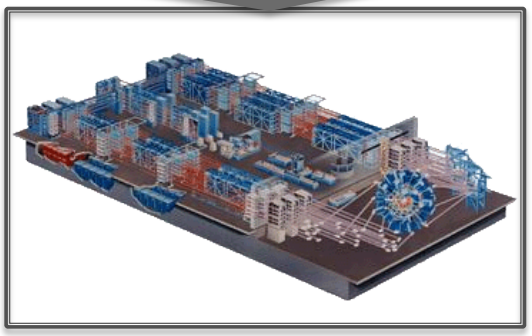
SSGF
STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP











Multi-Anvil — Few GPa

DAC — ~100 GPa

D” — *135 GPa*

Gas Gun — ~250 GPa

Earth’s Core — *360 GPa*

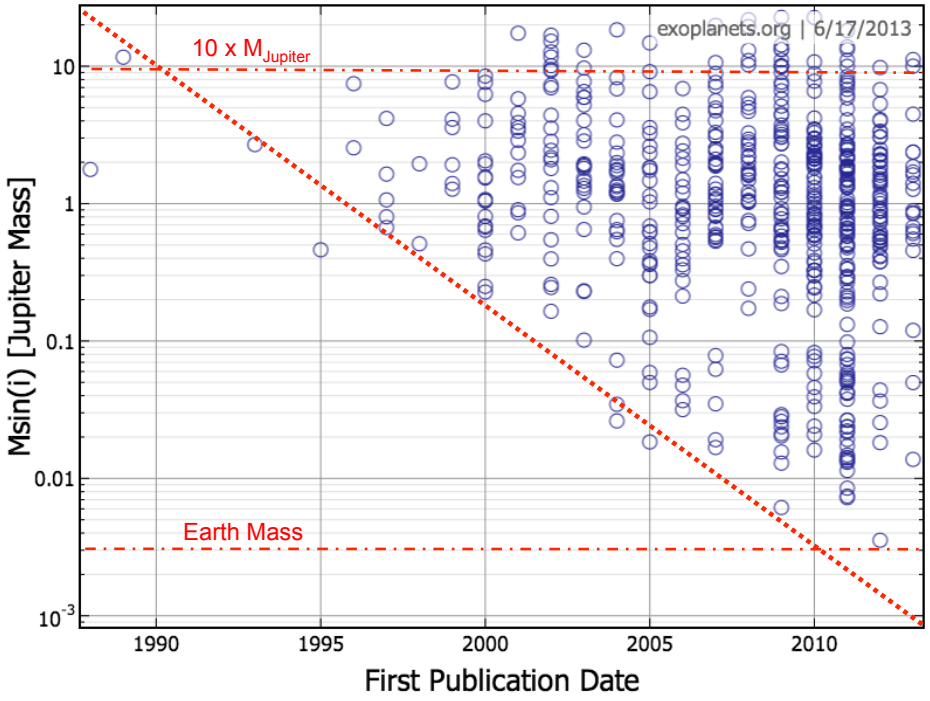
Lasers — >>10^3 GPa

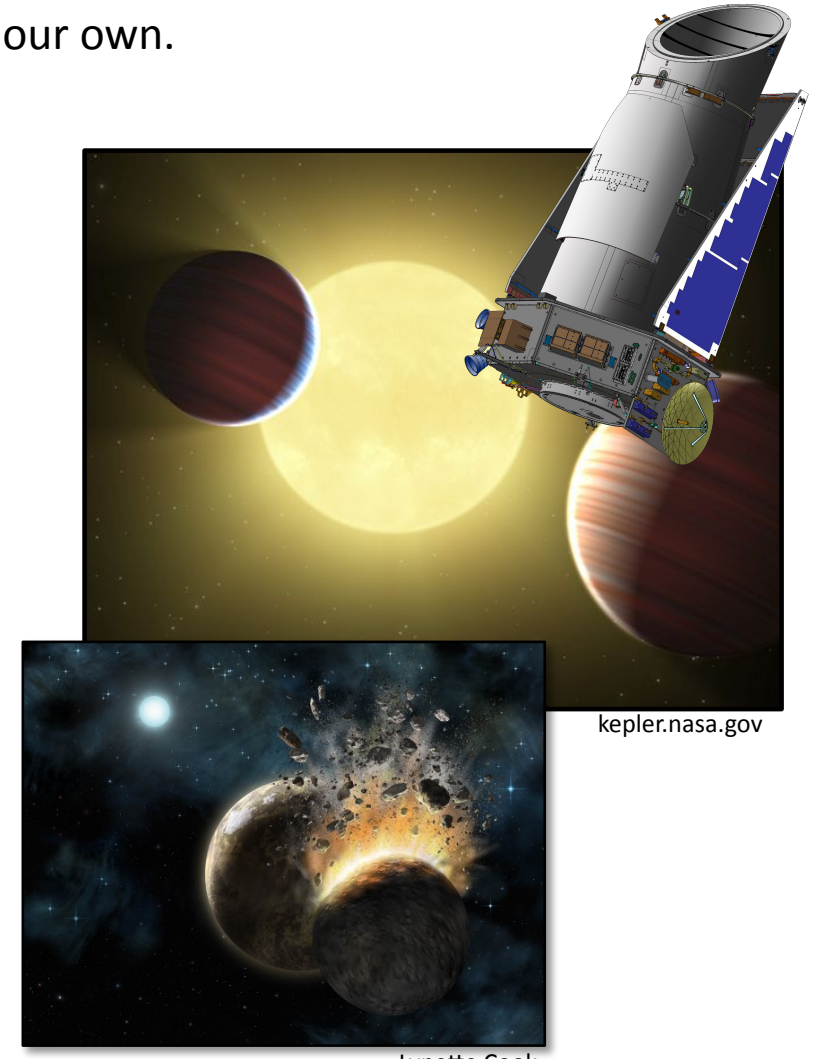
Increasing Pressure

Understanding Planetary Diversity – What are the Rules?

- The 'end-states' of planetary evolution are clearly very diverse and we now know there are many solar systems completely unlike our own.

- Is Earth a 'Goldilocks' planet?

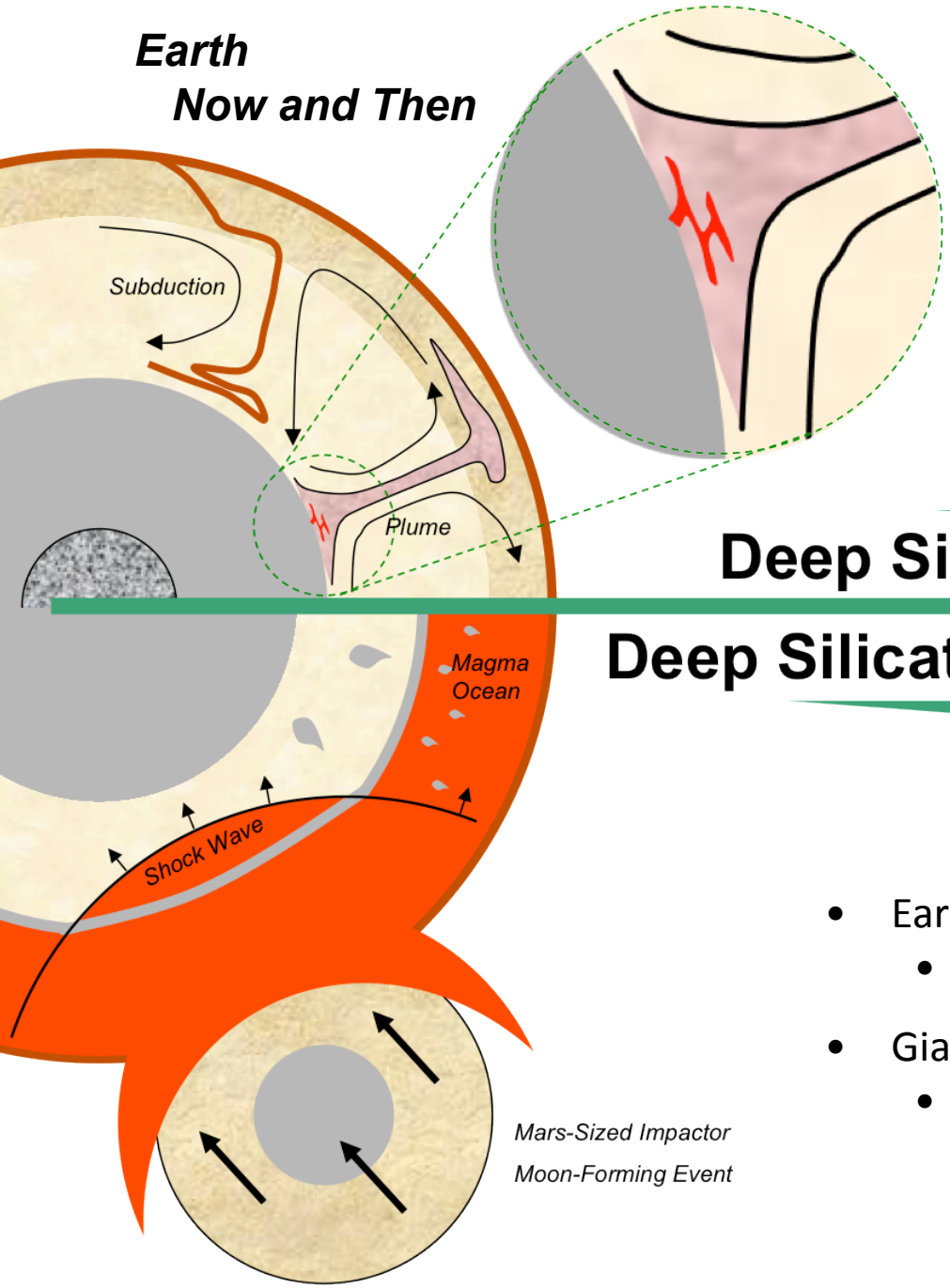




kepler.nasa.gov

Lynette Cook

Earth
Now and Then

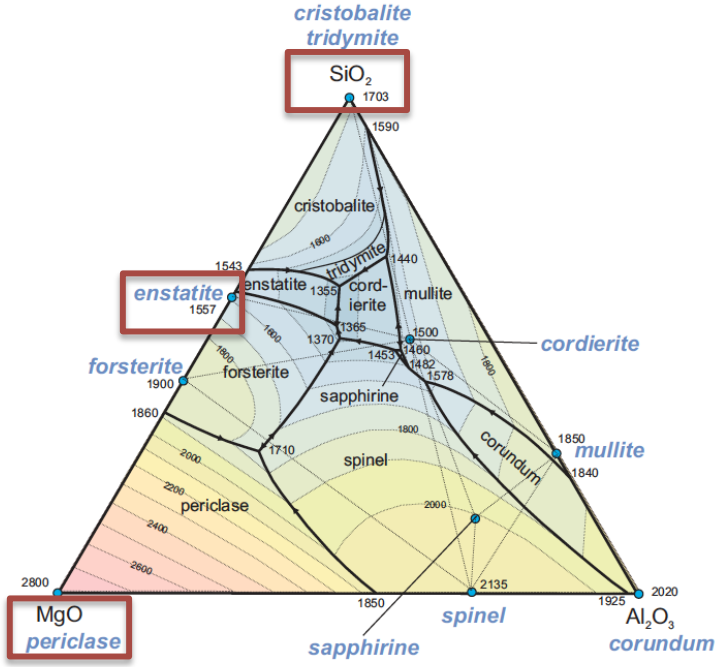


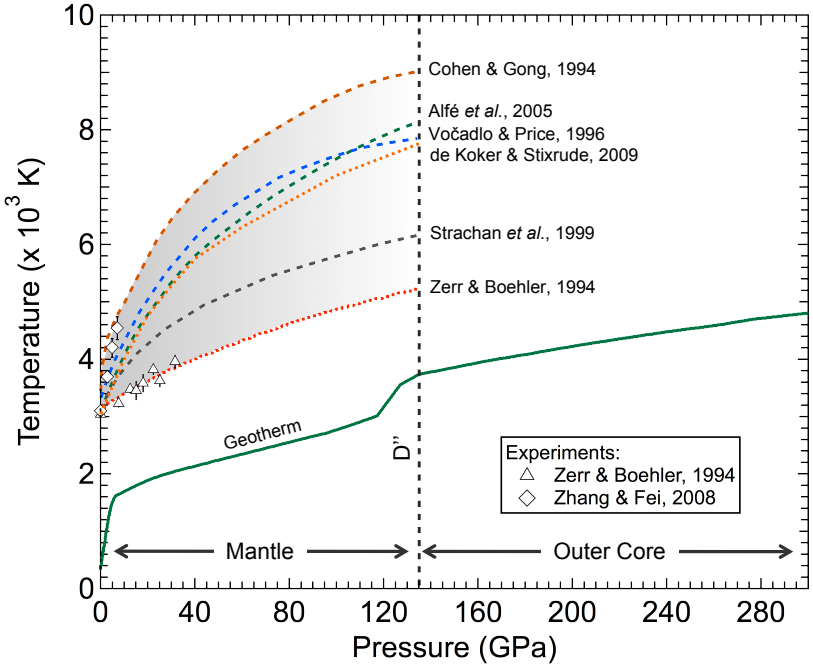
- Silicate Liquid Near Core-Mantle Boundary (D")?
- Likely at regions of high heat flow? →Transport properties?

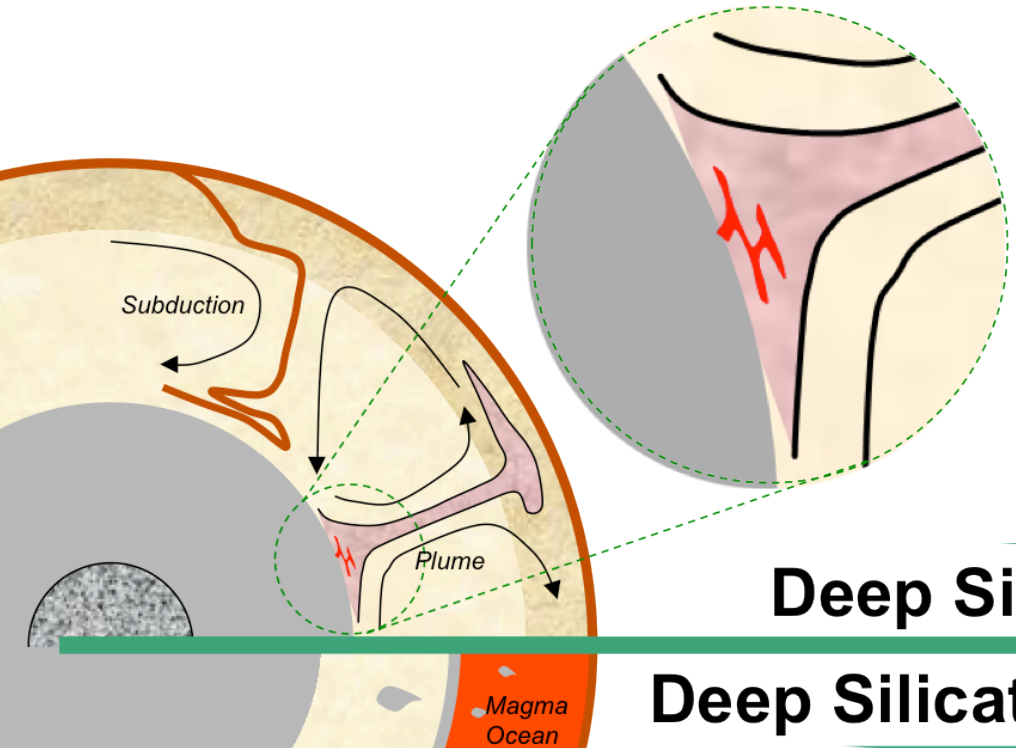
Deep Silicate Melt in the Present Earth

Deep Silicate Melt in the Ancient Earth

- Early Magma Ocean
  - Silicate Liquid at Depth
- Giant Impacts
  - Shock Melting Of Mantle







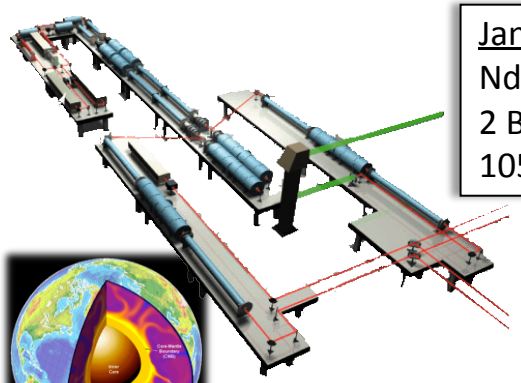
Numerous questions remain about the deep interior, formation and thermal evolution.

→ Calls for improved data on silicate and oxide liquids!

Deep Silicate Melt in the Present Earth

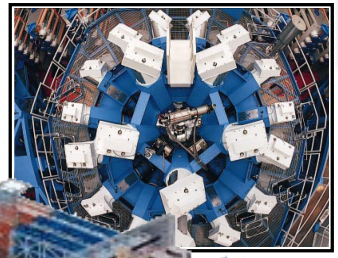
Deep Silicate Melt in the Ancient Earth

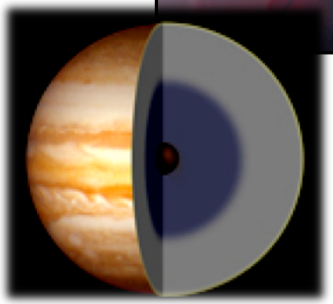
Exploring Planetary Interiors in the Laboratory



Janus Laser
Nd:glass
2 Beams: 1kJ/beam
1053nm, 527nm, 351nm

The OMEGA Laser
Nd:glass
Wavelength: UV
60 beams, 30kJ





The NIF (LLNL)
192 beams, 2Megajoules
Wavelength: 351nm

Images: Jlf.llnl.gov, lle.rochester.edu, NIF

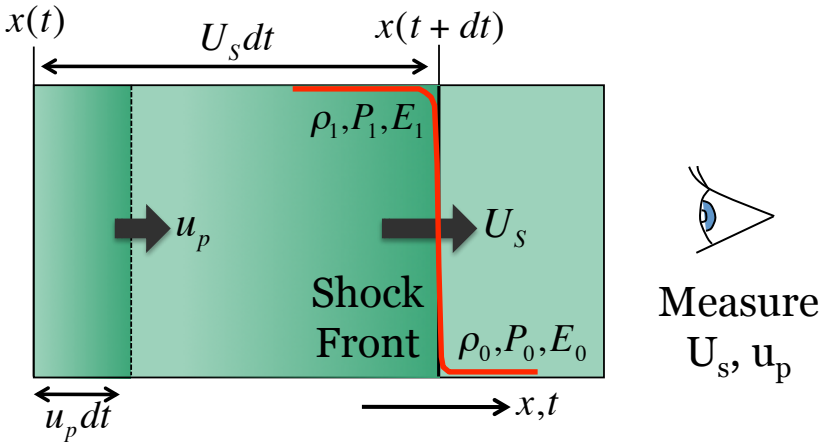
What Can We Measure?

Rankine-Hugoniot Equations

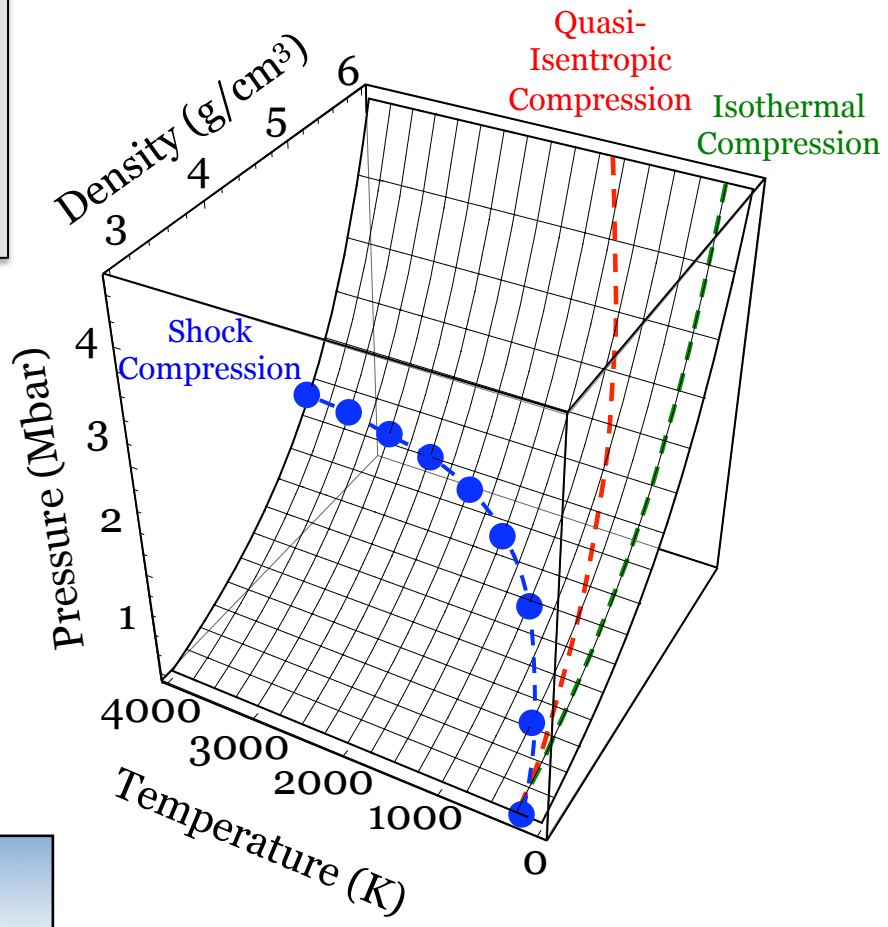
Conservation of mass $\longrightarrow$ $\rho_0 U_S = \rho_1 (U_S - u_P)$

Conservation of Momentum $\longrightarrow$ $P_1 = \rho_0 U_S u_p$

Conservation of Energy $\longrightarrow$ $(E_1 - E_0) = \frac{1}{2} P_1 (V_0 - V_1)$



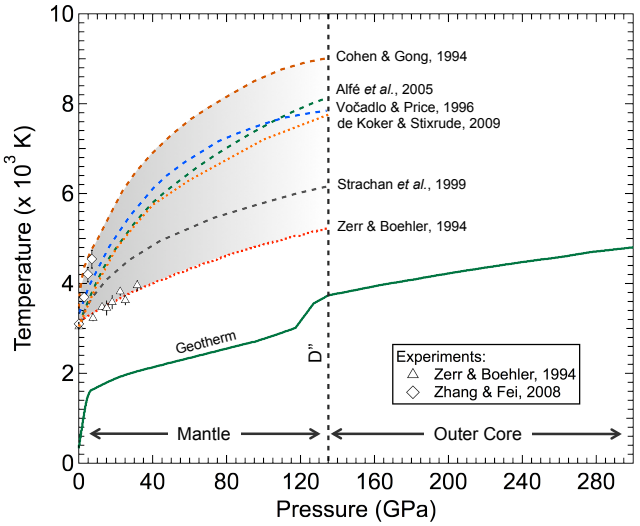
Measure
U_s, u_p

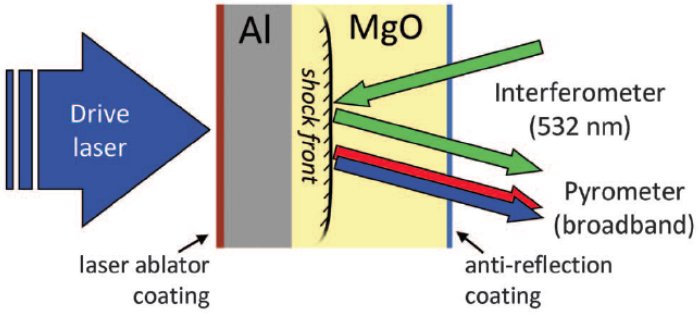


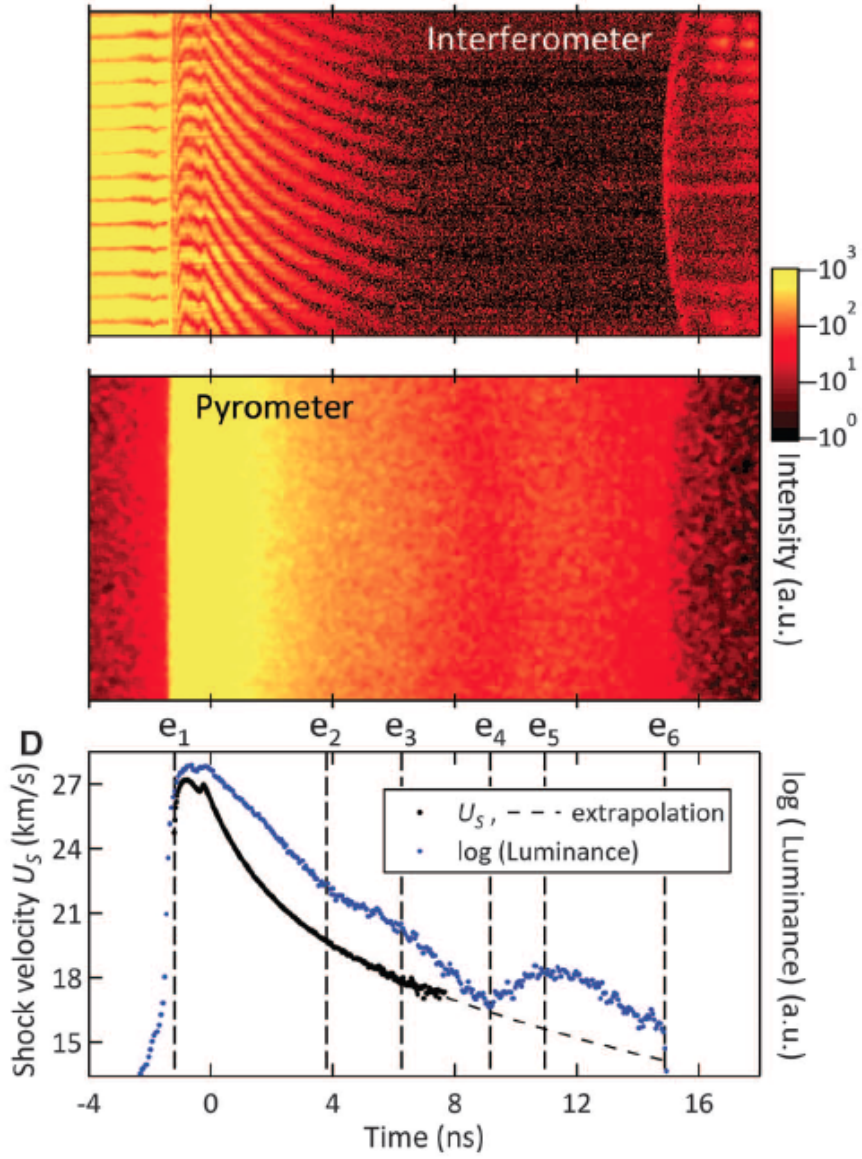
Conservation Equations	+	Material Properties	=	Wave Properties

Probing the Earth's Deep Mantle – Periclase (MgO)

Looking for phase changes with 'Shock Calorimetry'





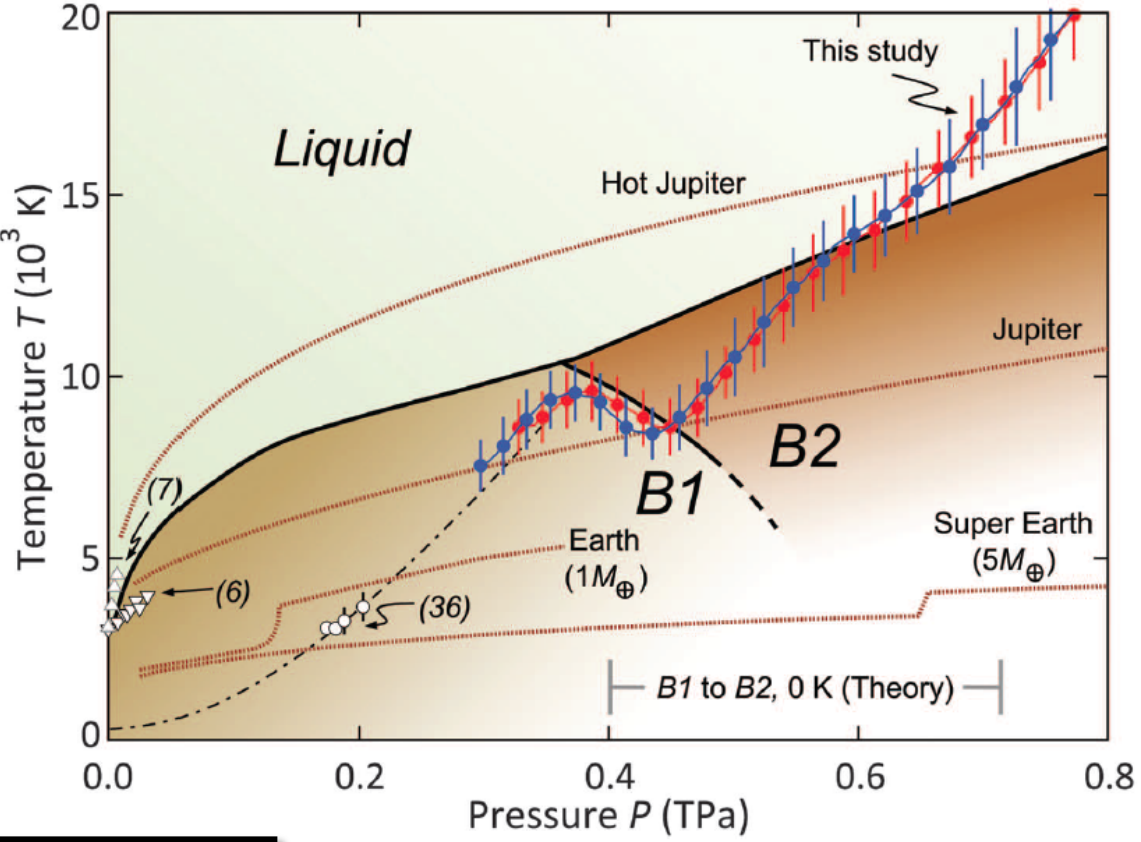


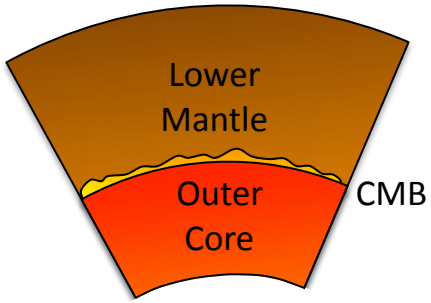
R. Stewart McWilliams, D. K. Spaulding, J. H. Eggert, P. M. Celliers, D. G. Hicks, R. F. Smith, G. W. Collins, R. Jeanloz, **Phase Transformations and Metallization of Magnesium Oxide at High Pressure and Temperature** , Science, 338, 2012.

Probing the Earth's Deep Mantle – Periclase (MgO)

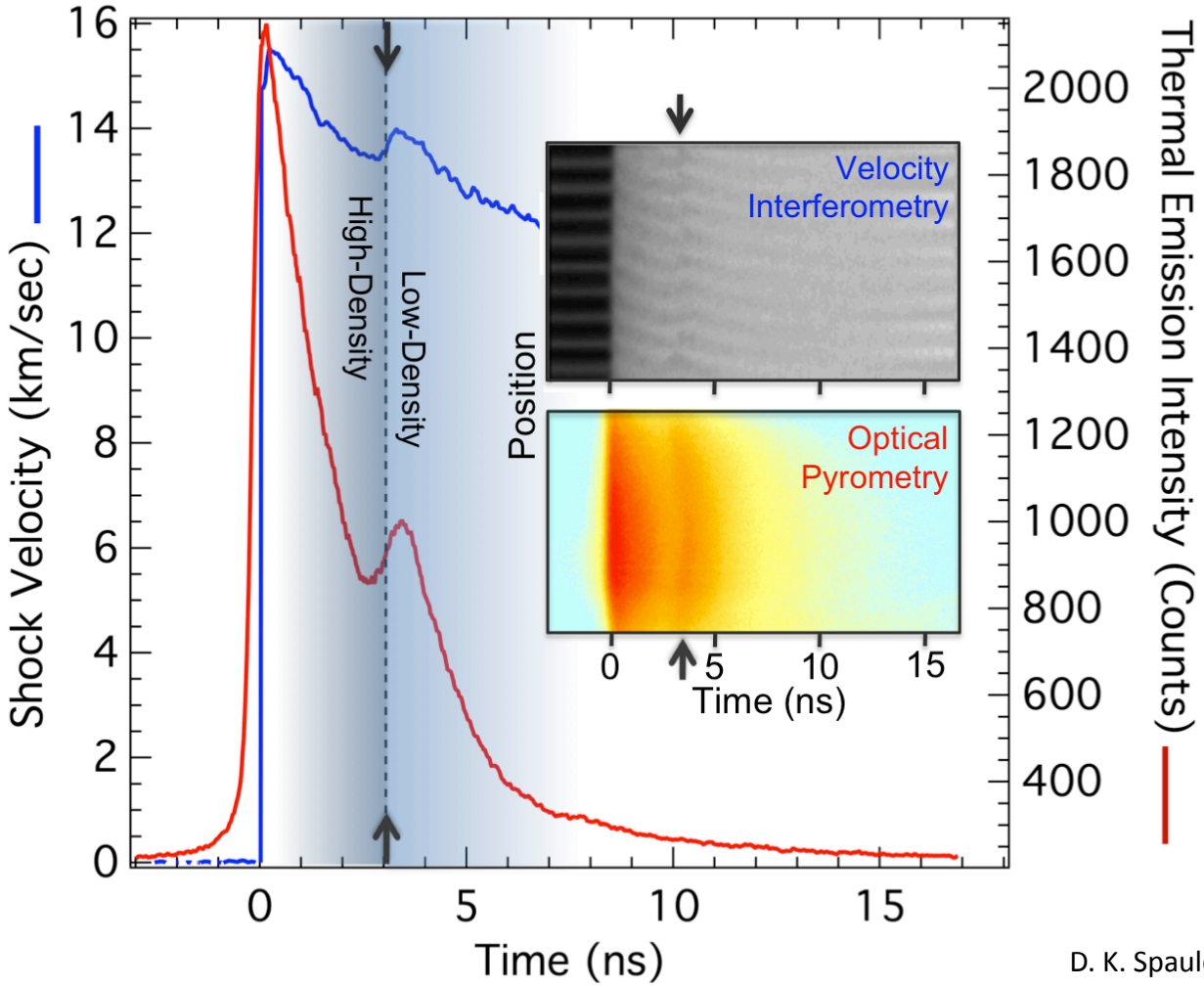
- Putting our pressure (velocity) and temperature data together, allows us to identify phase boundaries in P/T space

- Demonstrates remarkable stability of MgO over a vast domain





Probing the Earth's Deep Mantle – Enstatite ($MgSiO_3$)



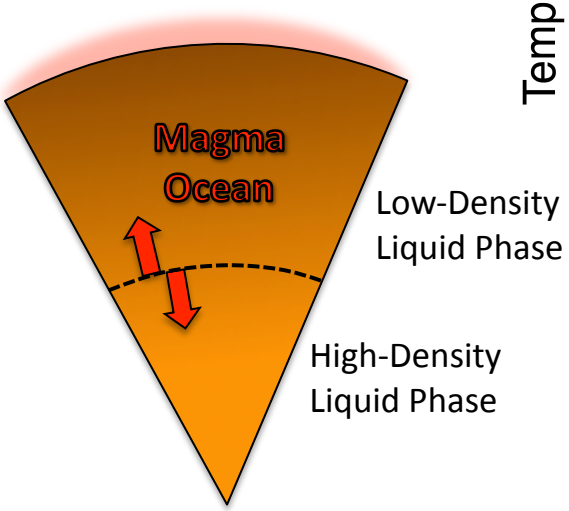
- Discontinuity in velocity suggests a volume change – first such observation
- Experiments on two different polymorphs reveals a whole different sort of phase transition

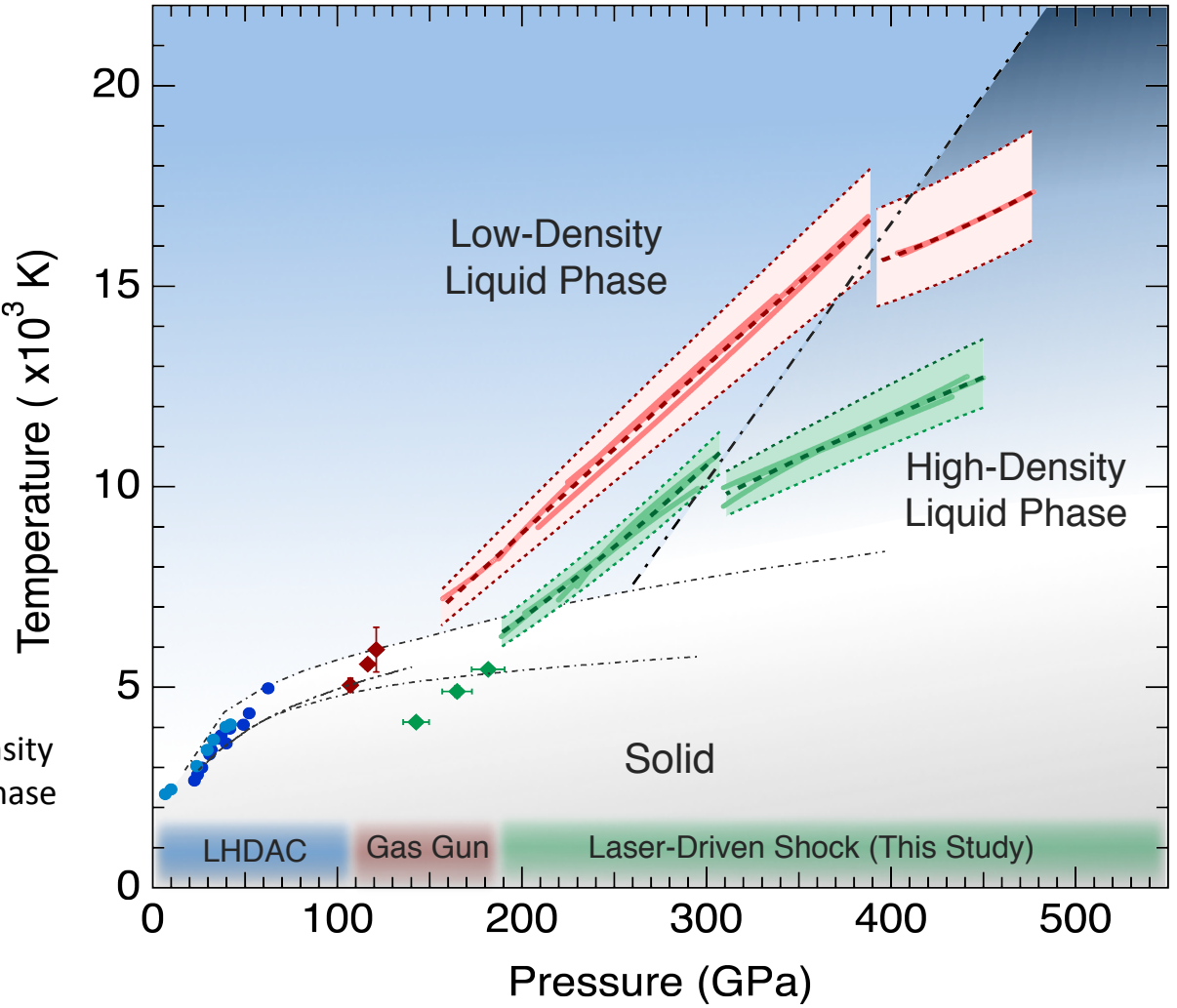
D. K. Spaulding, R. S. McWilliams, R. Jeanloz, J. H. Eggert, P. M. Celliers, D. G. Hicks, G. W. Collins, R. F. Smith, **Evidence for a Phase Transition in Silicate Melt at Extreme Pressure and Temperature Conditions,** Physical Review Letters **108**, 065701 (2012).

$MgSiO_3$ Phase Diagram – First Observations of a Liquid-Liquid Phase Transition in a Silicate Material

$MgSiO_3$ undergoes a transition between liquid states distinguished by density and entropy.

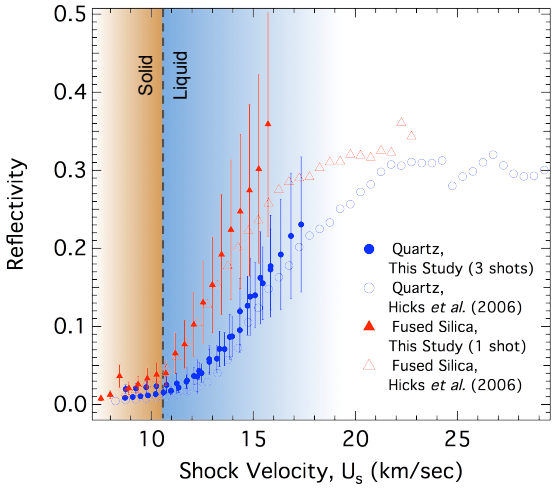
From the low-pressure to the high-pressure phase:
$\Delta V = -6.25 \pm 2.2\%$ and
$\Delta S = -2.9 \pm 0.6$ J/K · mol of atoms

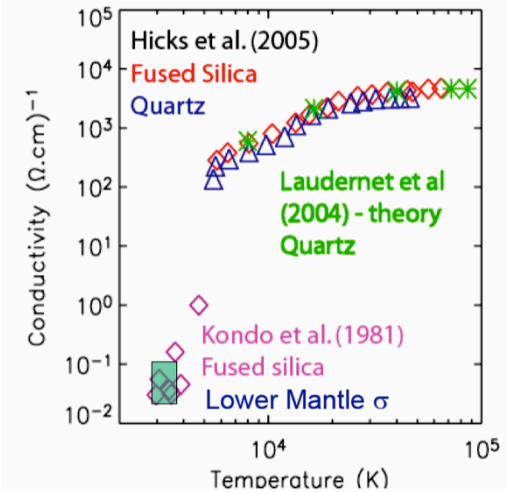




Not Melted Rock, but Rather Hot, Fluid Metal!

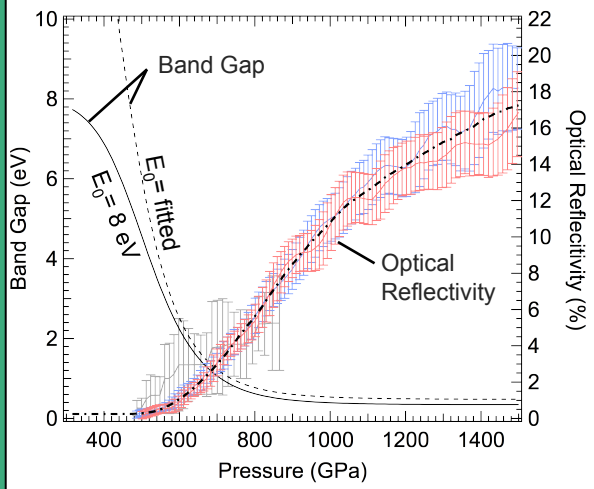
SiO_2



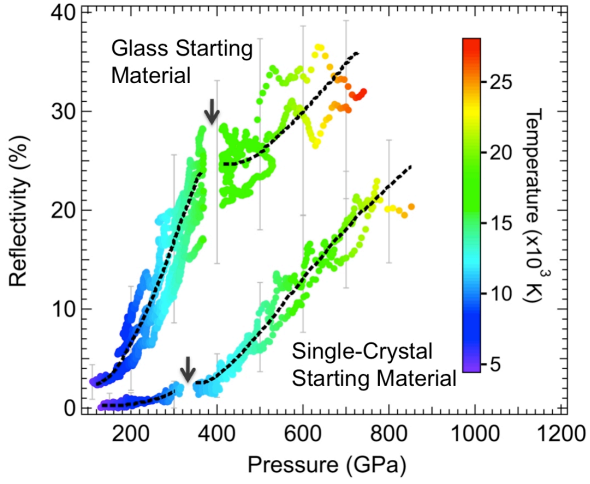


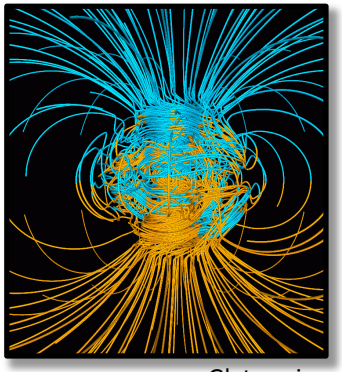
SiO_2, MgO, $MgSiO_3$ have conductivities like poor metals in the liquid state and could contribute to magnetic field generation in planets.

MgO



$MgSiO_3$





Glatzmaier

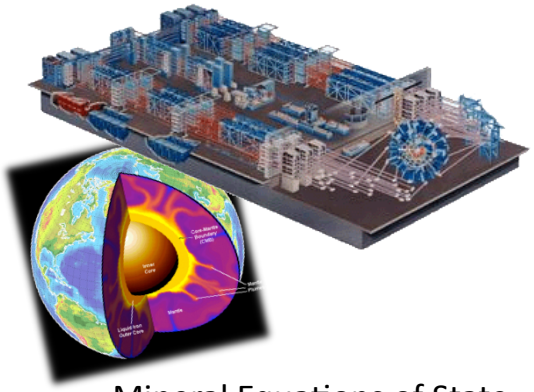
Delving Deeper into High Pressure Chemistry

Equations of state are key to understanding planetary structure and evolution

Material properties show dramatic change under extreme pressures and temperatures

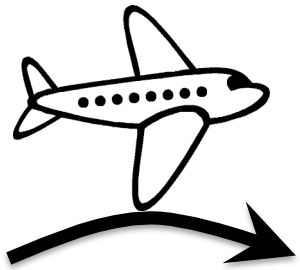
The potential for new chemistry is rich under these conditions but difficult to characterize

UC Berkeley, LLNL

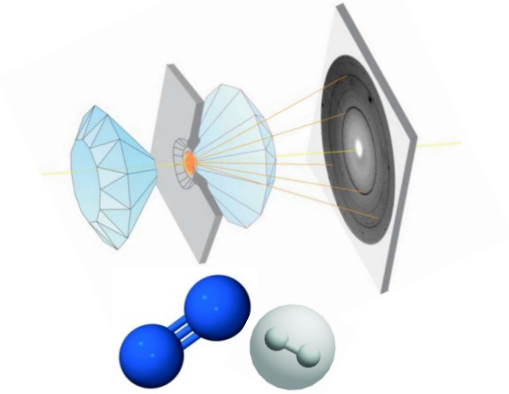


Mineral Equations of State
Laser-Driven Shocks

SSGF
STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP



CEA, France



Molecular Fluids
Static High Pressure
Spectroscopy, Synchrotron
Techniques

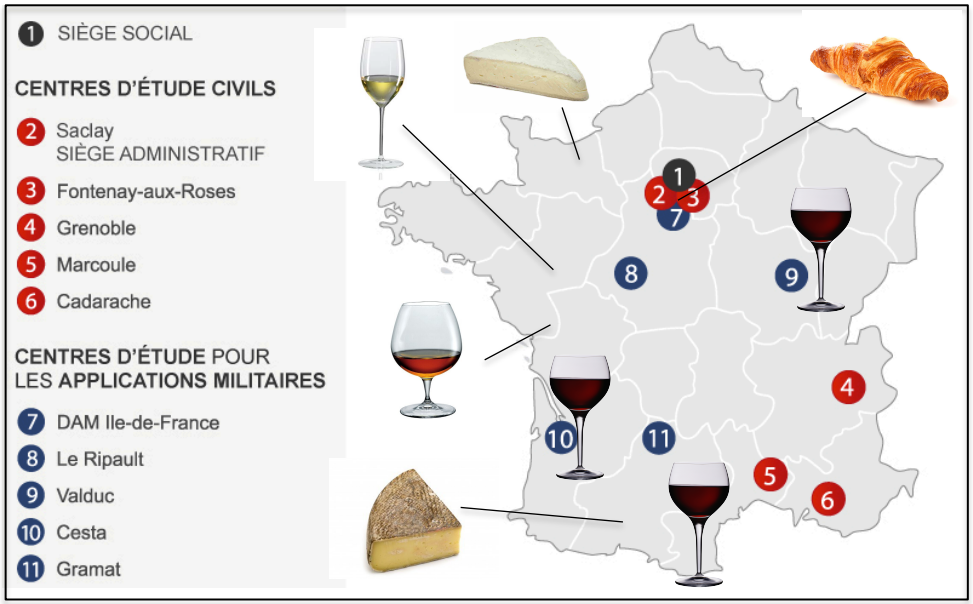
Commissariat à l'Énergie Atomique (CEA) – About the Lab

- Going abroad – why or why not?

- Cultural and scientific differences can be both good and bad
  - Choice of Projects
  - Work schedules
  - Hierarchy
  - Opportunity to broaden one's community, see parallel efforts on large projects
  - Develop collaborations and familiarity with other groups

- *YOU* are the foreign national!

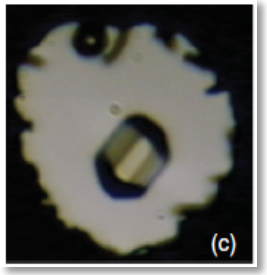
- Opportunities to travel…



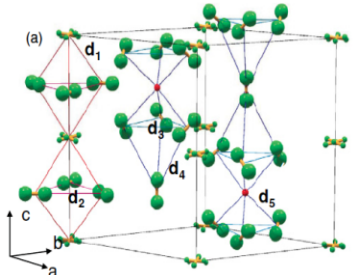
Pressure-Induced Chemistry in Molecular Mixtures

- Unique means of probing interatomic bonding and testing fundamental condensed matter theory
- These systems display surprisingly complex and subtle chemistry at high pressure and temperatures
- Possible synthesis of new materials with novel physical and energetic properties, ie Van der Waals Solids
- Simple molecular compounds are common reaction products – high P/T chemistry
- Knowledge of equations of state are critical for modeling in planetary astrophysics

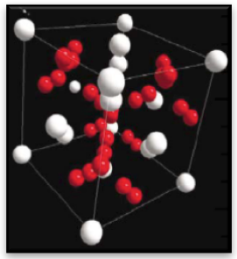
$(N_2)_{11}He$



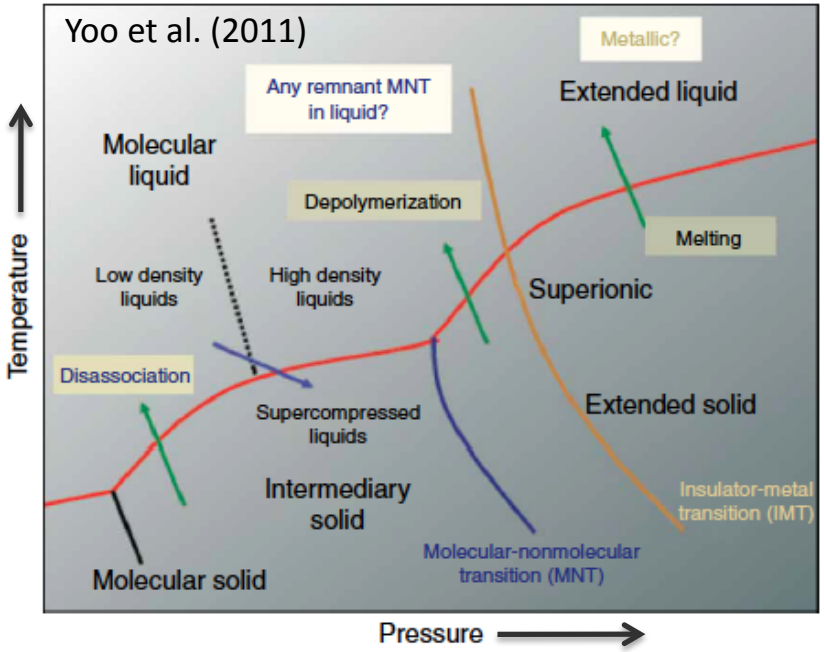
Ninet (2011)



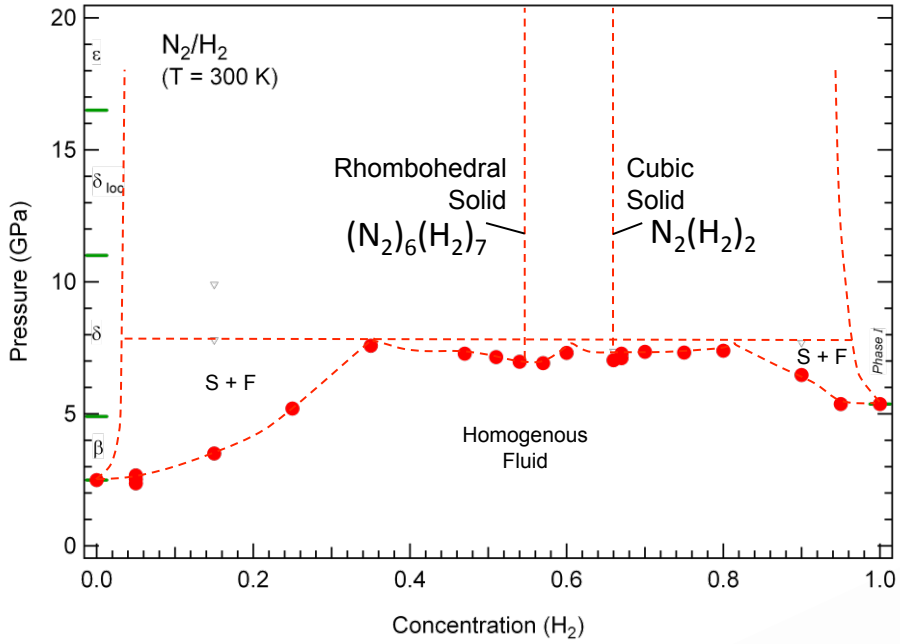
$Xe(O_2)_2$

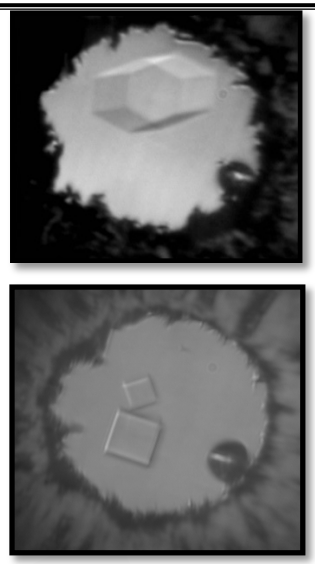


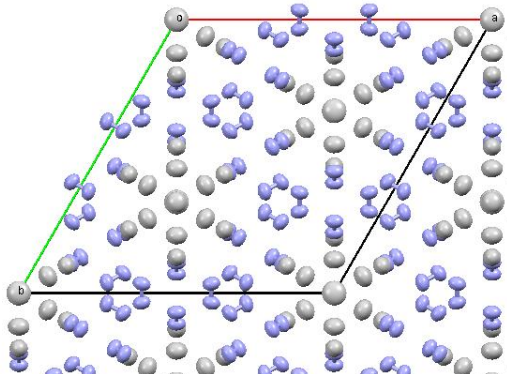
Weck (2010)



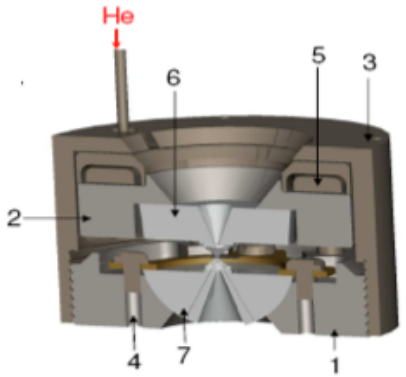
Nitrogen/Hydrogen Mixtures



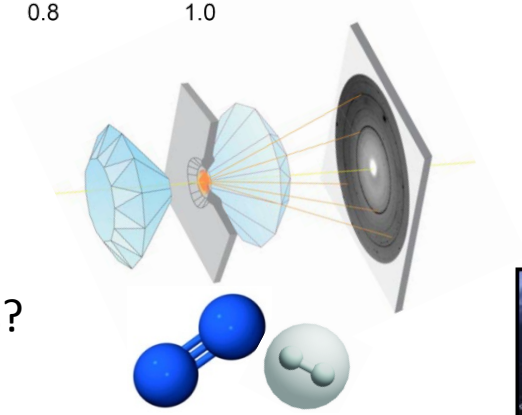


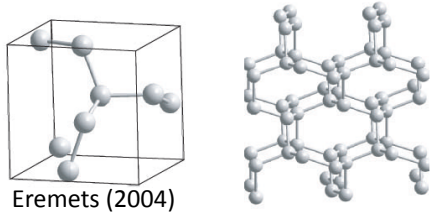


$(N_2)_6(H_2)_7$



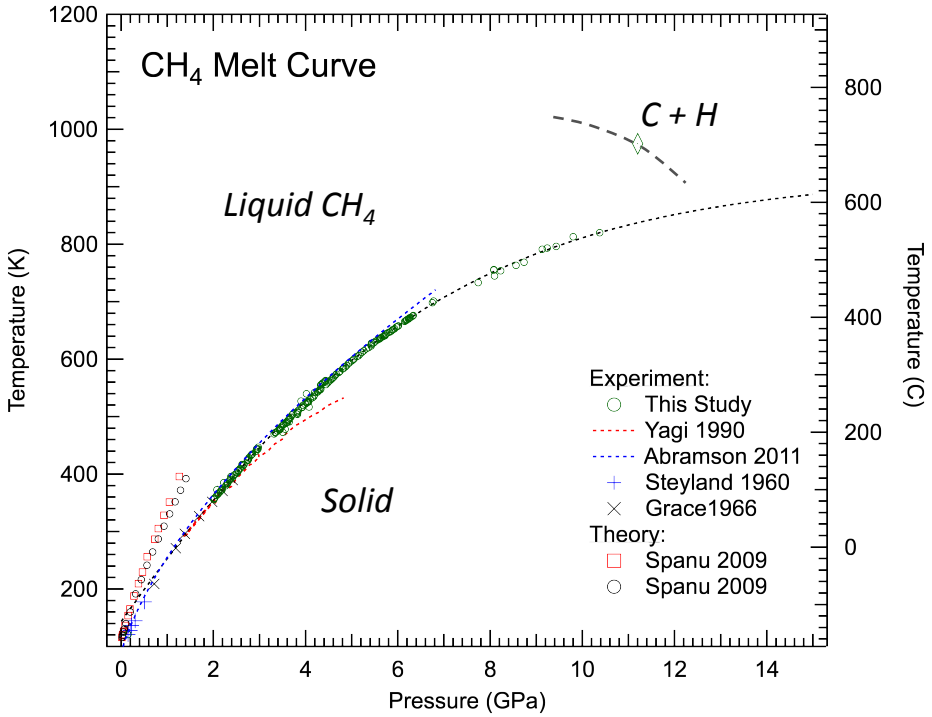
- Paths to metallisation?
- New high-pressure compounds?
- Lowering the threshold of the polymeric transition?

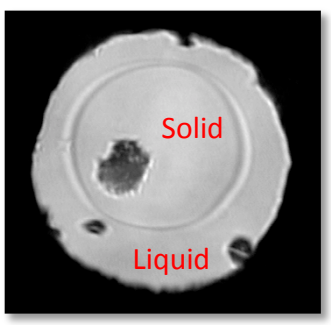


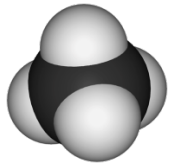


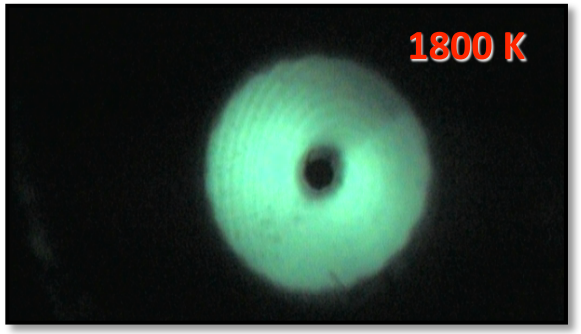
Eremets (2004)

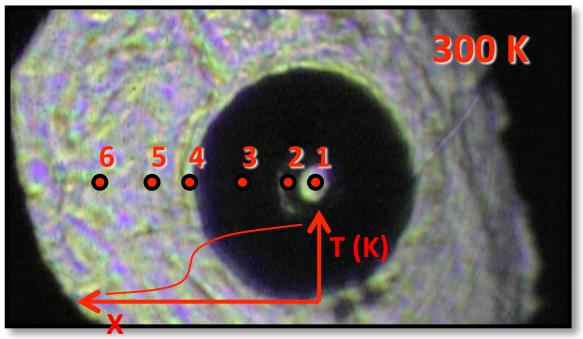
Methane Melting and Stability – Developing New Techniques

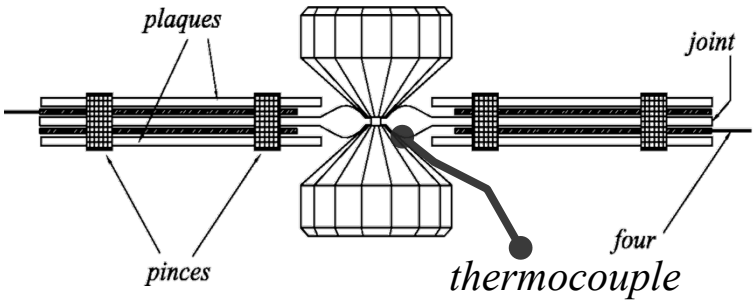


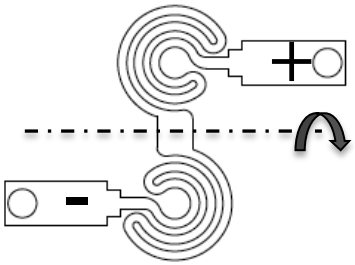




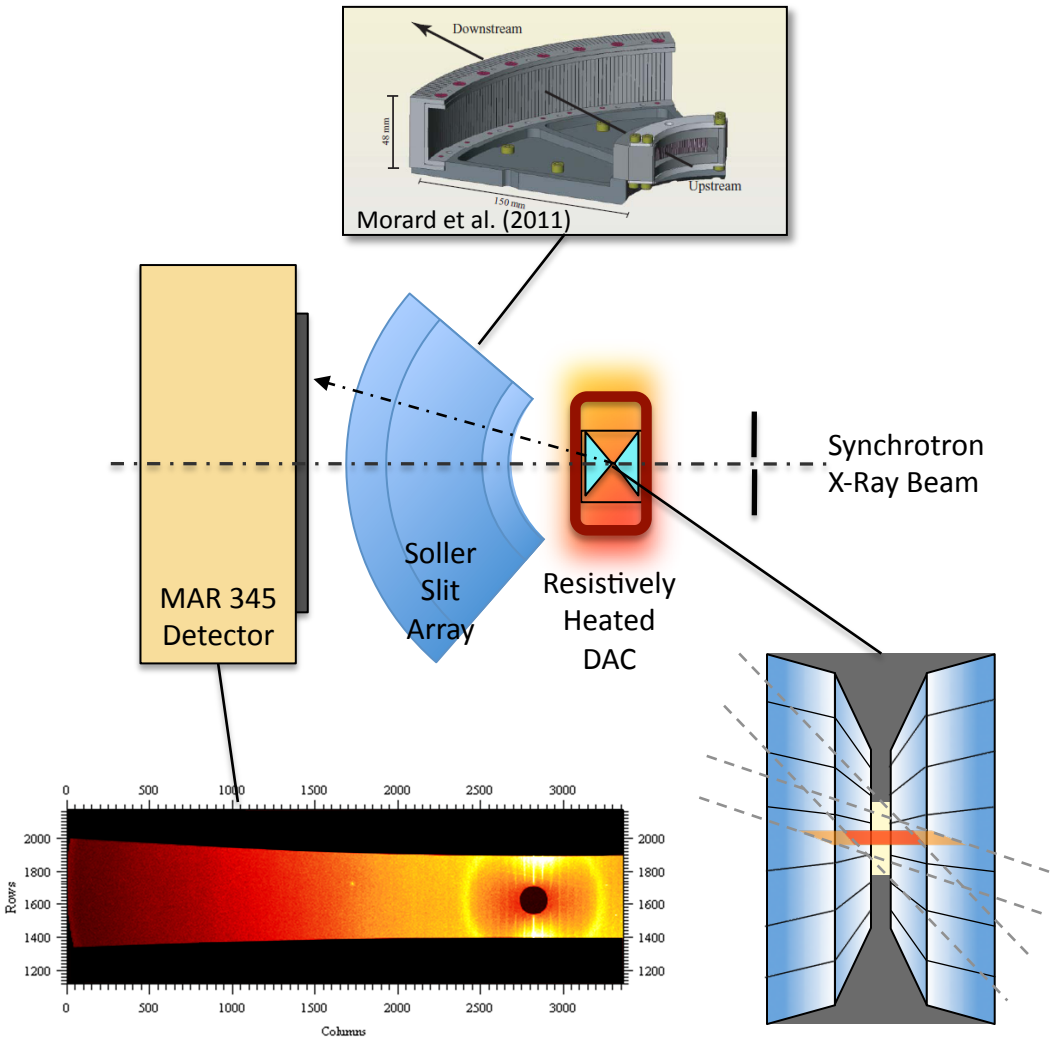


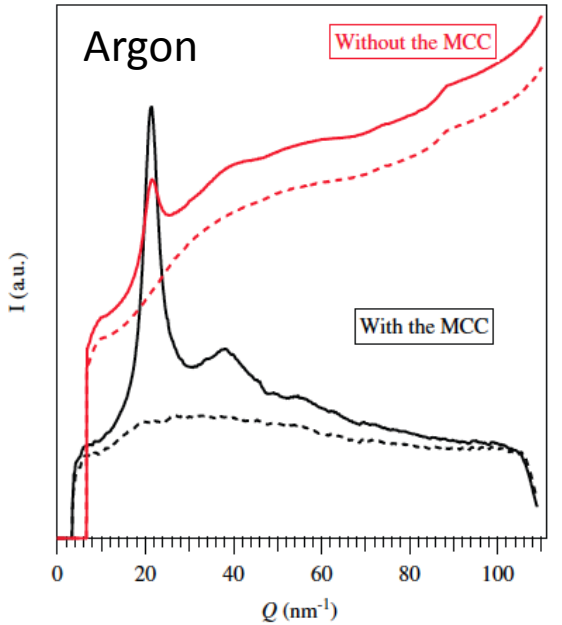


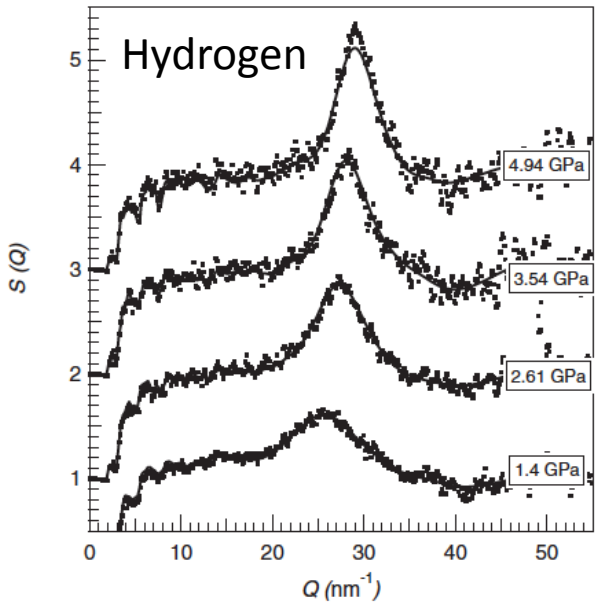




And Seeing How Far We Can Push These New Techniques…

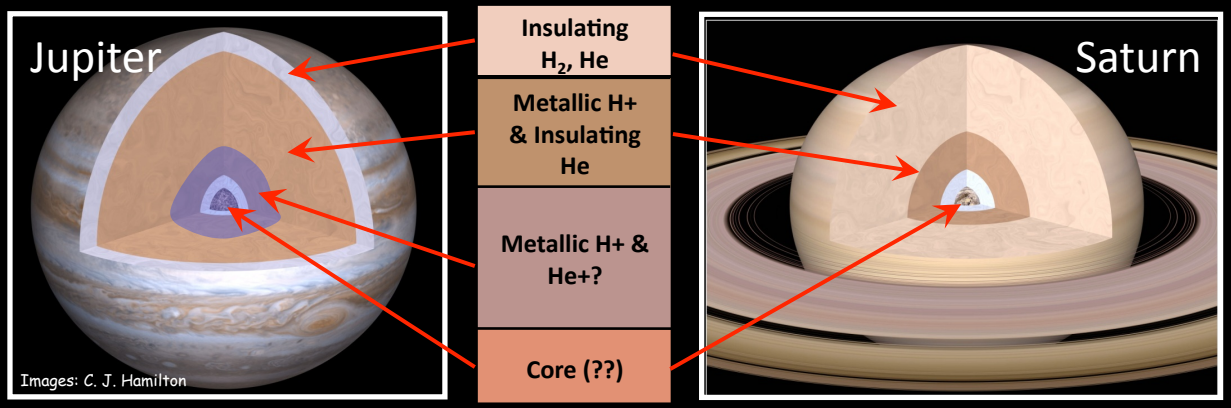




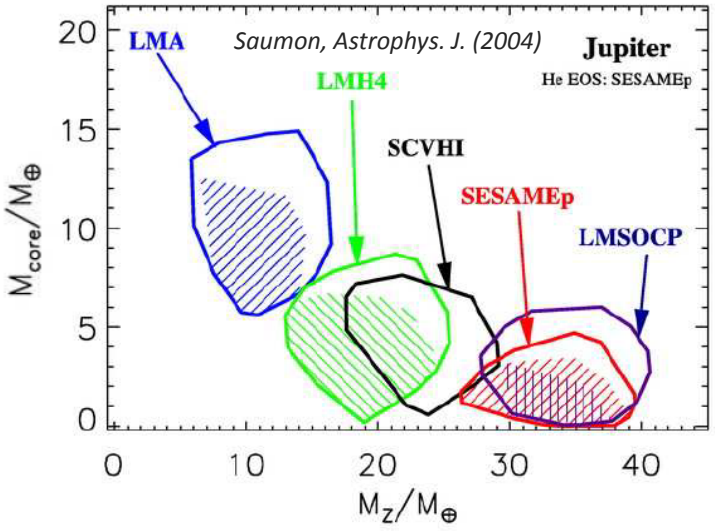


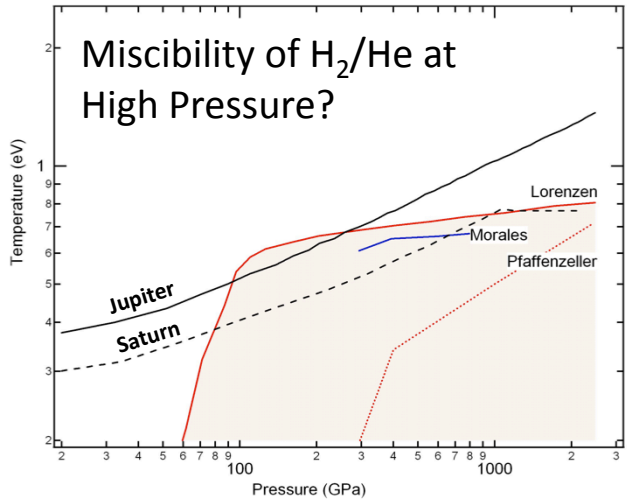
Weck, G., Garbarino, G., Ninet, S., Spaulding, D., Datchi, F. et al., Rev. Sci. Instrum. **84**, 063901 (2013)

Combing Tools to Reach New Phase Space – the Giant Planets

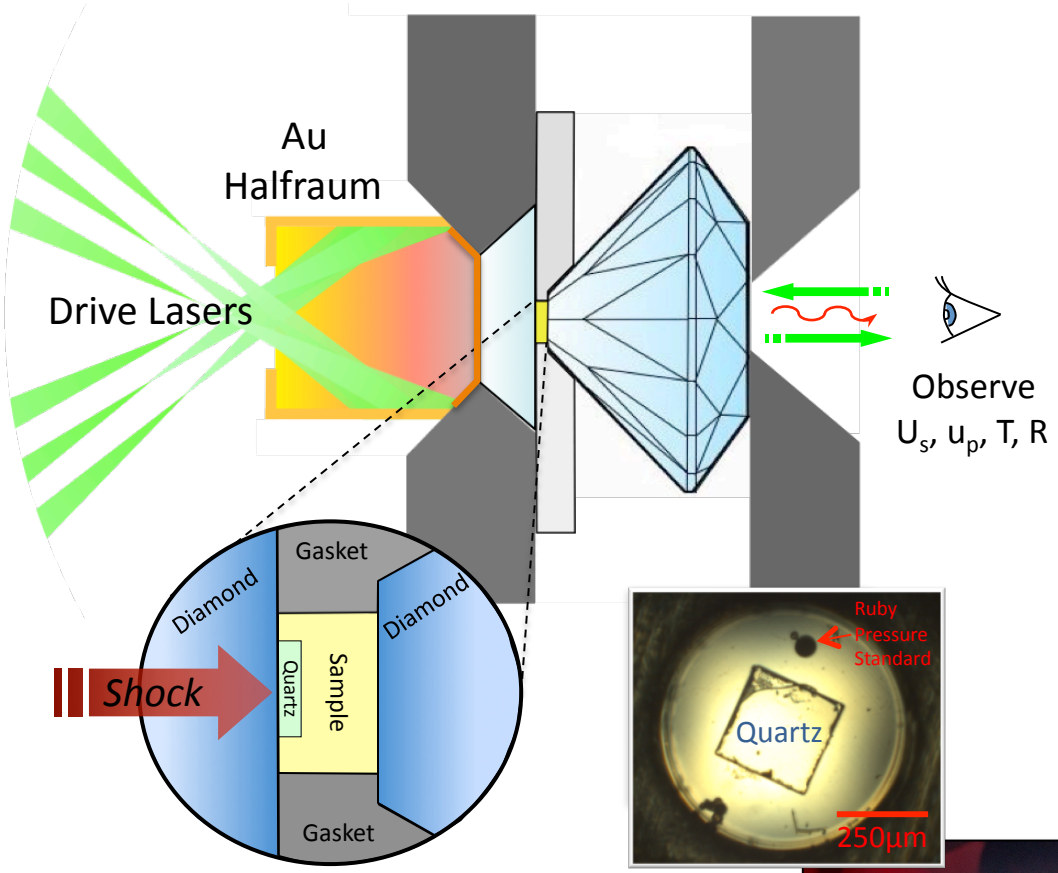


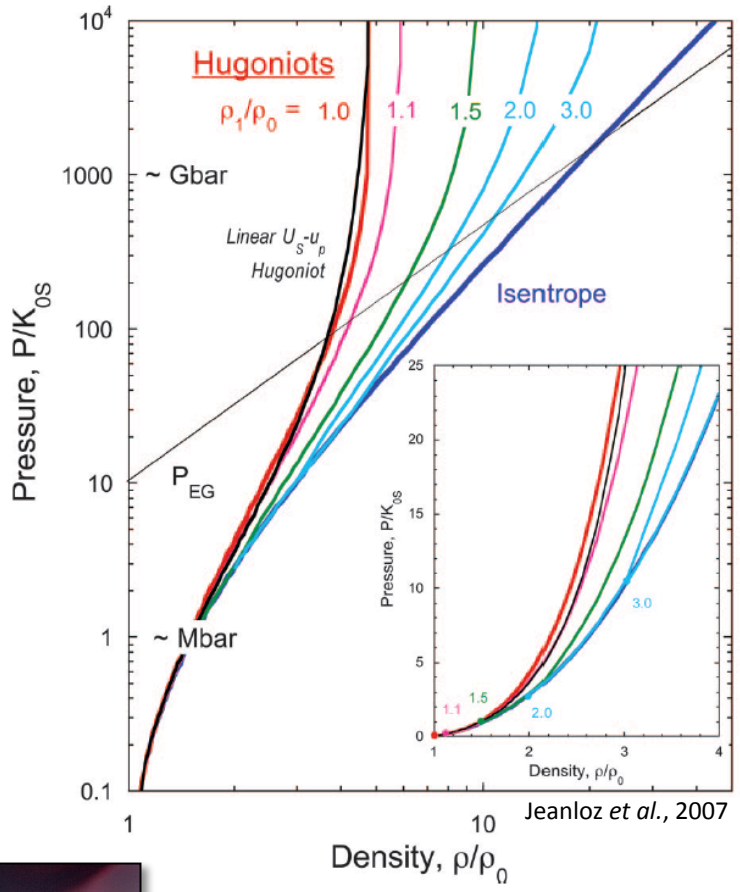
The structure and evolution of giant planets depends on the equations of state of their constituents (H_2, He and molecular fluids) under extreme conditions

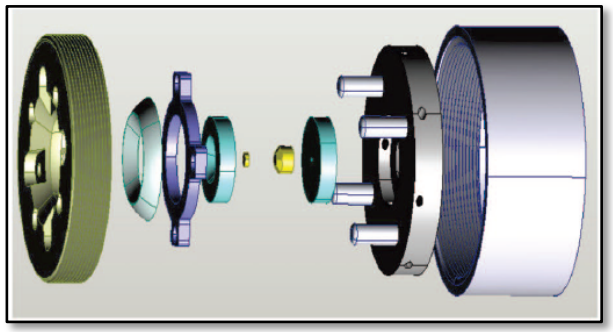


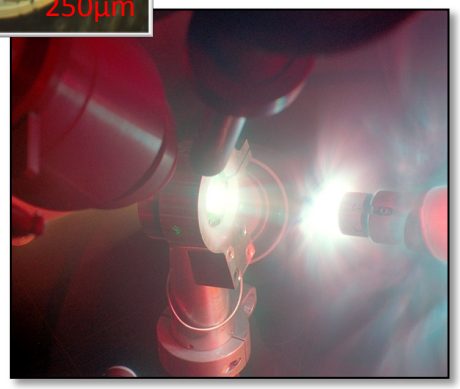


Combining Tools to Reach New Phase Space



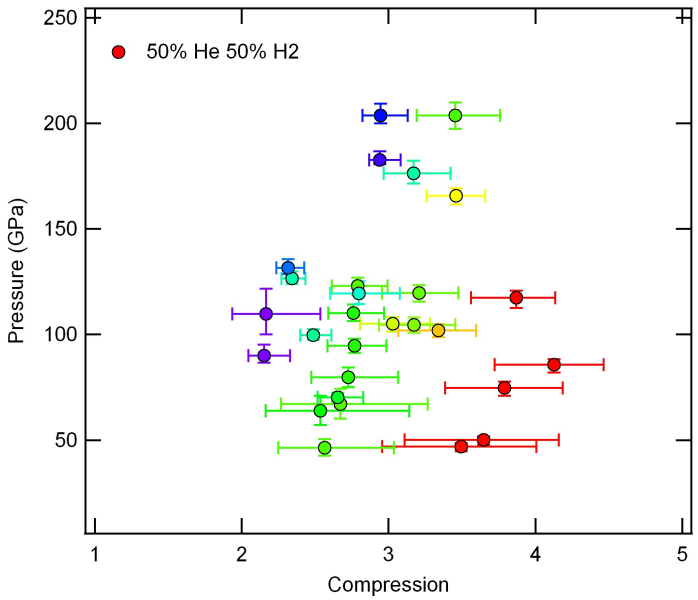


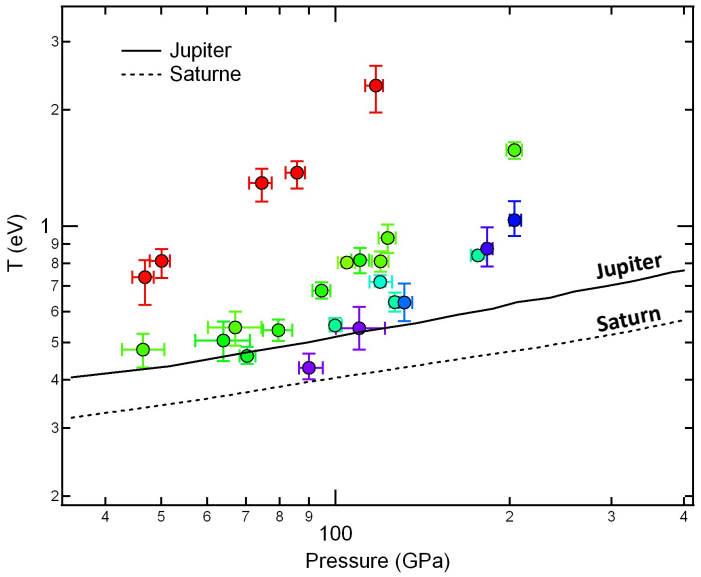




Shocking H_2/He Mixtures to Planetary Conditions

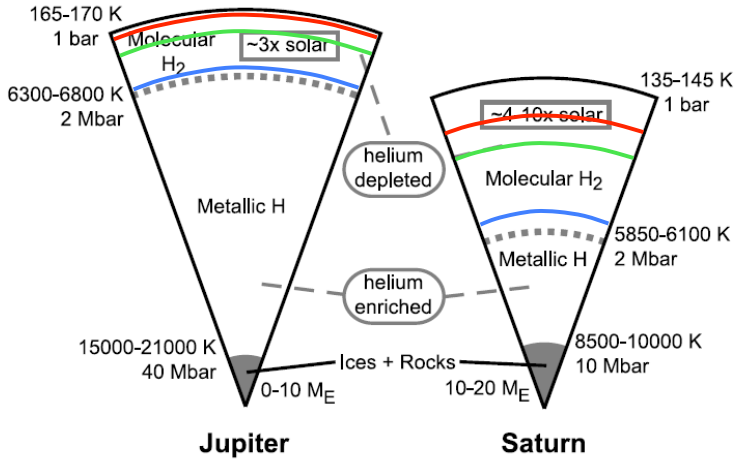
- Velocity, reflectivity and temperature were measured were three different initial pre-compressions: **0.4**, **2** and **4** GPa



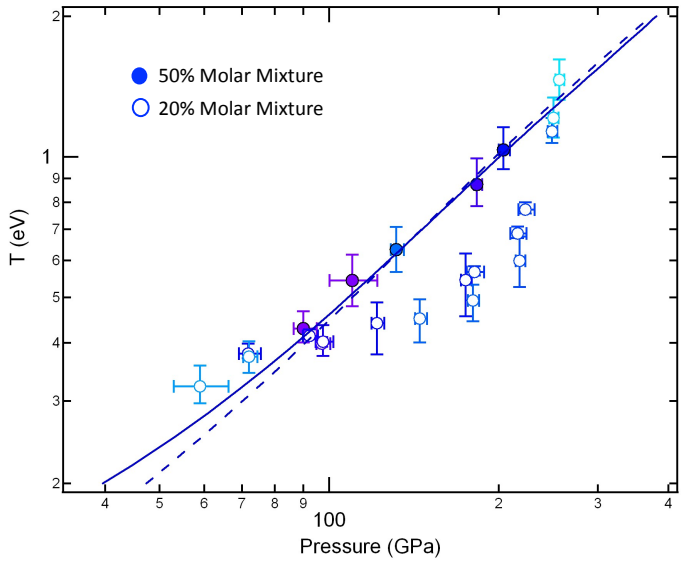


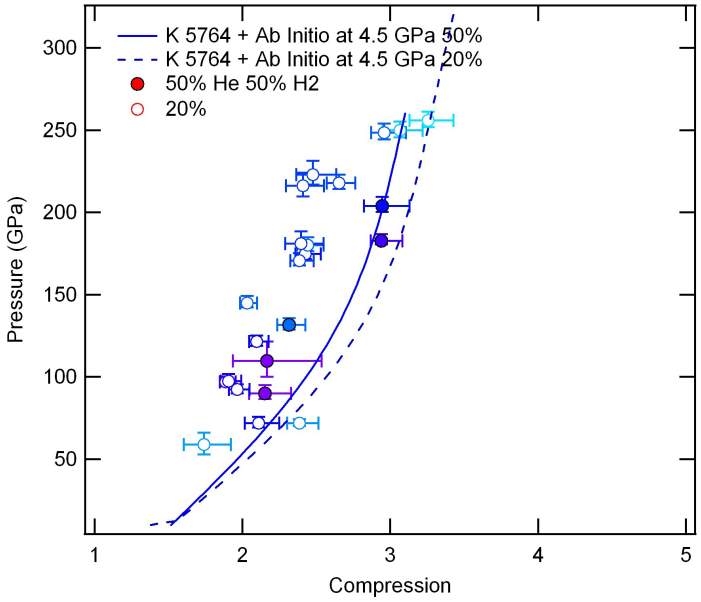
- Samples pre-compressed to 4 GPa cross the planetary isentropes and can test theoretical predictions for demixing in the planets

Higher precompression..
'Cooler' Temperatures..
Deeper Planetary Conditions..



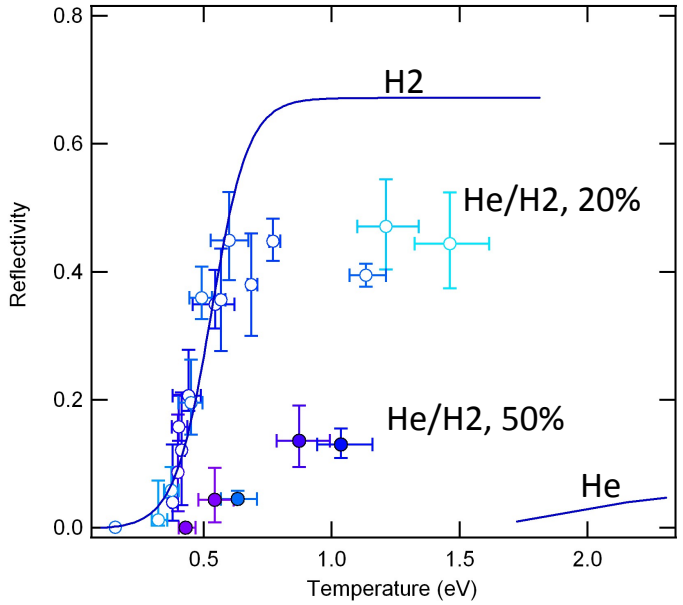
Demixing in H_2/He Mixtures – Compositional Effect



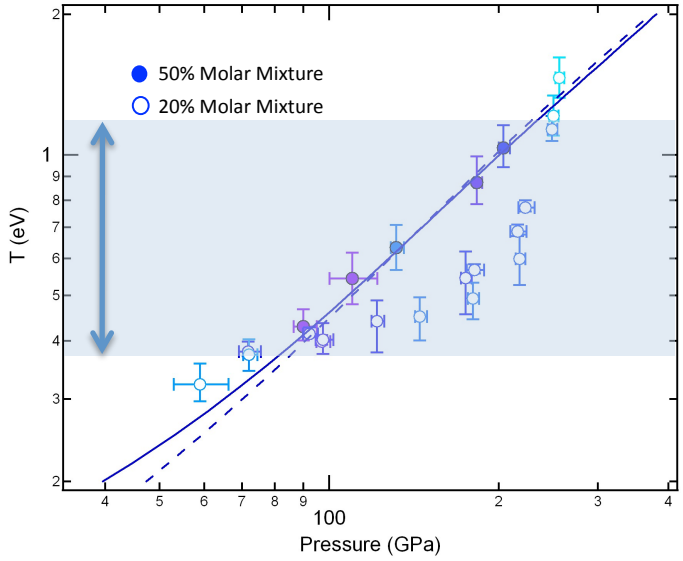


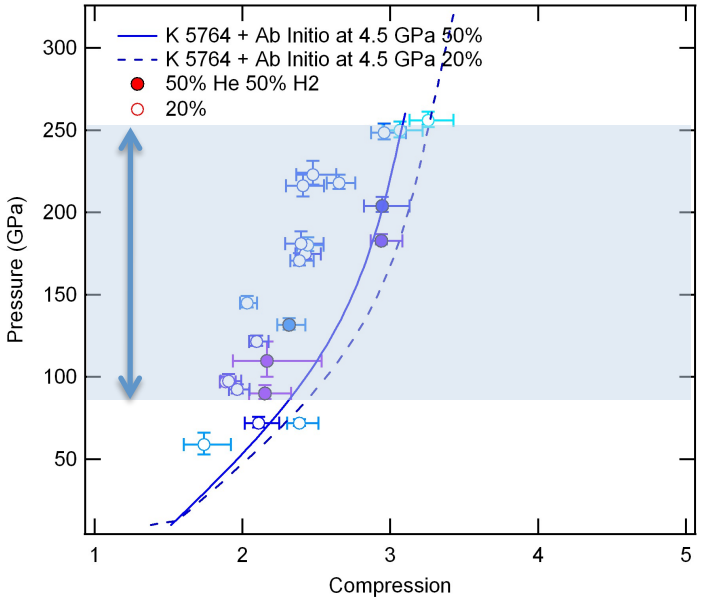
Look for Signs of Demixing by Comparing Mixtures at 20% and 50%

- At 20%, Hugoniot temperatures deviate from what is predicted by a simple mixing model - Energy change due to demixing?
- A deviation in volume is observed over the same pressure range
- Observed reflectivities confirm the limits of the demixing range.



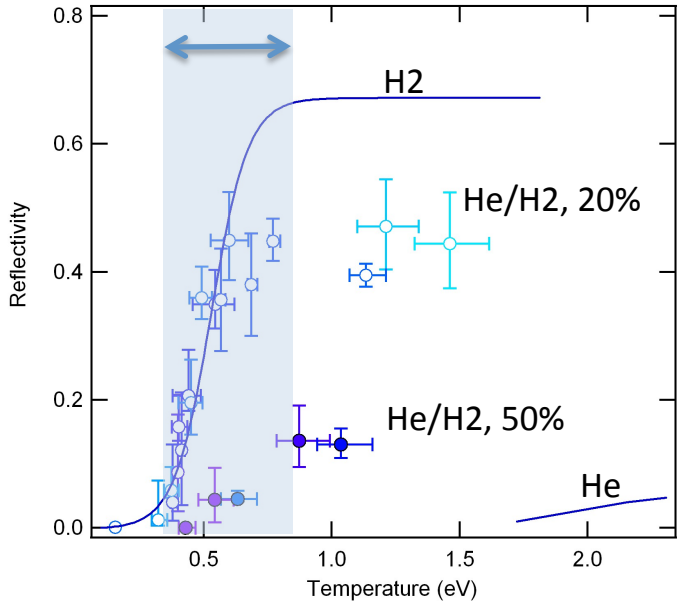
Demixing in H_2/He Mixtures – Compositional Effect



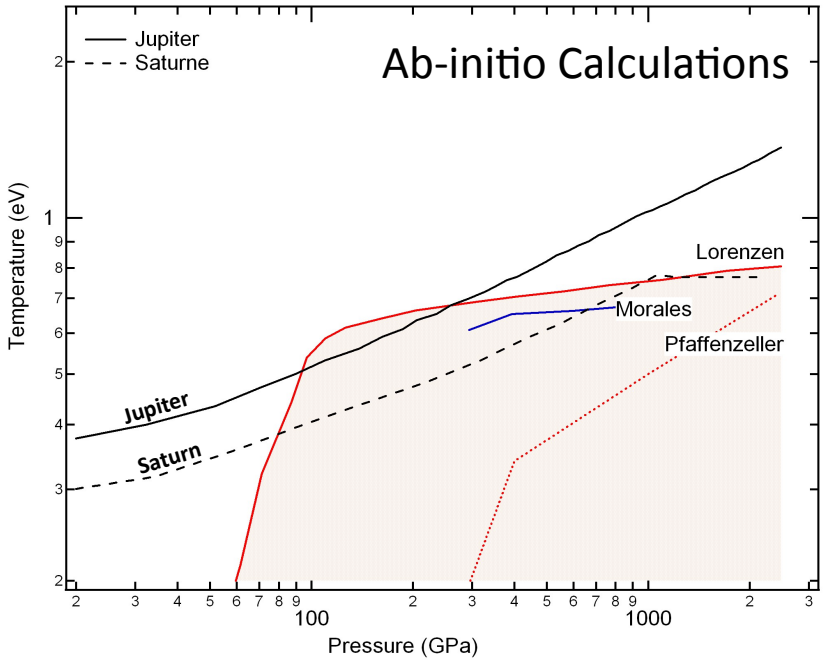


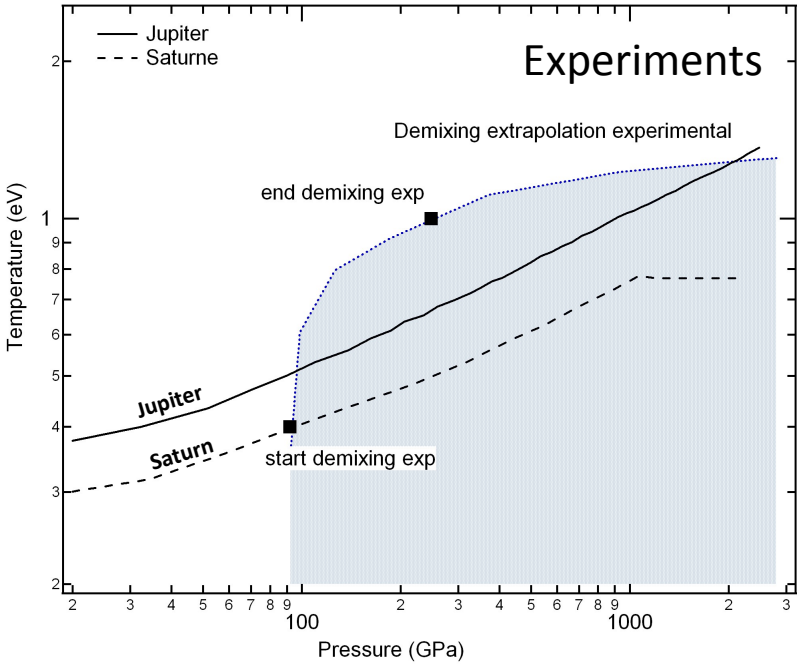
Look for Signs of Demixing by Comparing Mixtures at 20% and 50%

- At 20%, Hugoniot temperatures deviate from what is predicted by a simple mixing model - Energy change due to demixing?
- A deviation in volume is observed over the same pressure range
- Observed reflectivities confirm the limits of the demixing range.



Demixing in H_2/He Mixtures – Theory and Experiment





<u>Difficult Calculations:</u>

- Ab-initio models underestimate the gap energy
- Difficult to take into account entropy of mixing

Consequently, the predicted demixing regime is at lower temperature than observed

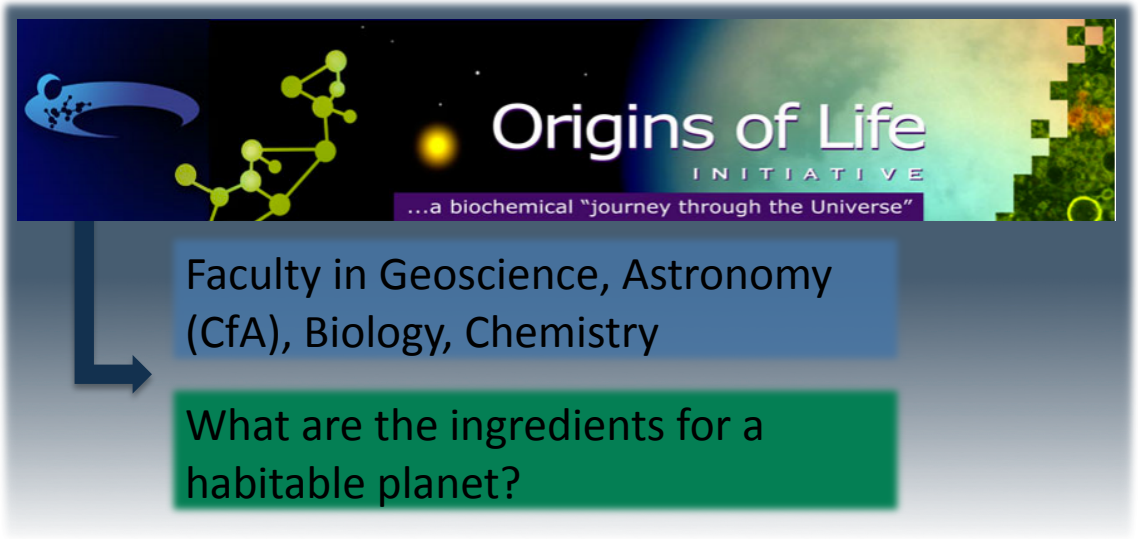
<u>Experiments:</u>

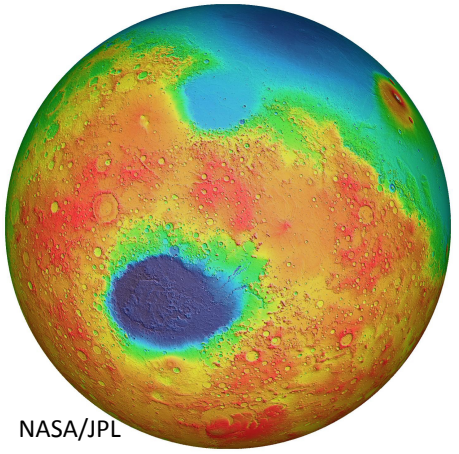
- Jupiter's isentrope is mostly in the demixing regime
- Saturn is entirely within it

Demixing could explain the observed He depletion in Jupiter's atmosphere

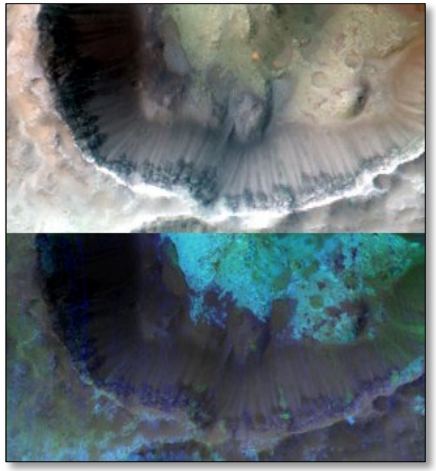
Demixing might contribute to Saturn's excess luminosity

And the Last Stop.. Planetary Surfaces and Life





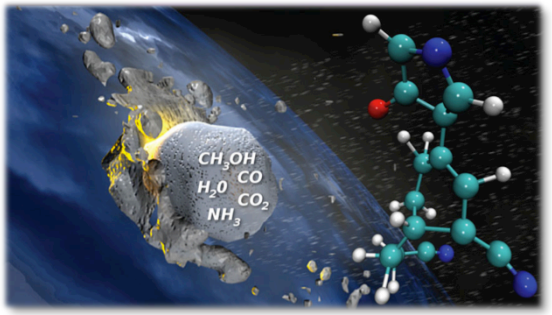
NASA/JPL



NASA/JPL

Problems I'm trying to address:

- Tracing acqueous mineralogy on Mars, history of clay minerals, devolatilization by impact
- Identifying shock-induced chemistry that could lead to significant pre-biotic molecules
- Using shocks to overcome reaction barriers and explore how geology gave way to biology

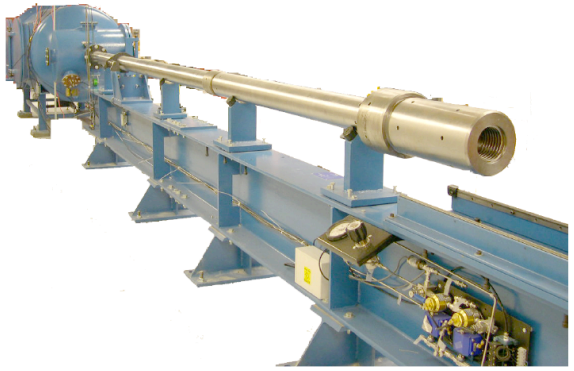


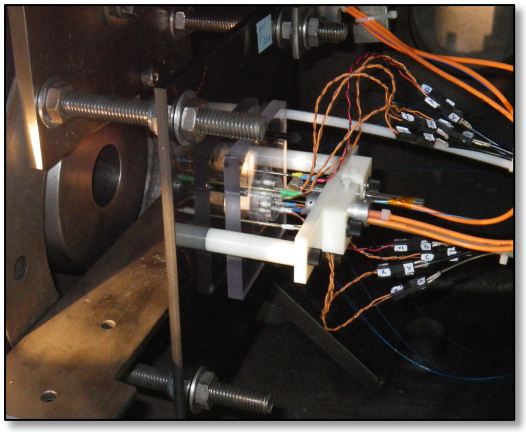
LLNL

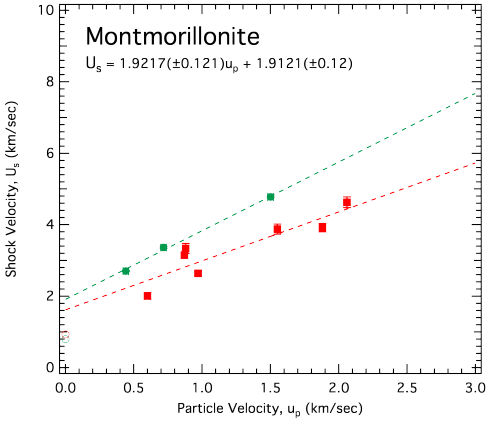
Experiments on the Harvard Gas Gun

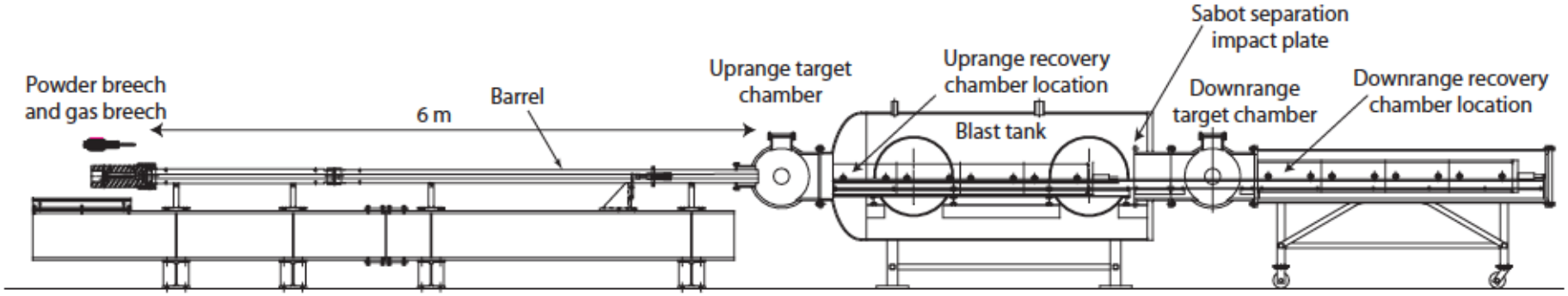
Measuring equations of state, temperature histories of shocked clays and heterogeneous mixtures

Working towards controlled recovery experiments





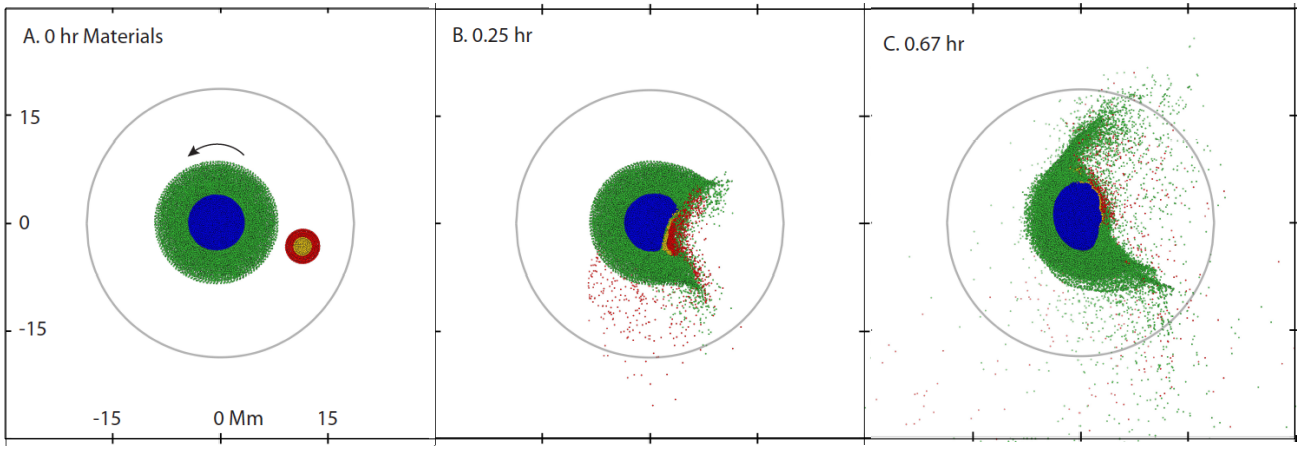




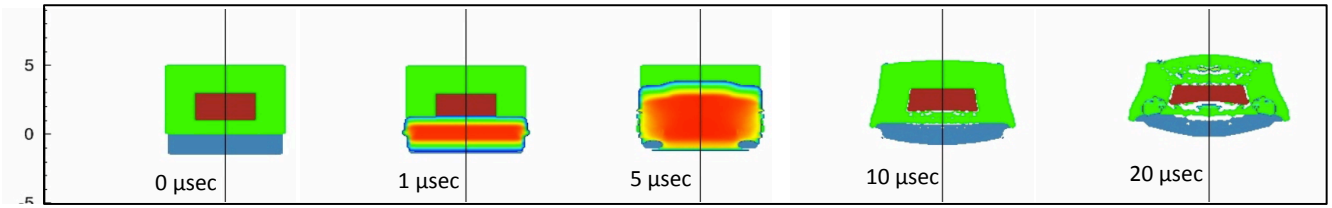
Incorporating Computational Tools

- Another advantage of a new place → Chances to increase one's skillset and capabilities
- Models allow a new perspective and more possibility to test applications

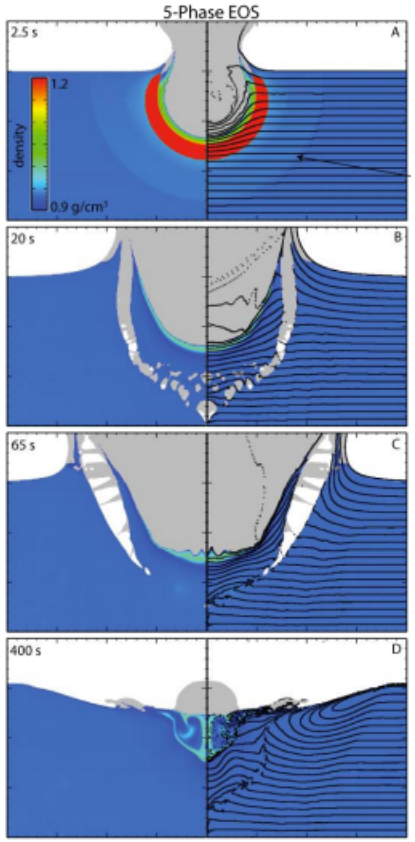
Moon Forming Impact – Cuk and Stewart, 2012



Designing Shock Recovery Capsules -



Cratering in Icy Materials - Stewart, 2010



‘Lessons Learned’

- Look for overlap in research opportunities and chances to attack dual-purpose problems, incorporate basic science

- Attack problems at the boundaries of your discipline and try to use your tools in unconventional ways

- Invite collaboration and look for ways to open your research to others as much as possible

- Be aware of breadth vs. depth