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How computational mineral physics informs our understanding of deep planetary interiors

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High Energy Density Physics Theory
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Albuquerque, NM 87185



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Main thread: *Quantifying that which can not be measured*¹

Two examples:

- ▶ Water partitioning between lower mantle minerals
- ▶ The shock Hugoniot of forsterite to 10 Mbar

Collaborators: Steve Jacobsen, Craig Bina (Northwestern) Jun Tsuchiya (GRC, Matsuyama) Seth Root, Luke Shulenburg (Sandia) Sarah Stewart (UC Davis)

¹within reason!

How is water distributed in the Earth?



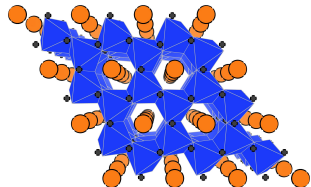
$$\frac{M^{H_2O}}{M^{\oplus}} \approx 0.00025$$

How is water distributed in the Earth?

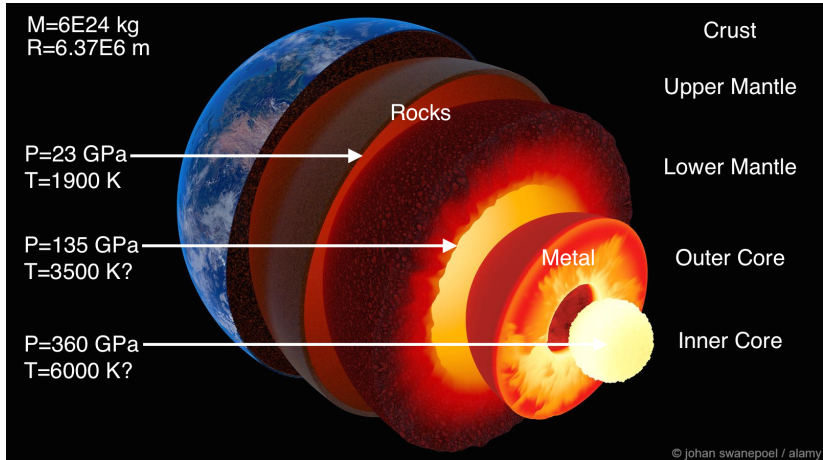


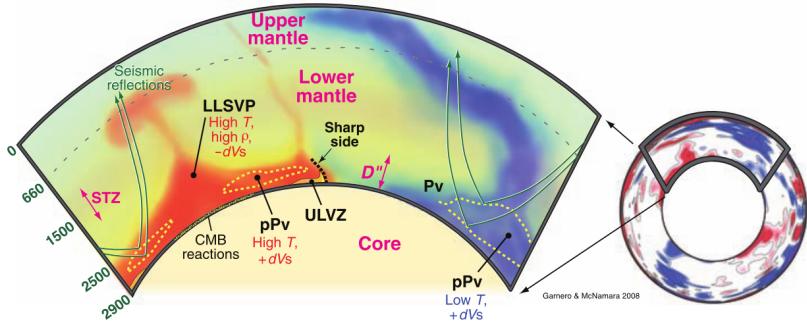
$$\frac{M^{H_2O}}{M^{\oplus}} \approx 0.00025$$

D.G.



Main constituents “nominally” anhydrous





The challenge is to explain:

- ▶ Anti-correlation of V_ϕ and V_S
- ▶ “Sharp sides” of some LLSVP’s
- ▶ Small regions of very low velocities

GEOCHEMISTRY

Evidence for primordial water in Earth's deep mantle

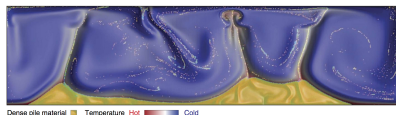
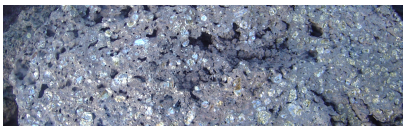
Lydia J. Hallis,^{1,2,*} Gary R. Huss,^{1,2} Kazuhide Nagashima,² G. Jeffrey Taylor,^{1,2} Sæmundur A. Halldórsson,² David R. Hilton,² Michael J. Mottl,³ Karen J. Meech^{1,5}

The hydrogen-isotope [deuterium/hydrogen (D/H)] ratio of Earth can be used to constrain the origin of its water. However, the most accessible reservoir, Earth's oceans, may no longer represent the original (primordial) D/H ratio, owing to changes caused by water cycling between the surface and the interior. **Thus, a reservoir completely isolated from surface processes is required to define Earth's original D/H signature.** Here we present data for Baffin Island and Icelandic lavas, which suggest that the deep mantle has a low D/H ratio (δD more negative than -218 per mil). Such strongly negative values indicate the existence of a component within Earth's interior that inherited its D/H ratio directly from the protosolar nebula.

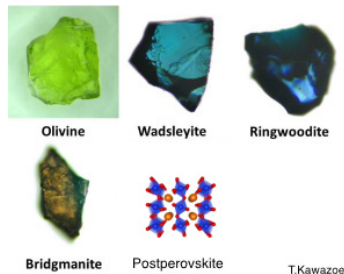
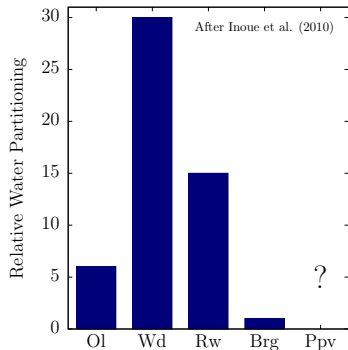
Episodic entrainment of deep primordial mantle material into ocean island basalts

Curtis D. Williams^{1,2}, Mingming Li^{2,1}, Allen K. McNamara², Edward J. Garnero² & Matthijs C. van Soest²

Chemical differences between mid-ocean ridge basalts (MORBs) and ocean island basalts (OIBs) provide critical evidence that the Earth's mantle is compositionally heterogeneous. MORBs generally exhibit a relatively low and narrow range of $^3\text{He}/^4\text{He}$ ratios on a global scale, whereas OIBs display larger variability in both time and space. The primordial origin of ^3He in OIBs has motivated hypotheses that high $^3\text{He}/^4\text{He}$ ratios are the product of mantle plumes sampling chemically distinct material, but do not account for lower MORB-like $^3\text{He}/^4\text{He}$ ratios in OIBs, nor their observed spatial and temporal variability. Here we perform thermochemical convection calculations which show the variable $^3\text{He}/^4\text{He}$ signature of OIBs can be reproduced by deep isolated mantle reservoirs of primordial material that are viscously entrained by thermal plumes. Entrainment is highly time-dependent, producing a wide range of $^3\text{He}/^4\text{He}$ ratios similar to that observed in OIBs worldwide and indicate MORB-like $^3\text{He}/^4\text{He}$ ratios in OIBs cannot be used to preclude deep mantle-sourced hotspots.



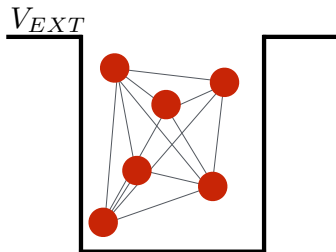
Emerging consensus on chemical heterogeneity in the lower mantle



Polymorphs of Mg_2SiO_4 (top), and MgSiO_3 (bottom).

- ▶ Well explored at low P , T , poorly constrained in LM
- ▶ Measurements @ 1 Mbar challenging!

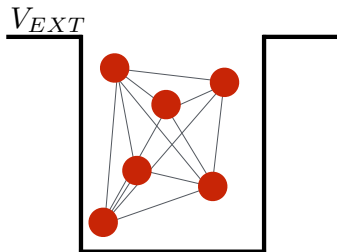
“Nature”
Fully interacting system



$$E = \int \Psi^* \hat{H} \Psi d\mathbf{r}_1 \dots d\mathbf{r}_N$$

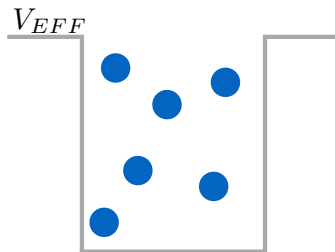
Adapted from Mattsson et al. 2005

“Nature”
Fully interacting system



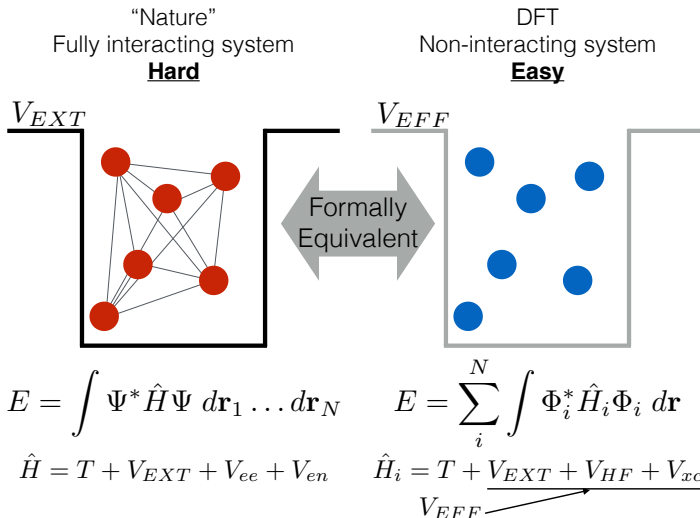
$$E = \int \Psi^* \hat{H} \Psi \, d\mathbf{r}_1 \dots d\mathbf{r}_N$$

DFT
Non-interacting system



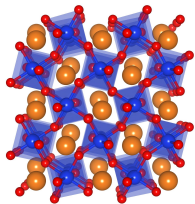
$$E = \sum_i^N \int \Phi_i^* \hat{H}_i \Phi_i \, d\mathbf{r}$$

Adapted from Mattsson et al. 2005

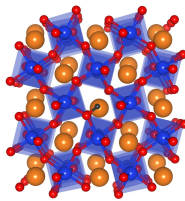


Adapted from Mattsson et al. 2005

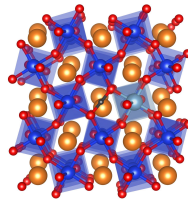
Two hydrogen defect models



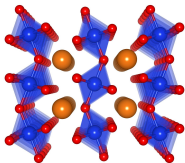
brg



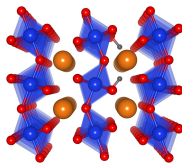
hbrg



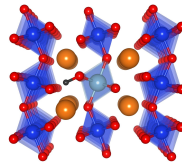
Al-hbrg



ppv

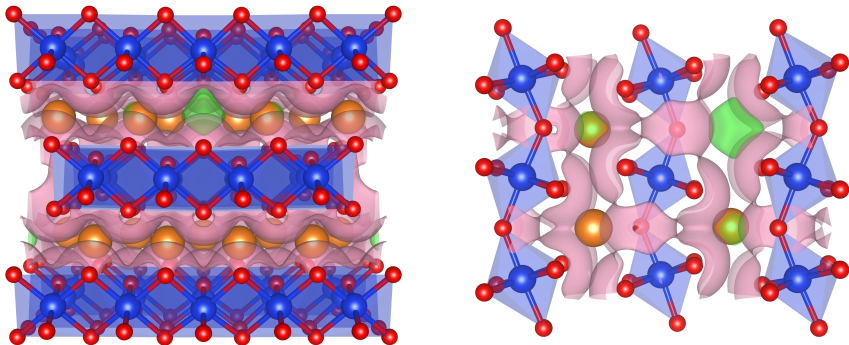


hppv

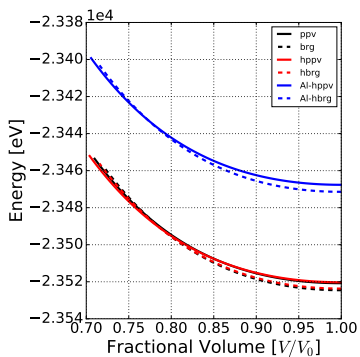


Al-hppv

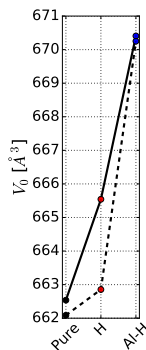
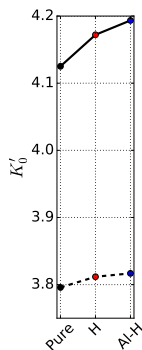
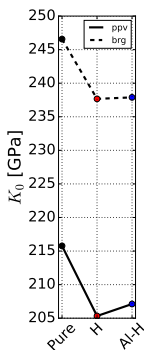
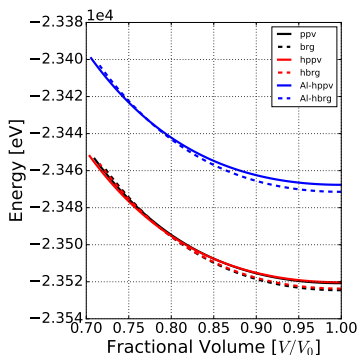
How to find where the hydrogen go



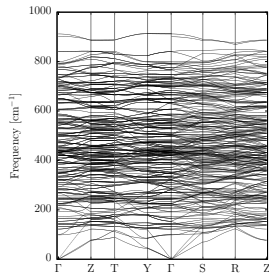
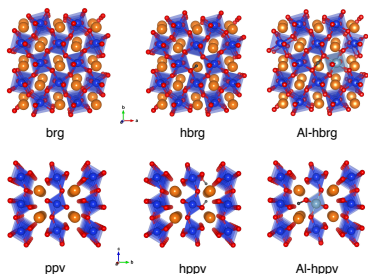
A good starting guess: Look at geometry of low density regions.



► 3rd order Birch-Murnaghan EOS

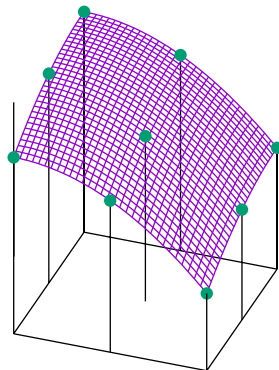
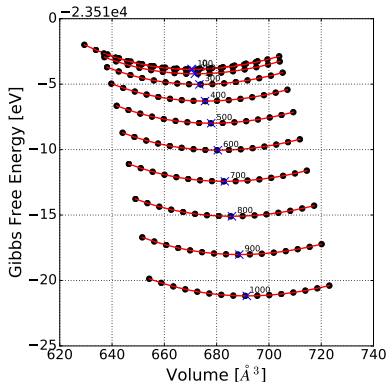


- ▶ 3rd order Birch-Murnaghan EOS
- ▶ H defects reduce K_0 , increase V_0 , resolved sensitivity of K'_0



Computational approach:

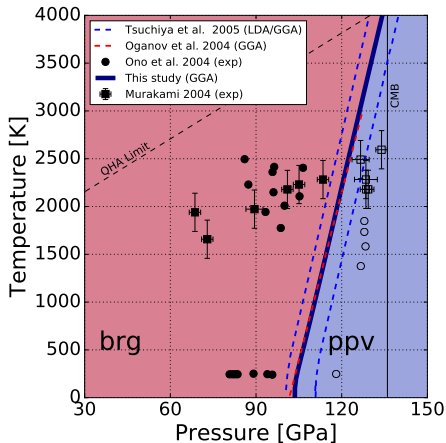
- ▶ Used Quantum ESPRESSO + PBE GGA
- ▶ DFPT phonon dispersions calculated on $2 \times 2 \times 2$ k -point grid
- ▶ Quasi-harmonic phonons $\rightarrow$ thermodynamic properties



The basic procedure:

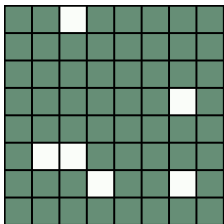
$$F^{vib}(T; V) = \sum_{\mathbf{q}, s} \left\{ \frac{\hbar}{2} \omega_s(\mathbf{q}; V) + kT \ln \left(1 - e^{-\hbar \omega_s(\mathbf{q}; V)/kT} \right) \right\}$$

$$G(P, T) = \min \left\{ U^{static}(V) + F^{vib}(T; V) + PV \right\}$$

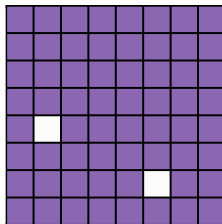


- ▶ Excellent agreement w/ experiment & theory.
- ▶ Clapeyron slope @ 125 GPa, 2500 K ≈ 7.5 MPa/K
- ▶ Self-consistency is vital!

Crystal A



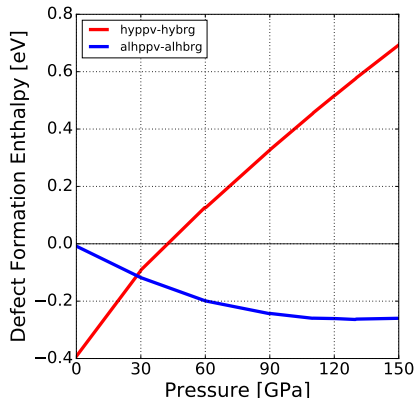
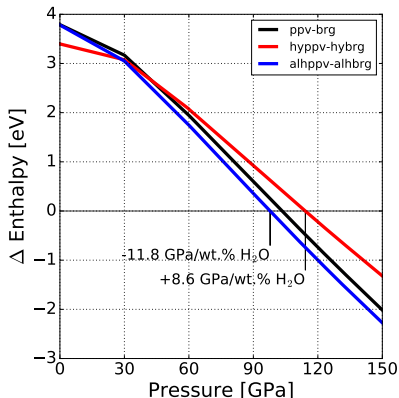
Crystal B



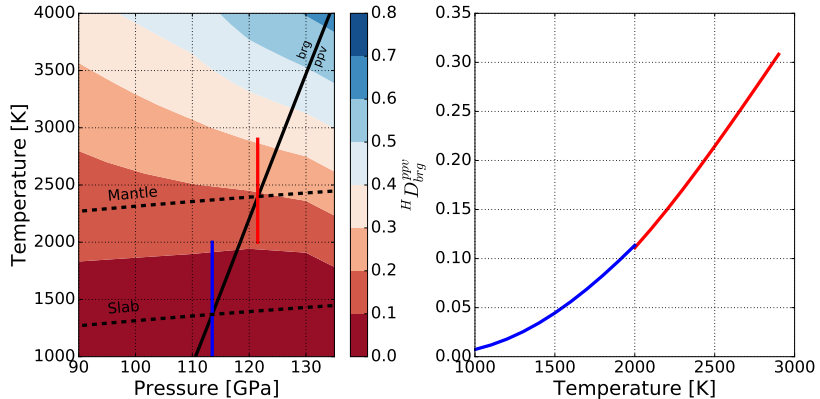
The equilibrium ratio of defect Y in phases a and b :

$${}^Y D_b^a = \frac{e^{G_b^f/kT} + 1}{e^{G_a^f/kT} + 1} \approx e^{\Delta G_{ba}^f/kT}$$

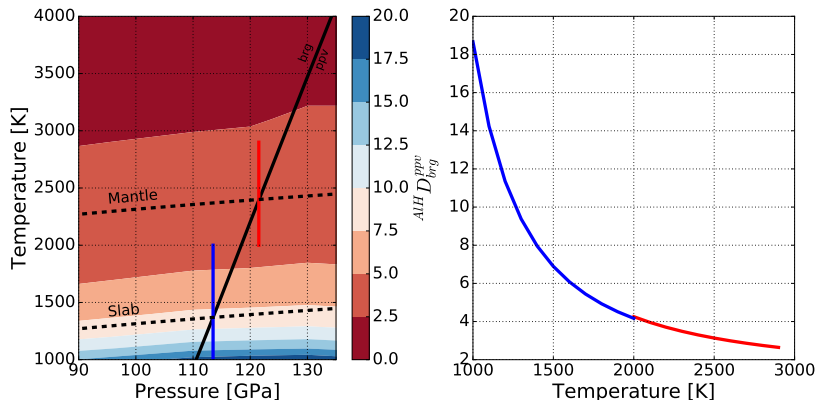
After Hernández et al. (2013)



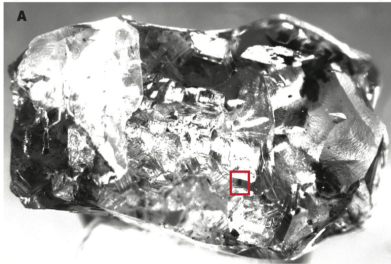
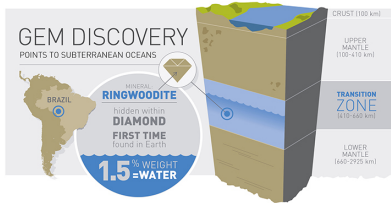
- ▶ Al-free defects stabilize brg, Al-bearing defects stabilize ppv.
- ▶ AIH defect formation energy is insensitive to pressure.



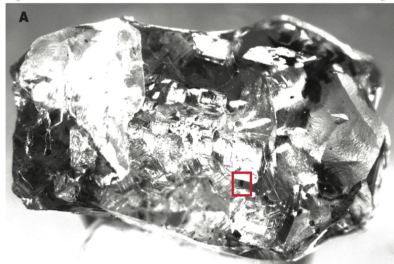
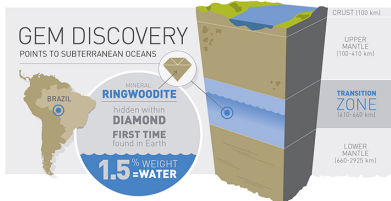
Al-free hydrous defects → more water in bridgmanite



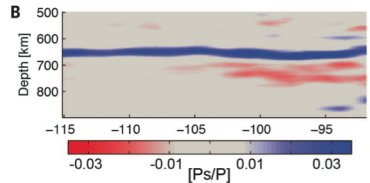
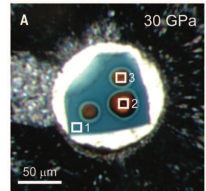
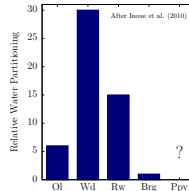
Al-bearing hydrous defects → more water in postperovskite



Pearson et al. (2014)



Pearson et al. (2014)

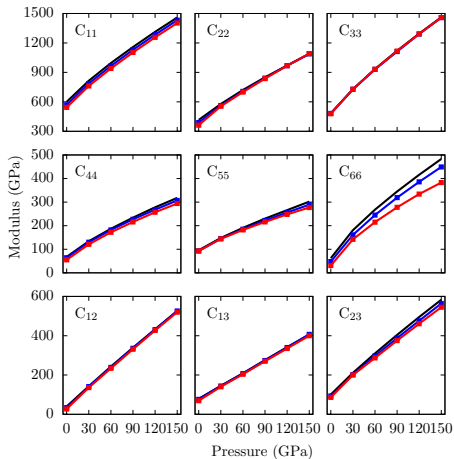


Schmandt et al. (2014)

Dehydration-induced melting?



email: jptowns@sandia.gov



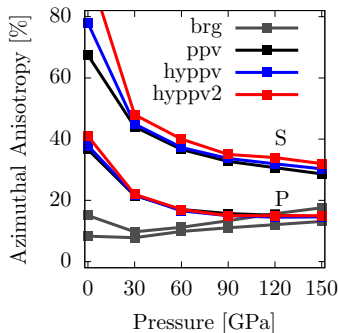
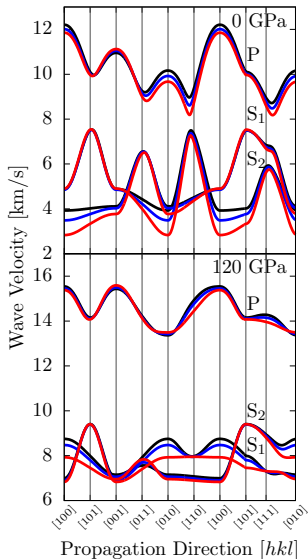
Hooke's Law:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

- ▶ All C_{ij} 's reduced
- ▶ Shear elements sensitive
- ▶ C_{66} reduced 10%/wt.% H_2O

Color change:

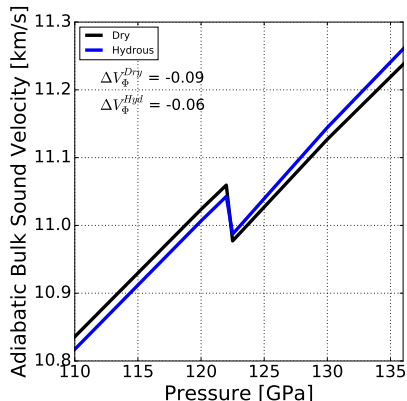
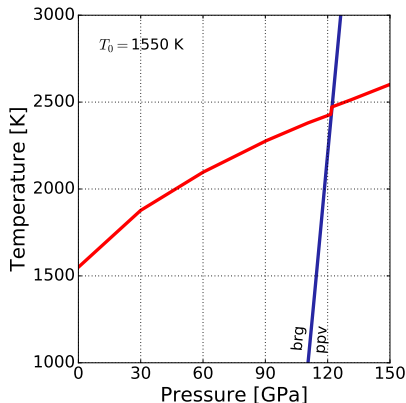
Dry, 1 wt.% H_2O , 2 wt.% H_2O



Cristoffel equation:

$$\det |c_{ijkl}n_jn_l - \rho V^2\delta_{ik}| = 0$$

► Influence of water small at CMB!

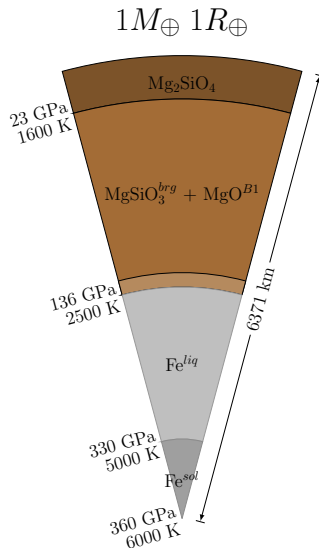


Focus on the brg-ppv transition:

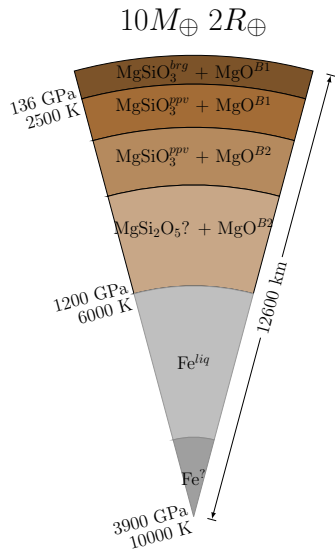
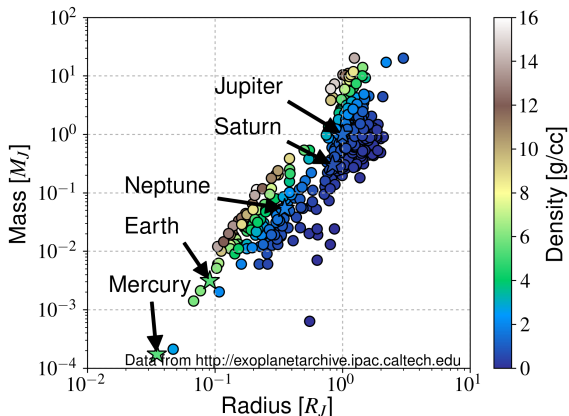
- ▶ Impedance contrast reduced by 40% w.r.t. dry
- ▶ Higher velocity gradient for hydrous ppv

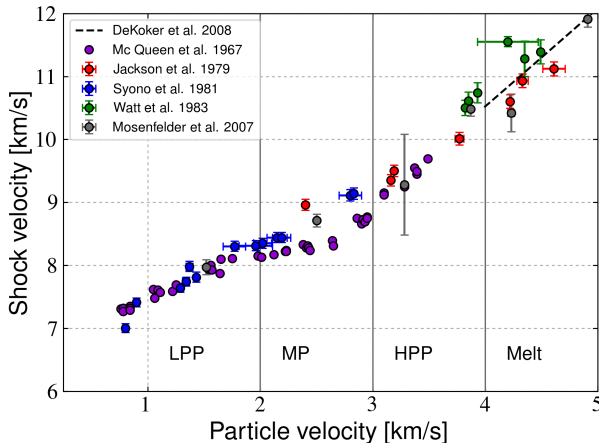
1. H partitioning between brg & ppv controlled by Al
2. Al-free ppv stores very little water
3. Al-bearing ppv stores up to 10x more water than brg
4. Seismic detection very challenging - but hopeful!
5. Ppv may be a host for primordial water - no DHMS needed
6. Possible mechanism for dredging primordial material via entrainment of primordial al-ppv back-transformation to brg

Giant impacts explore exotic P , T states



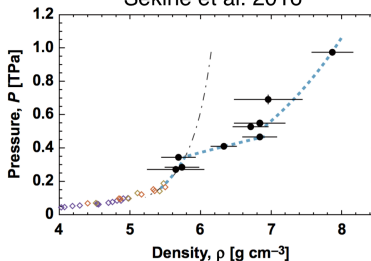
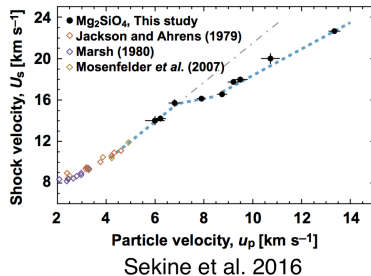
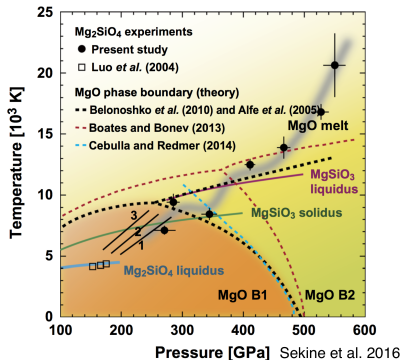
Super-Earth interiors poorly constrained



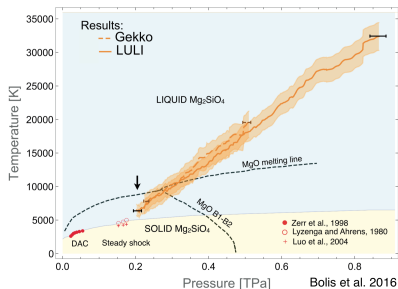
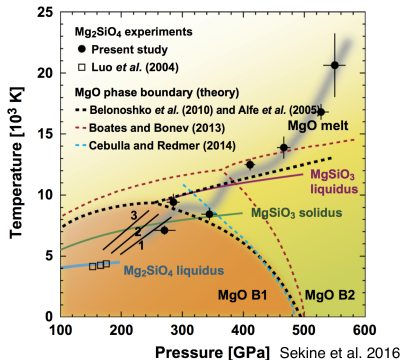


Giant impacts explore much higher velocities!

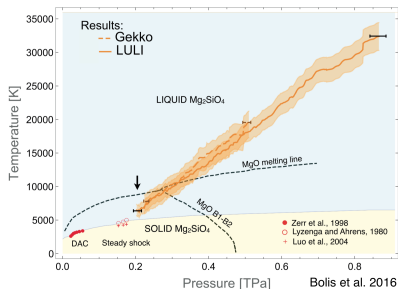
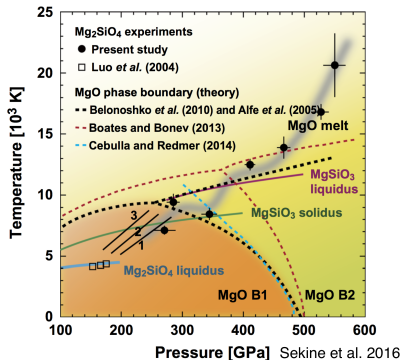
► Incongruent melting



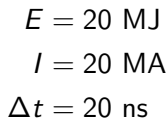
- Incongruent melting
- Single phase



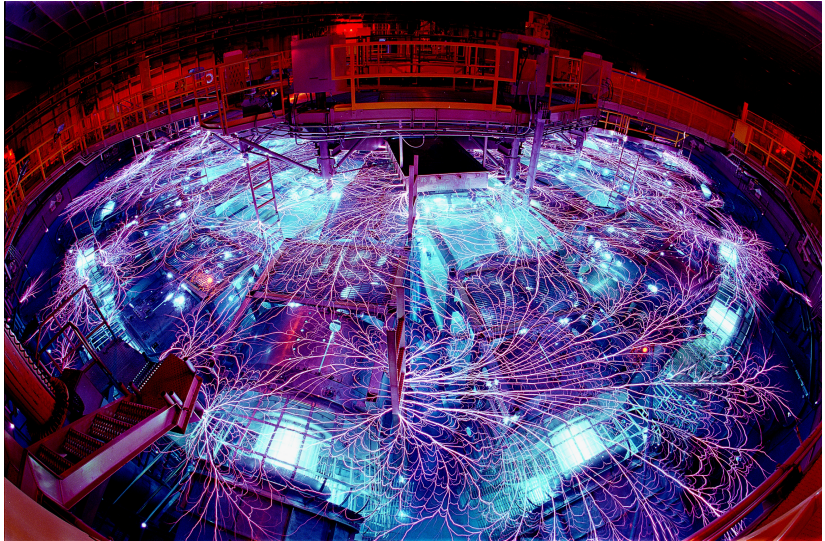
- ▶ Incongruent melting
- ▶ Single phase

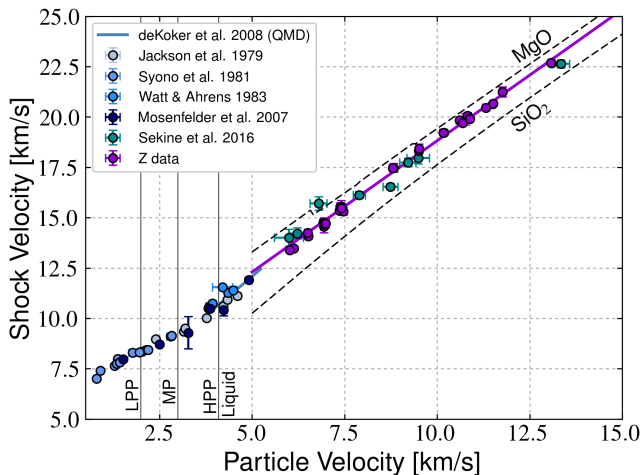


Two experiments two answers!

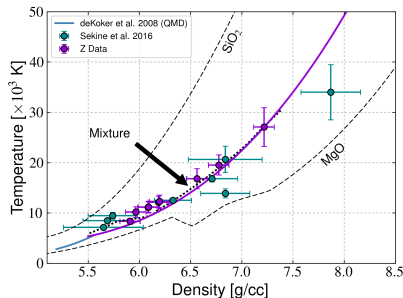
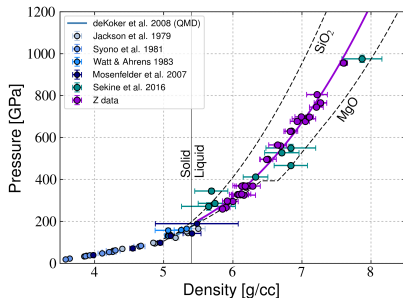


Credit: S. Root (SNL)

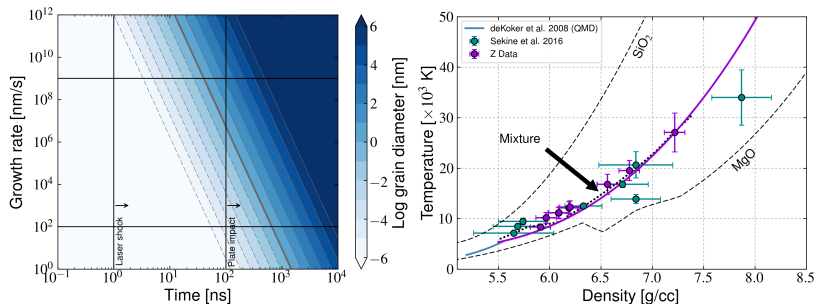




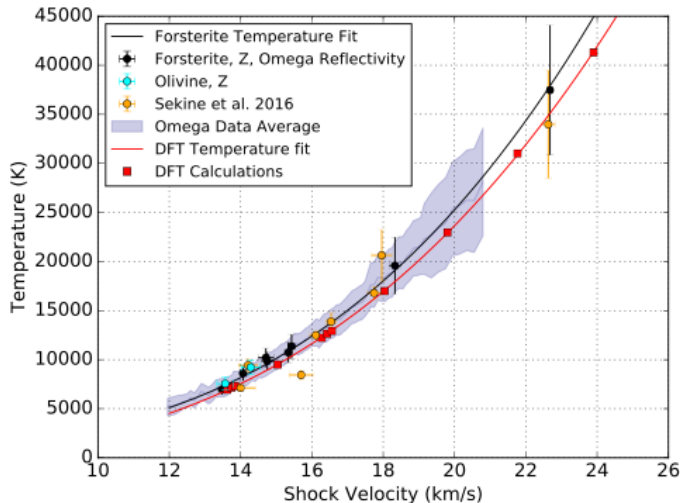
No incongruent melting on the Hugoniot



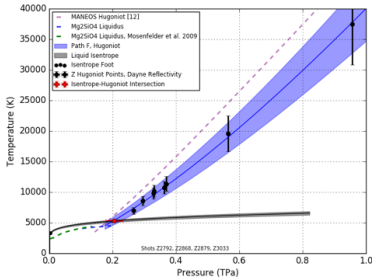
- ▶ Z expts. show no evidence of incongruent melting
- ▶ DFT of single fluid phase in excellent agreement with data
- ▶ DFT computed Hugoniot of hypothetical mixture would be most noticeable at low density



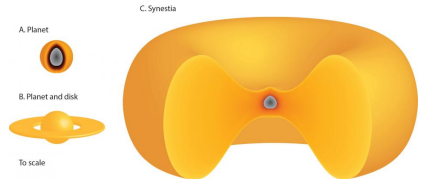
- ▶ Z expts. maintain Hugoniot state longer than laser shocks
- ▶ Estimate grain growth rates from Gleason et al. (2015)
- ▶ We can rule out possibility of kinetic effects



Courtesy S. Stewart



Courtesy S. Stewart



Lock and Stewart 2017

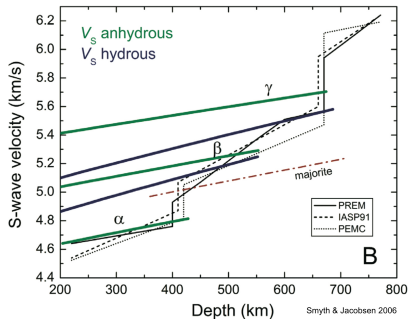
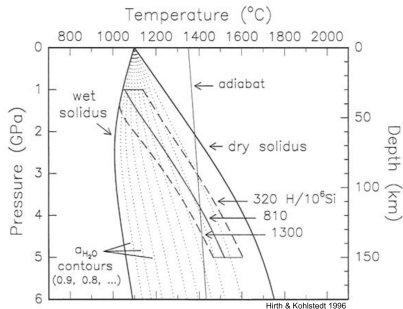
- Accretion models with old EOS under-predict vaporization

Thank you!
Questions?

Extra slides



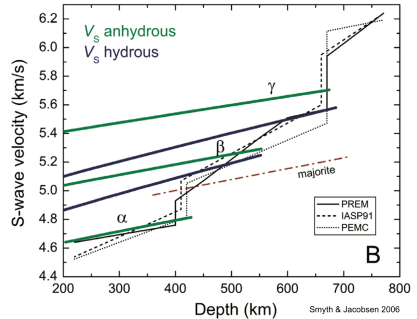
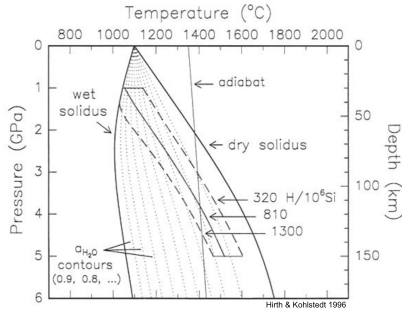
Why water is important



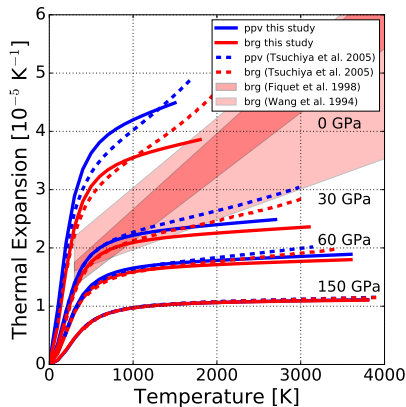
Trace amounts of water:

- ▶ Reduce melting temperature
- ▶ Reduce seismic velocity

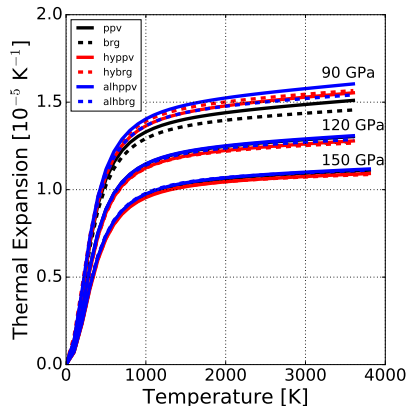
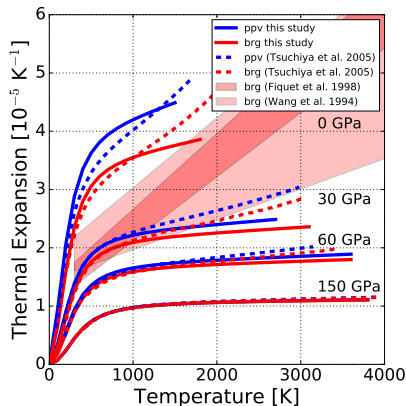
Why water is important



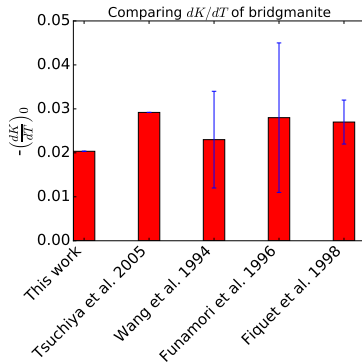
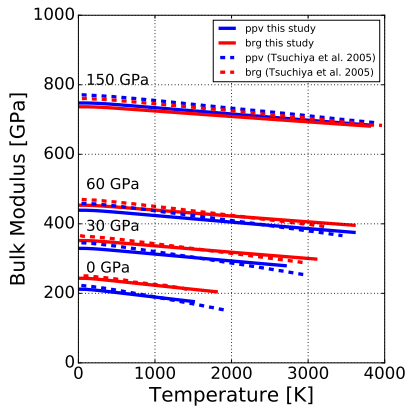
Does water have a role to play in the lowermost mantle?



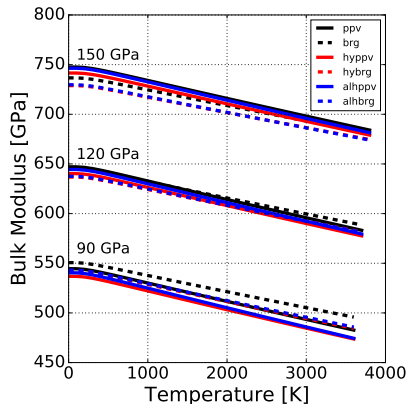
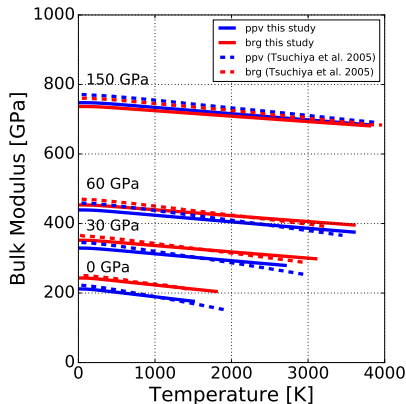
- ▶ Reasonable agreement with previous theory & experiment
- ▶ More experiments needed here



- ▶ Reasonable agreement with previous theory & experiment
- ▶ More experiments needed here
- ▶ Influence of defects negligible at high P, T



- Good agreement with previous theory & experiment.



- ▶ Good agreement with previous theory & experiment.
- ▶ Defects reduce K , but not $\left(\frac{\partial K}{\partial T}\right)_P$.