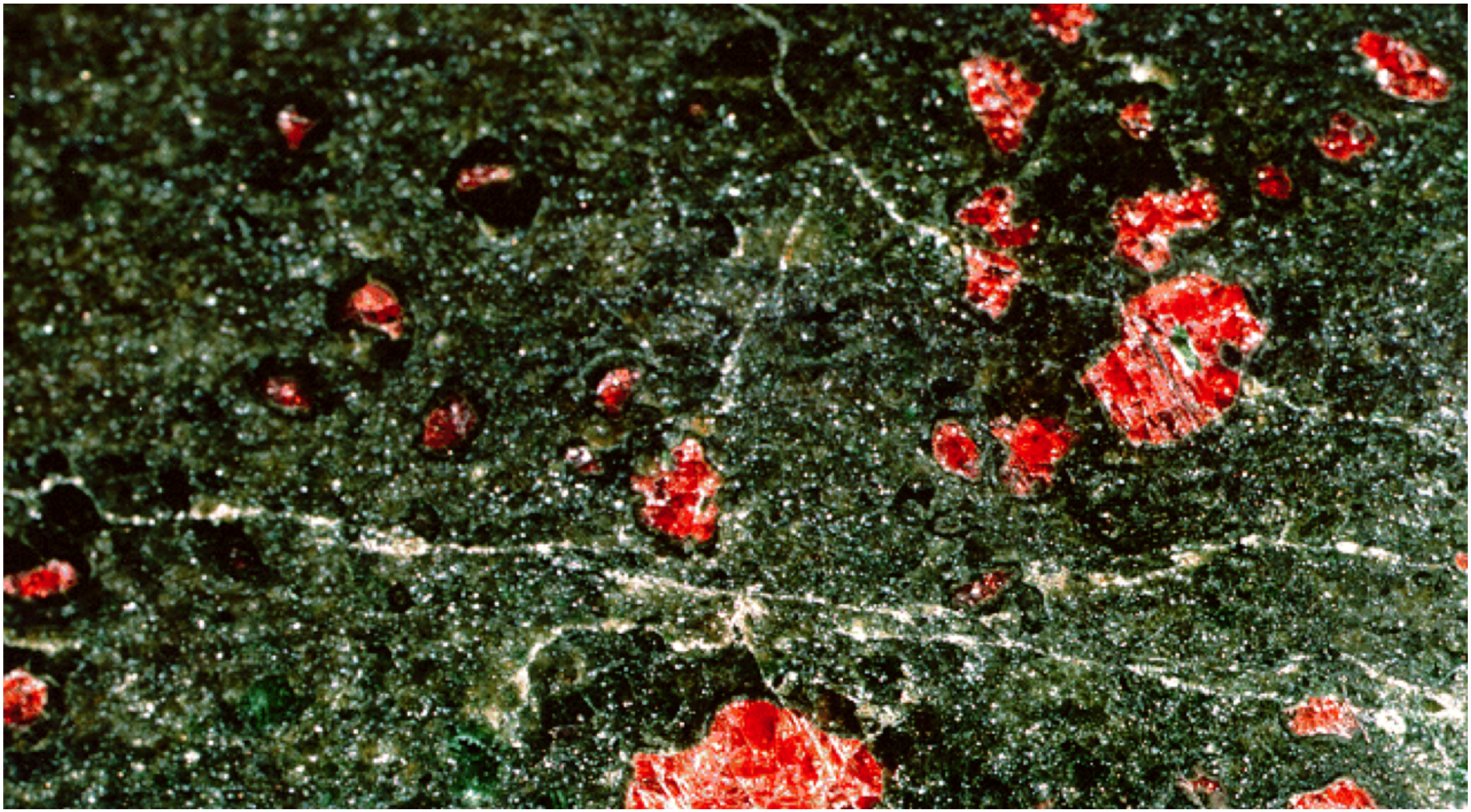
Advanced Grant
MOLTENEARTH

Fluid Silicates at Extreme Conditions and the Magma Ocean

Lars Stixrude[1,2], Roberto Scipioni[2], Michael Desjarlais[3], Eero Holmström[2,4], Bing Xiao[2]

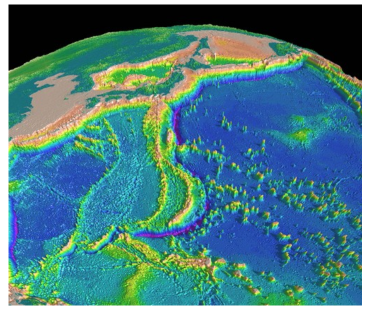
[1]UCLA; [2]University College London; [3]Sandia National Laboratory; [4]Aalto University

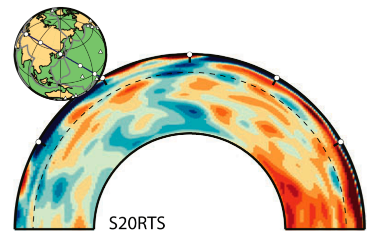


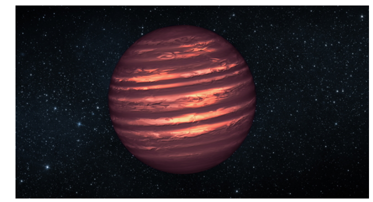
Francisco Negroni; Calbuco Volcano, Chile

Nakajima & Stevenson (2015) EPSL

Pressure

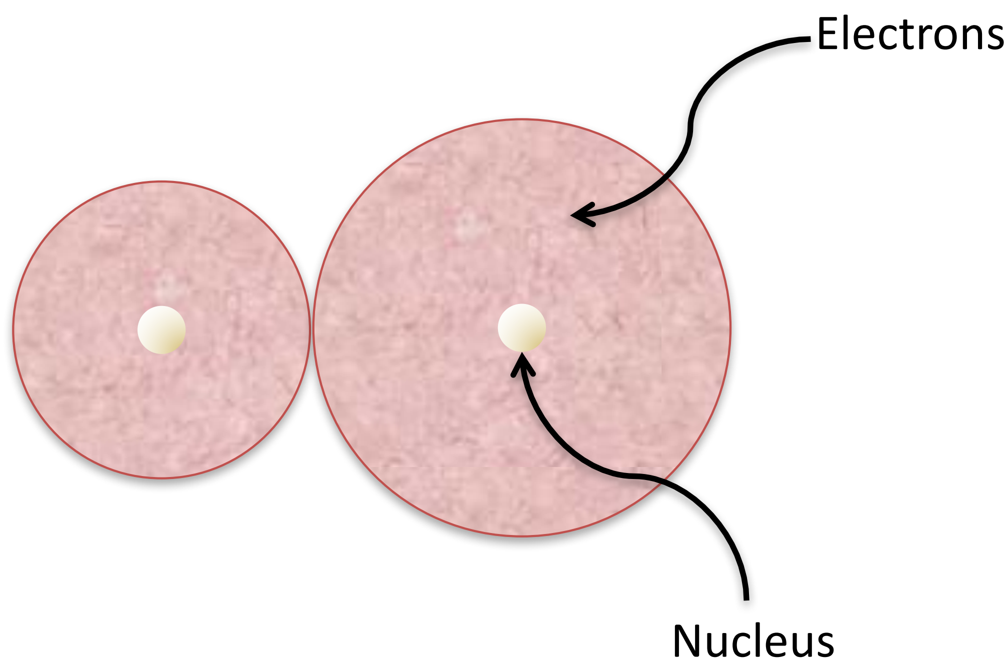


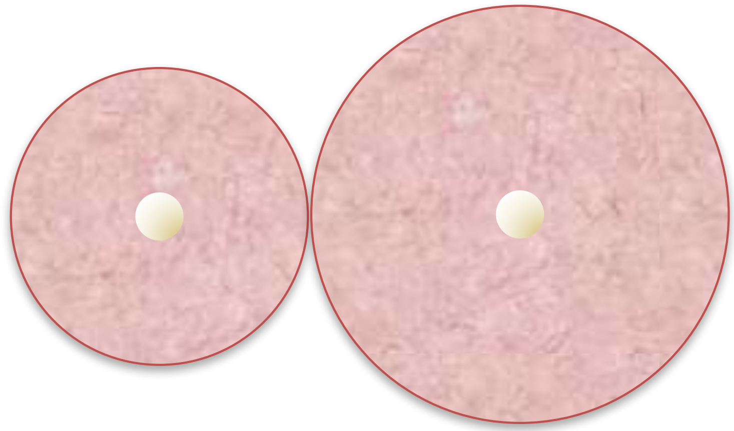




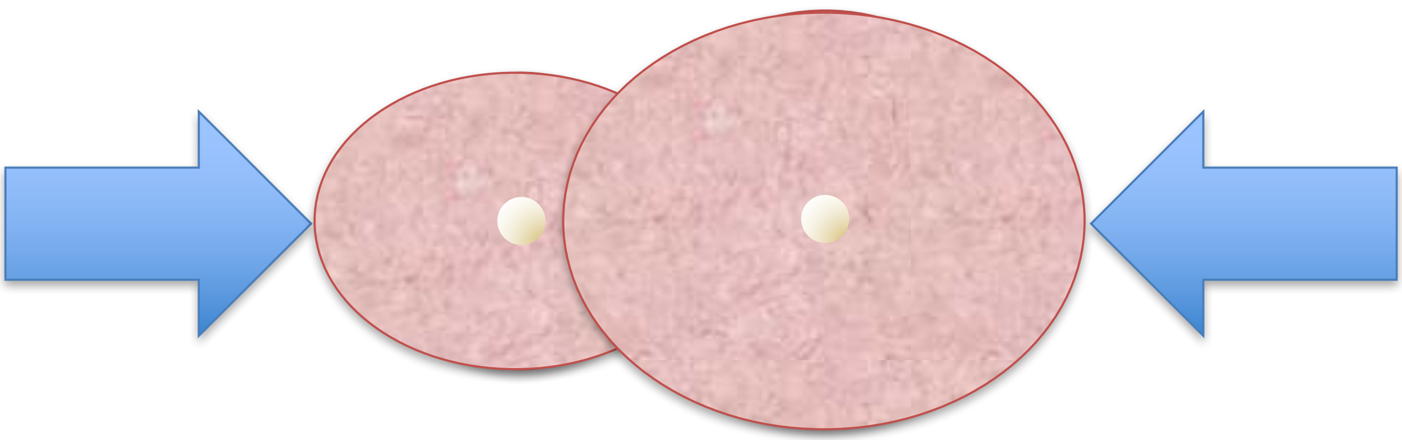
Stratopause	Surface	Challenger Deep	Core-Mantle Boundar	Brown Dwarf
1 millibar	1 bar	1 kilobar	1 Megab	Gigabar
		100 MPa	100 GPa	100 TPa

Most Matter in the Universe

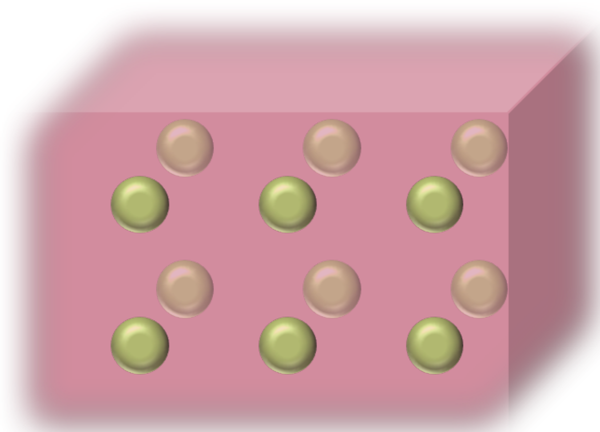

Electrons
Nucleus



Earth’s surface
Pauling-Goldschmidt



Planetary Interiors

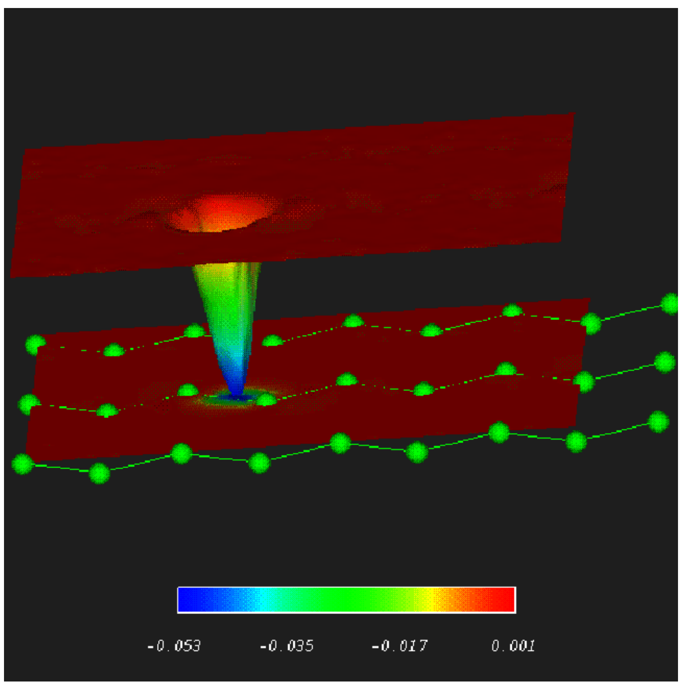


Stellar Interior
Uniform Electron Gas

Density Functional Theory

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \sum_{\alpha}^{N} \frac{Z_\alpha e^2}{|\mathbf{R}_\alpha - \mathbf{r}|} + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}' + V_{xc}\left[\rho(\mathbf{r})\right] - \varepsilon_i\right]\psi_i(\mathbf{r}) = 0$$

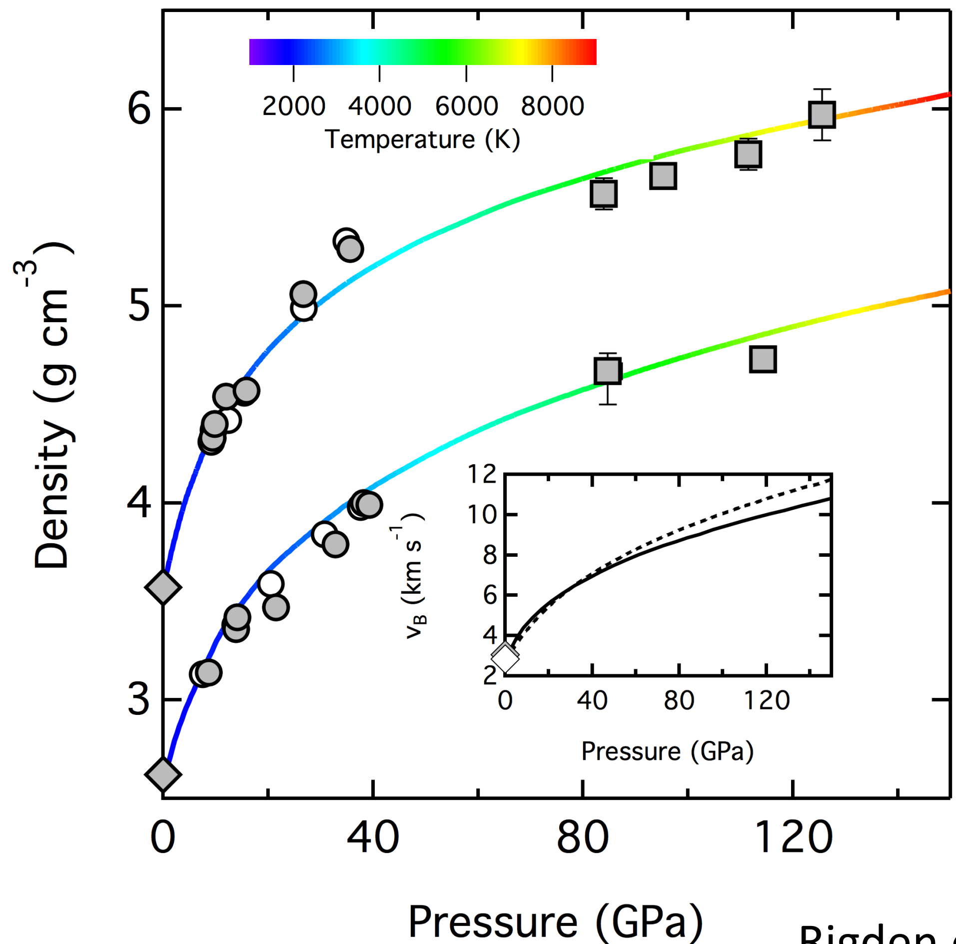
Approximate the eXchange-Correlation Potential



Hood et al. (1997) *PRL*

Hohenberg & Kohn (1964) *Phys Rev*
Kohn & Sham (1965) *Phys Rev*

Density Functional Theory

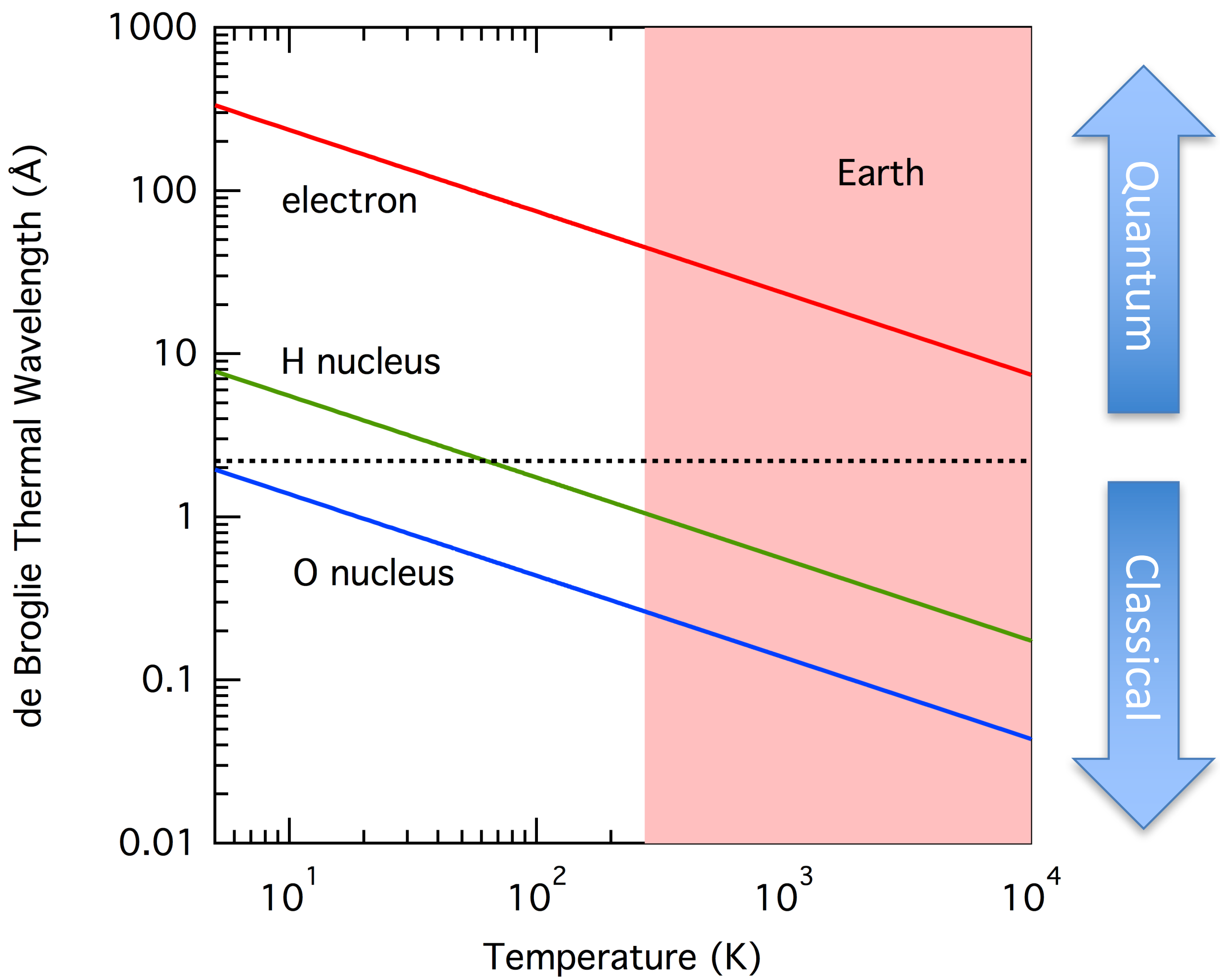


$CaAl_2Si_2O_8$
$CaMgSi_2O_6$

Rigden et al. (1989) *JGR*
Asimow & Ahrens (2010) *JGR*
Sun et al. (2011) *GCA*
Karki et al. (2012) *Am. Min.*

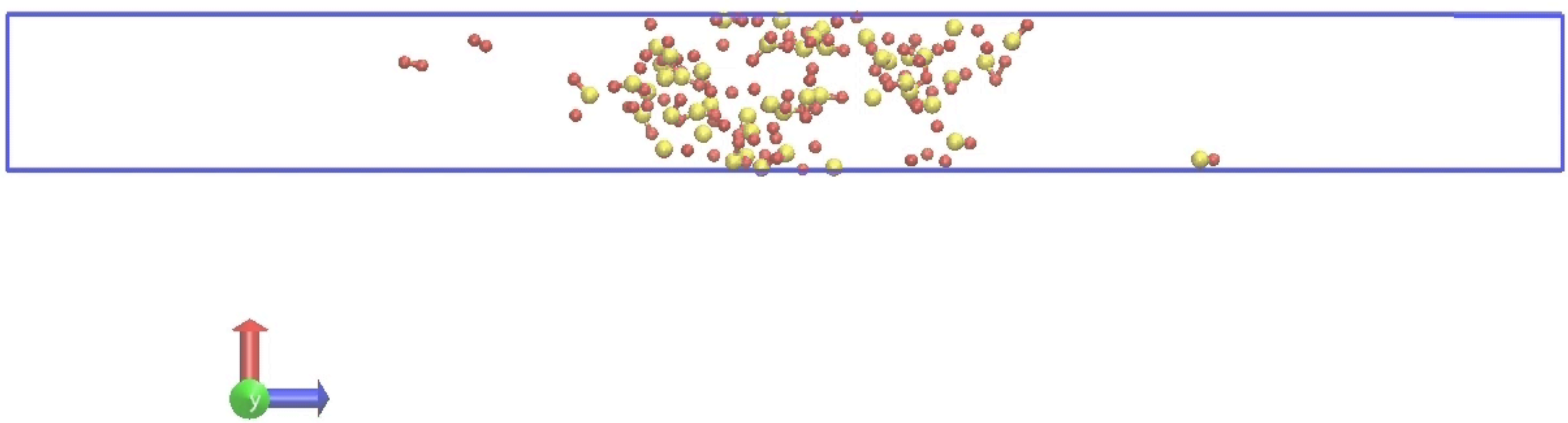
VASP: Kresse et al. (1992); Kresse and Joubert (1996)
LAPW: Wei & Krakauer (1985); Singh (1994)

Temperature



First Principles Molecular Dynamics

$$F_{\alpha i}\left(R^N\right) = m_\alpha \ddot{R}_{\alpha i}$$



SiO_2

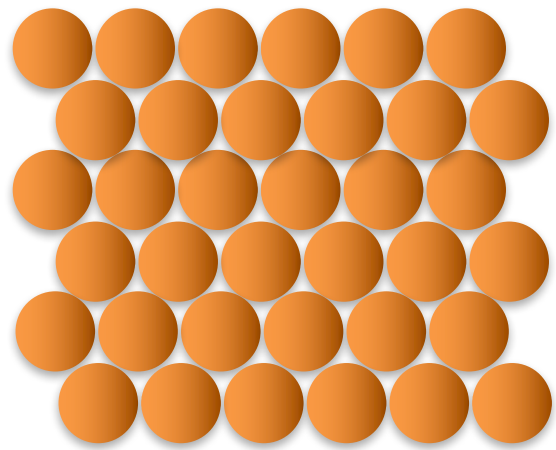
Xiao and Stixrude (2018) PNAS

FPMD

- Density Functional Theory
- Born-Oppenheimer Molecular Dynamics
- Mermin Functional
- Projector Augmented Wave Method
- Exchange-Correlation: PBEsol, HSE06, +U
- NVT Ensemble
- Kubo-Greenwood

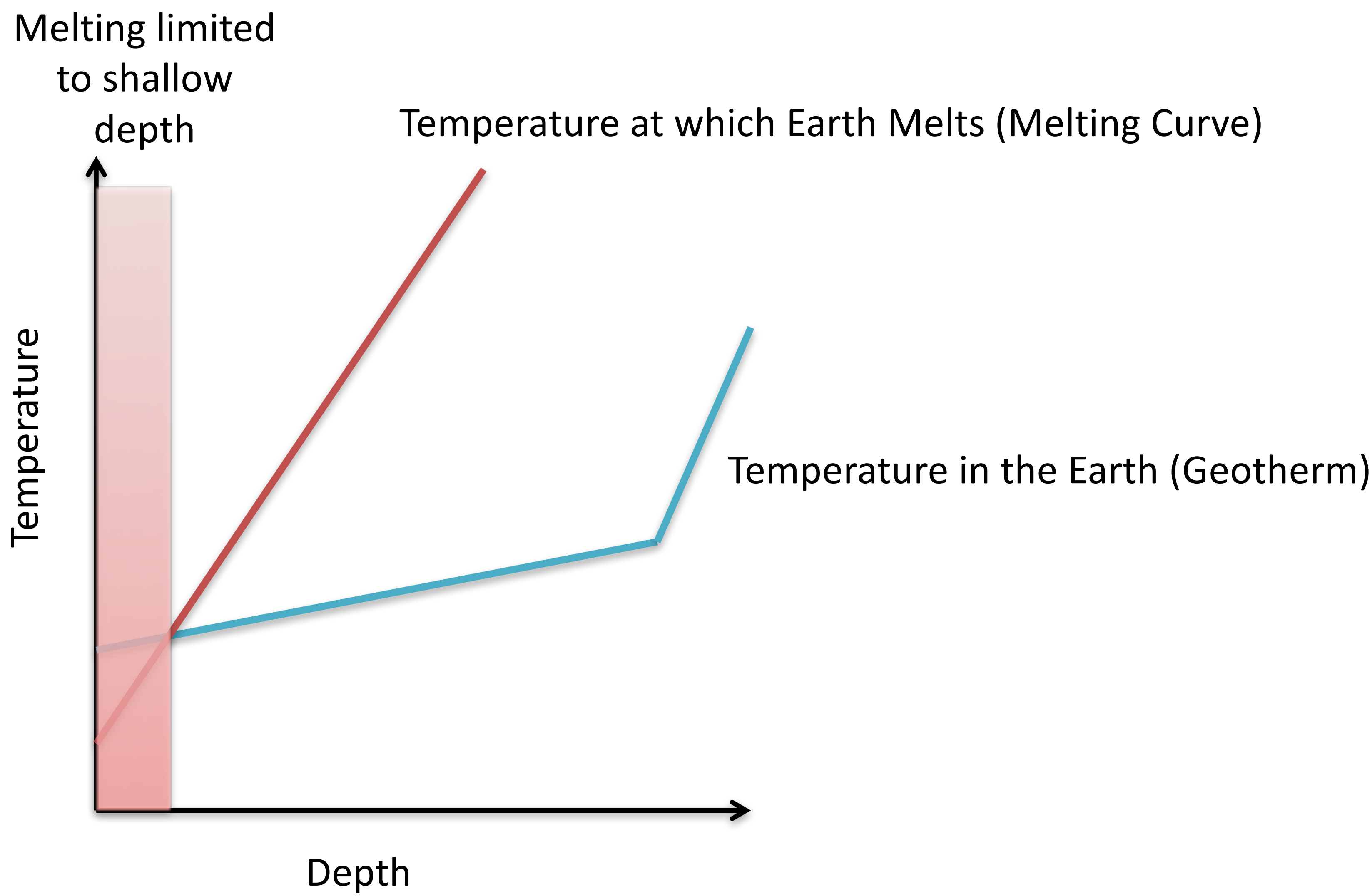
Kresse et al. (1992); Kresse and Joubert (1996); Mermin (1965); Perdew et al., (2008); Nosé (1984); Hoover (1985); Desjarlais et al. (2002)

Liquid Structure

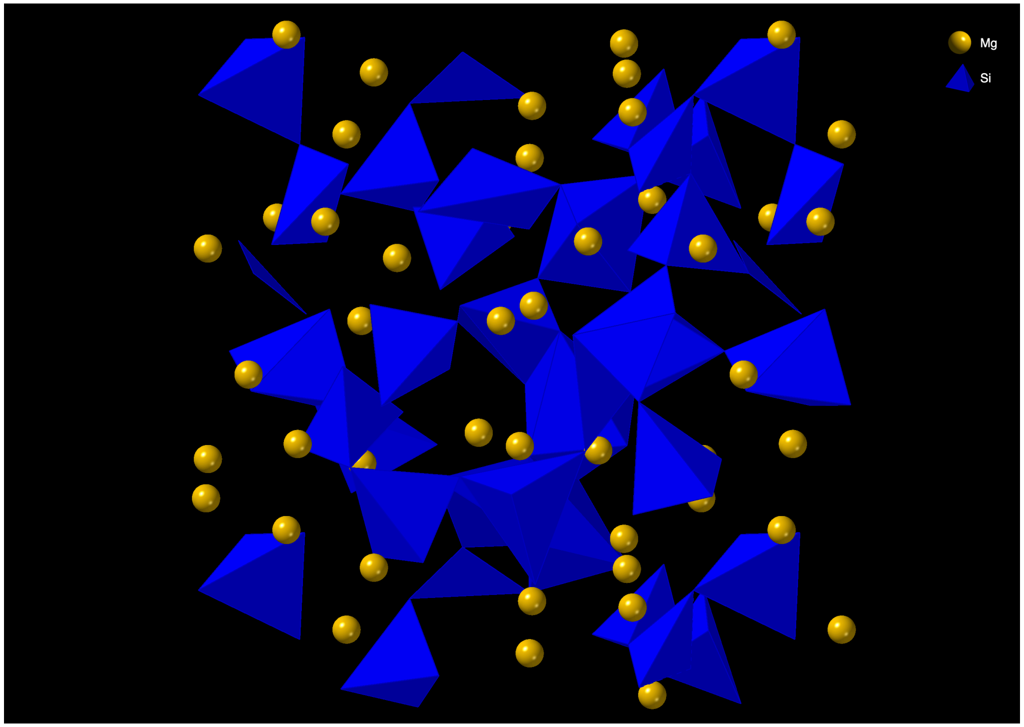


Liquid Volume > Solid Volume

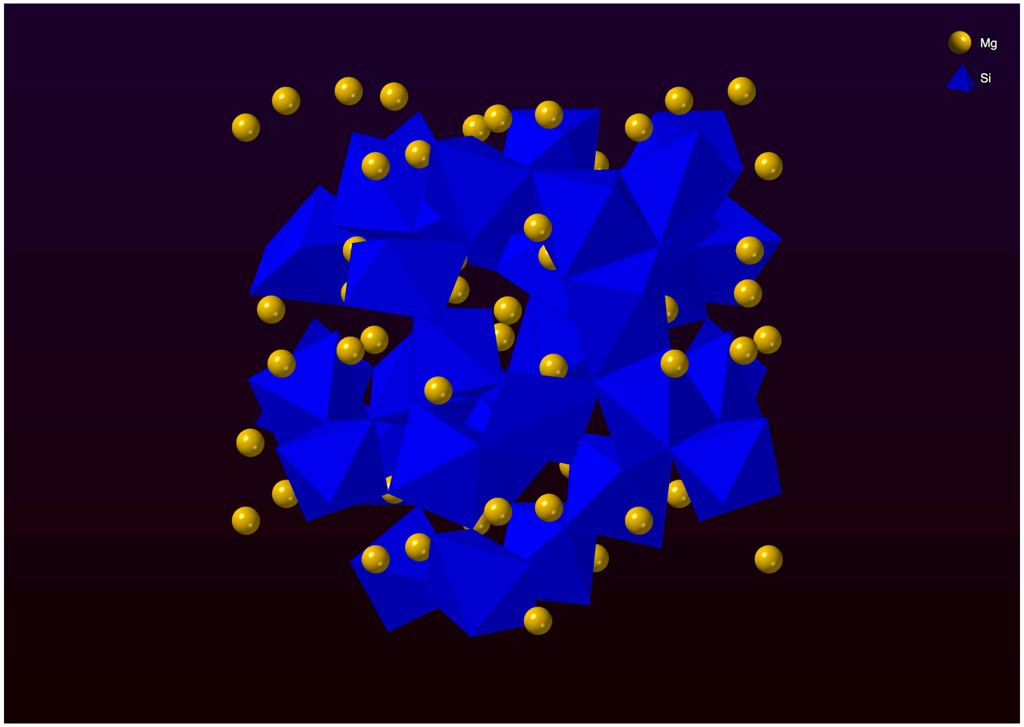
$$\left(\frac{\partial T}{\partial P}\right)_{melt} = \frac{\Delta V_{melting}}{\Delta S_{melting}}$$


Melting limited to shallow depth
Temperature at which Earth Melts (Melting Curve)
Temperature in the Earth (Geotherm)
Temperature
Depth

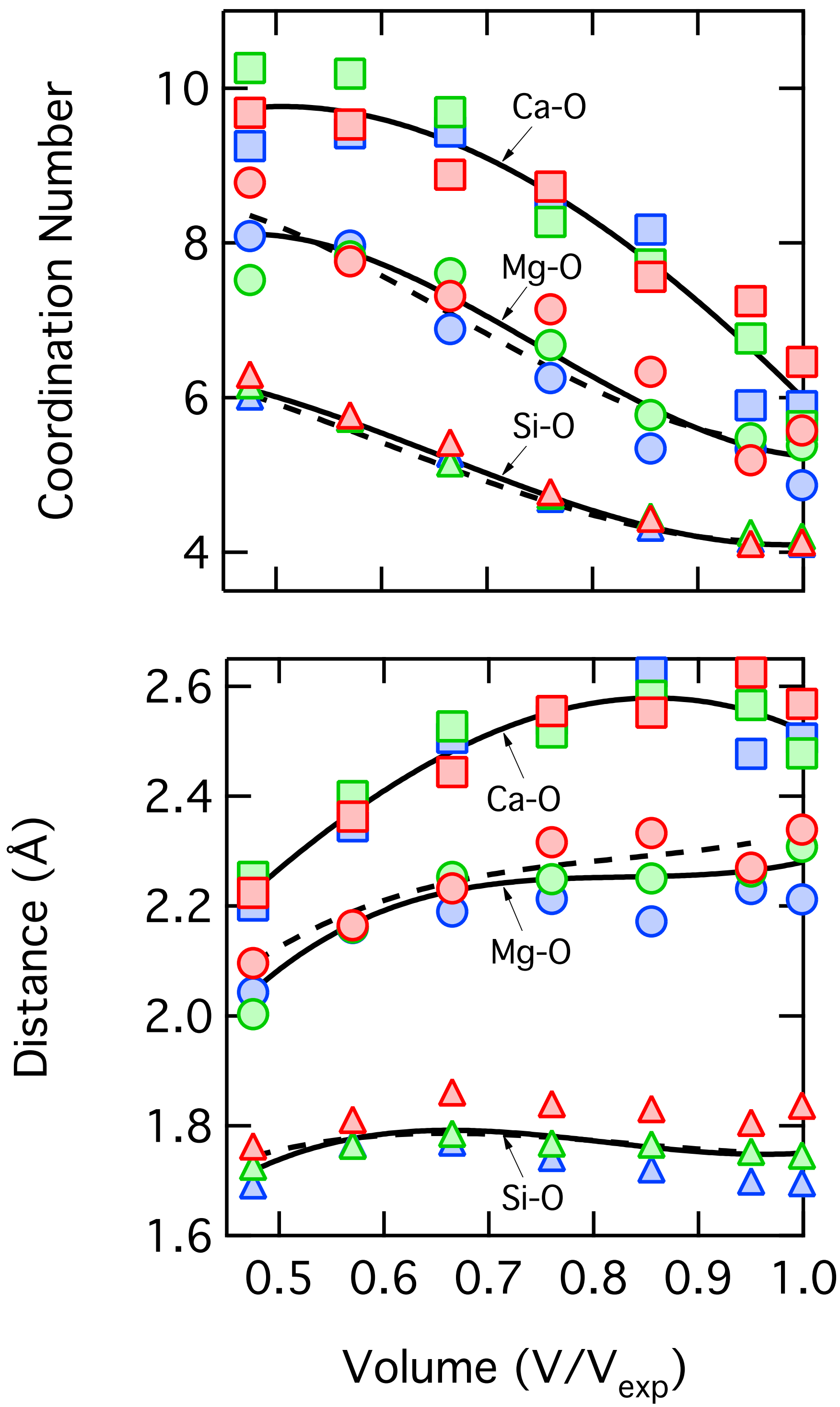
$MgSiO_3$ Liquid



10 GPa

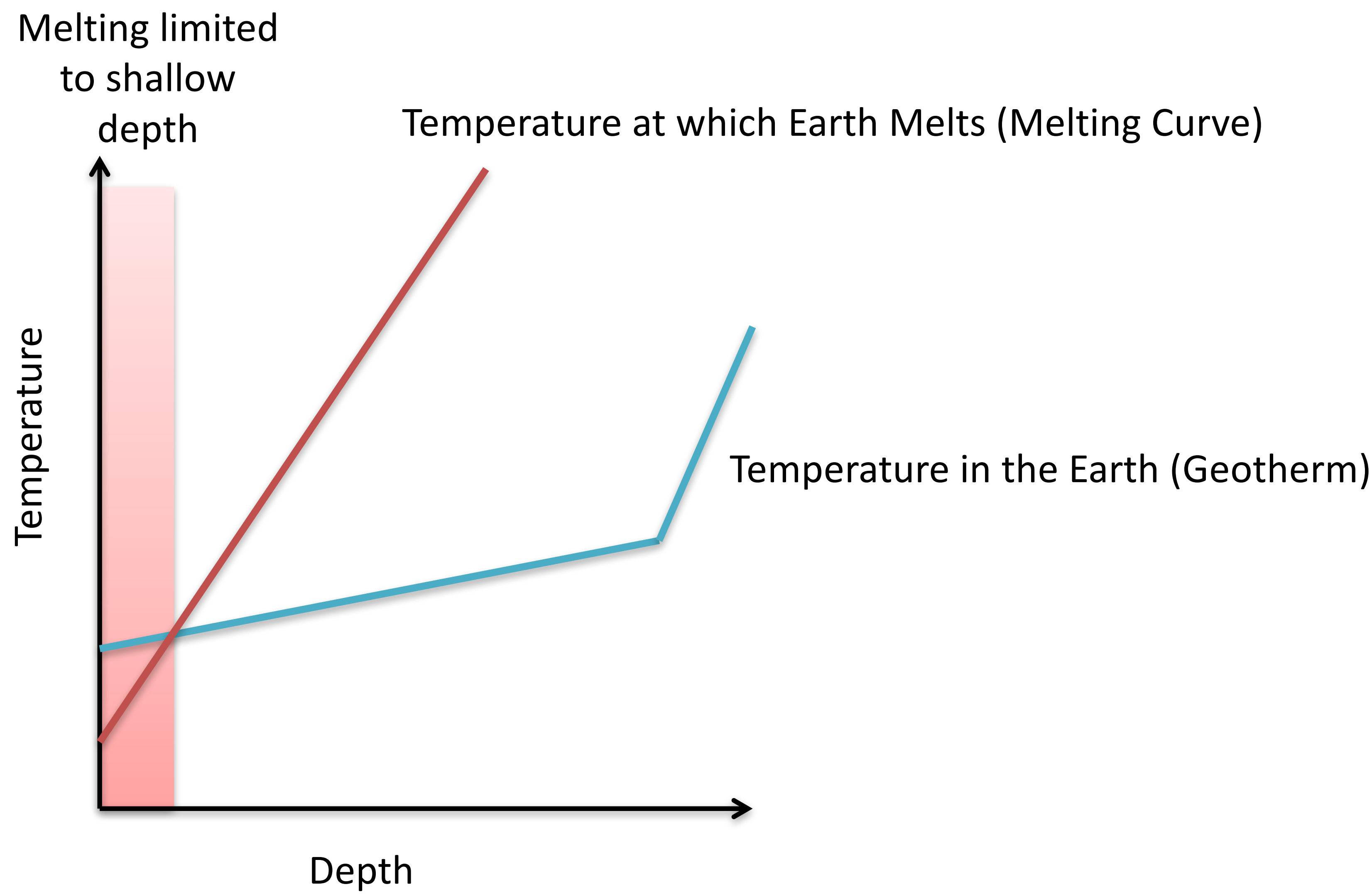


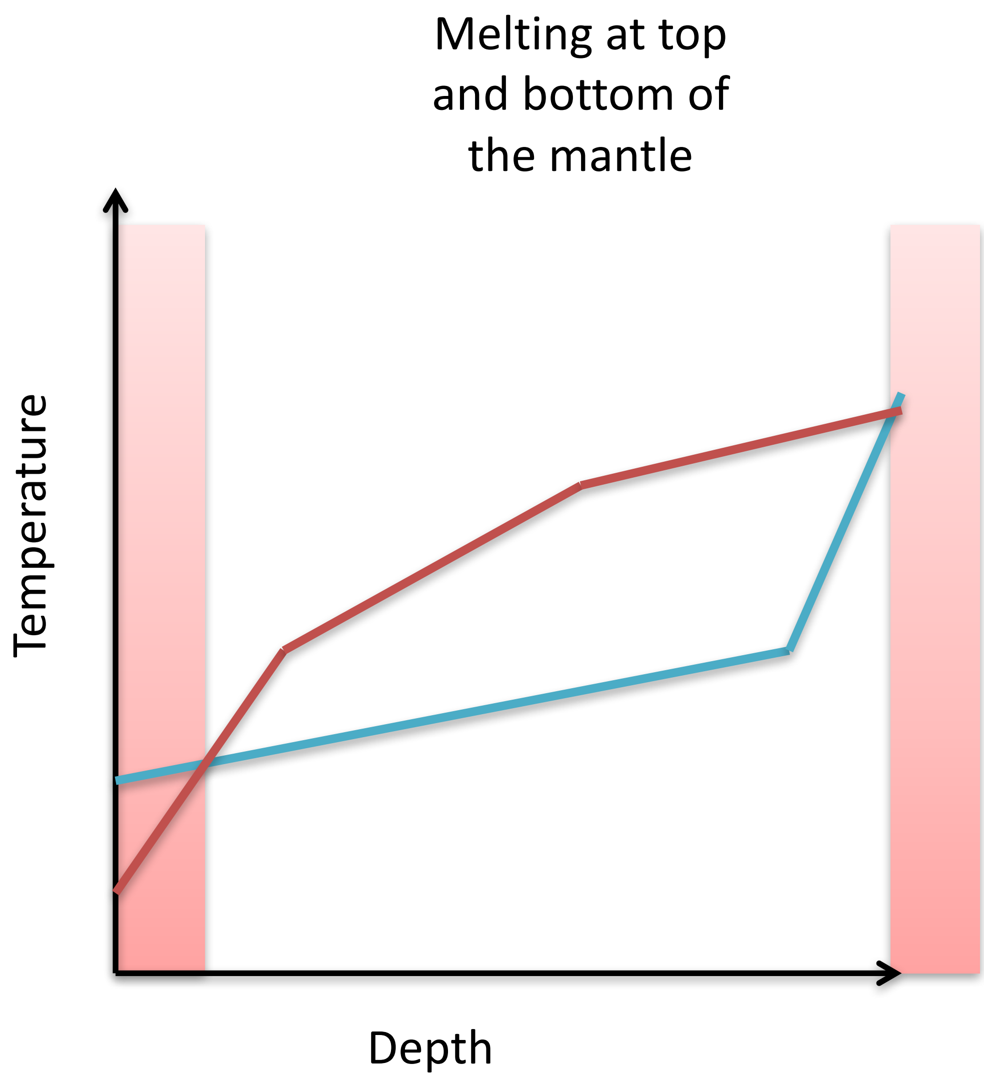
150 GPa



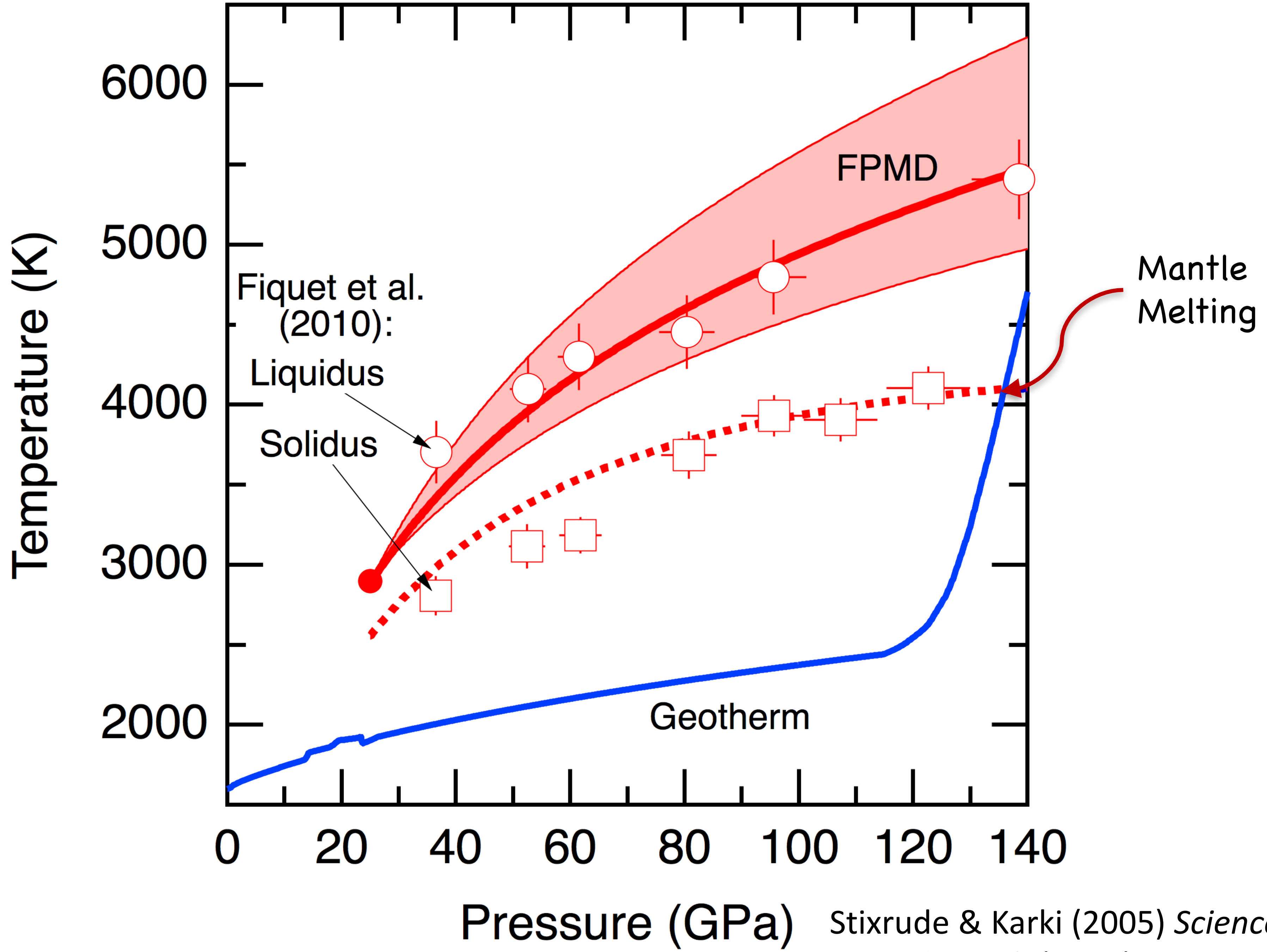
$CaMgSi_2O_6$

Ni et al. (2011) *GCA*


Melting limited to shallow depth
Temperature at which Earth Melts (Melting Curve)
Temperature in the Earth (Geotherm)
Temperature
Depth

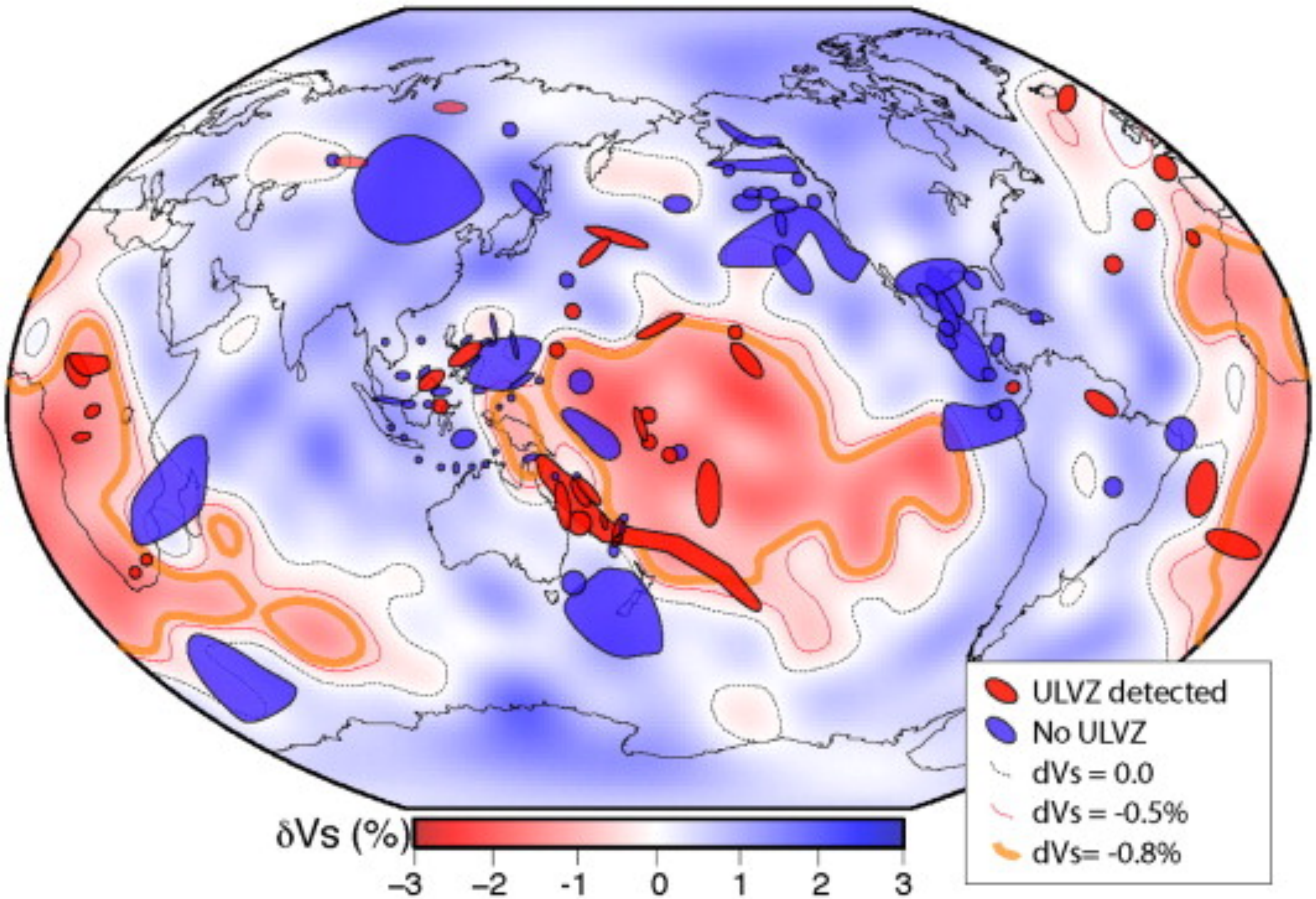


Melting at top and bottom of the mantle
Temperature
Depth



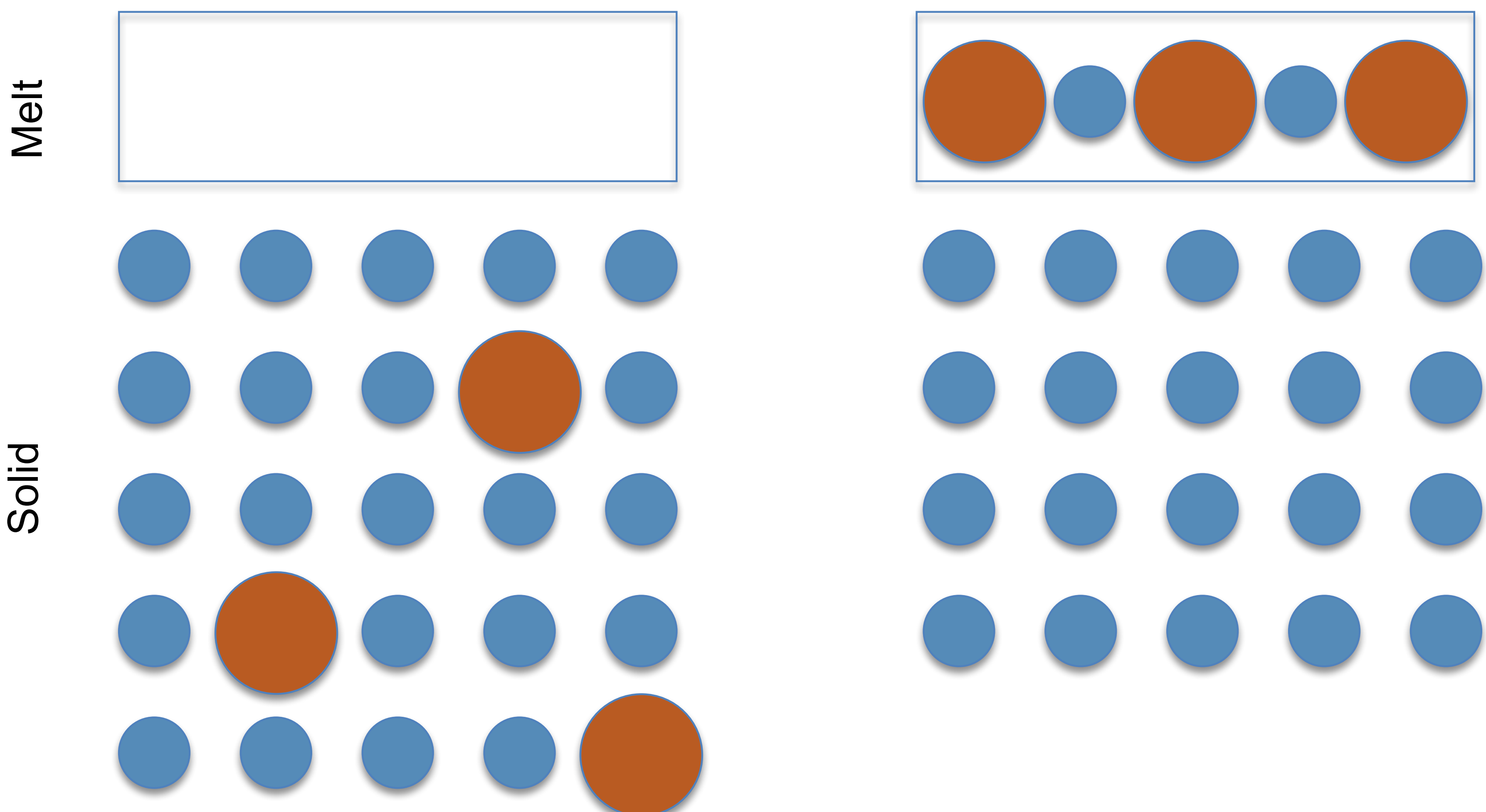
Stixrude & Karki (2005) *Science*
Stixrude et al. (2009) *EPSL*

Ultra-low velocity zones (ULVZ)



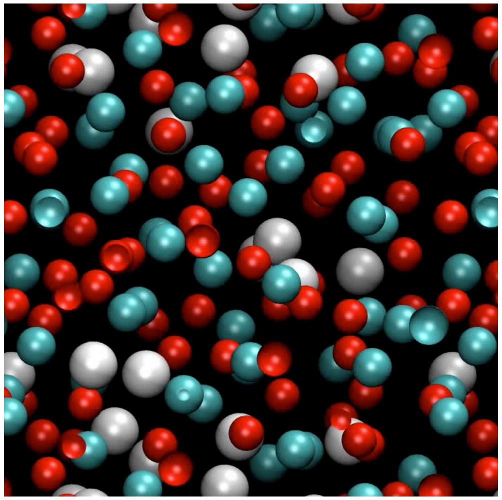
McNamara et al. (2010) EPSL

Liquids denser than solids?

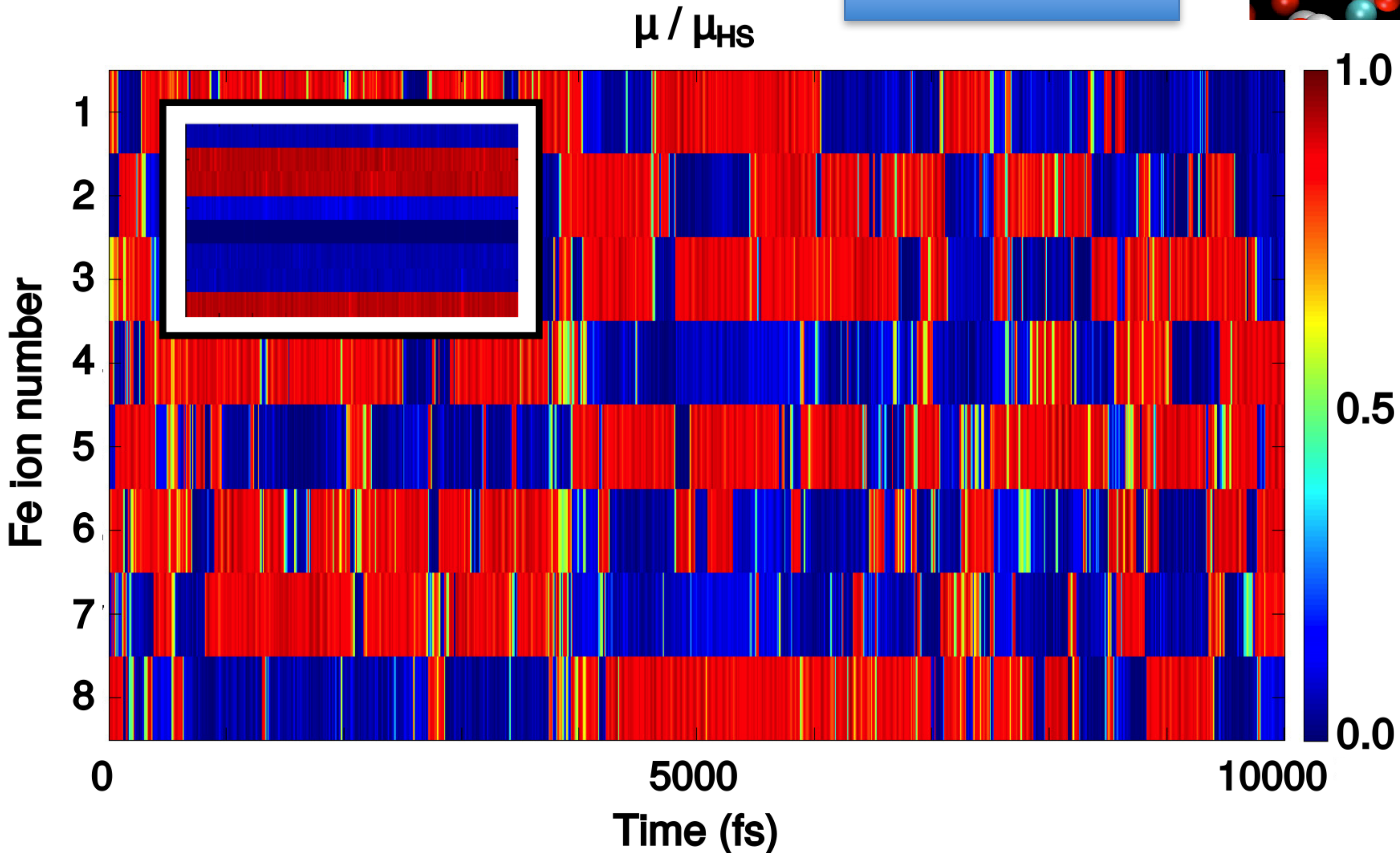


Holmstrom & Stixrude (2015) *PRL*; (2016) *PRB*

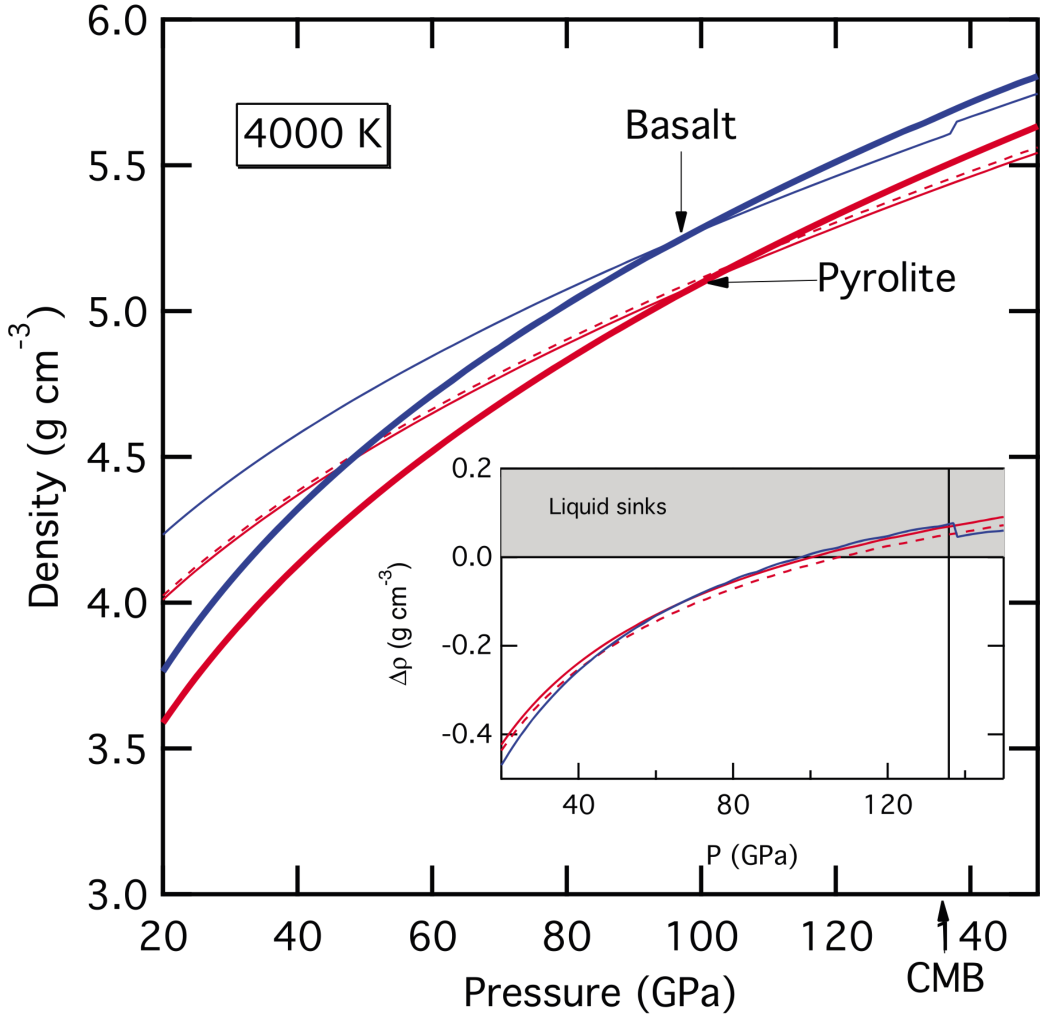
Magnetic Collapse via FPMD



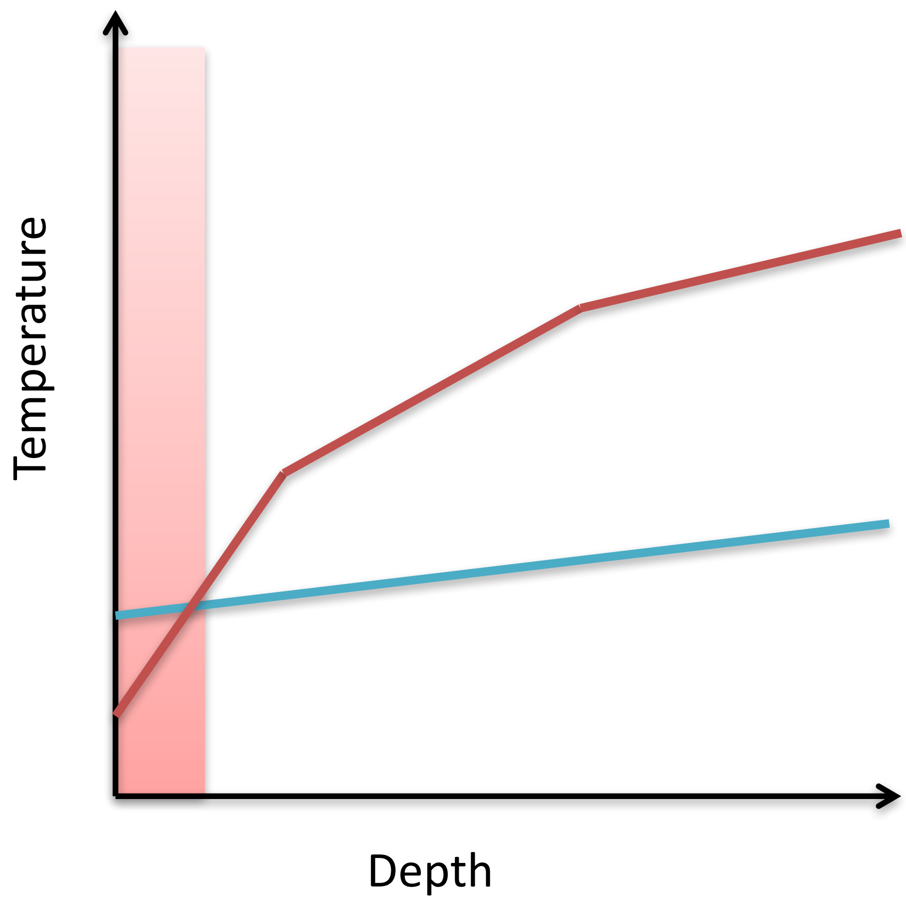
$Mg_{0.75}Fe_{0.25}O$



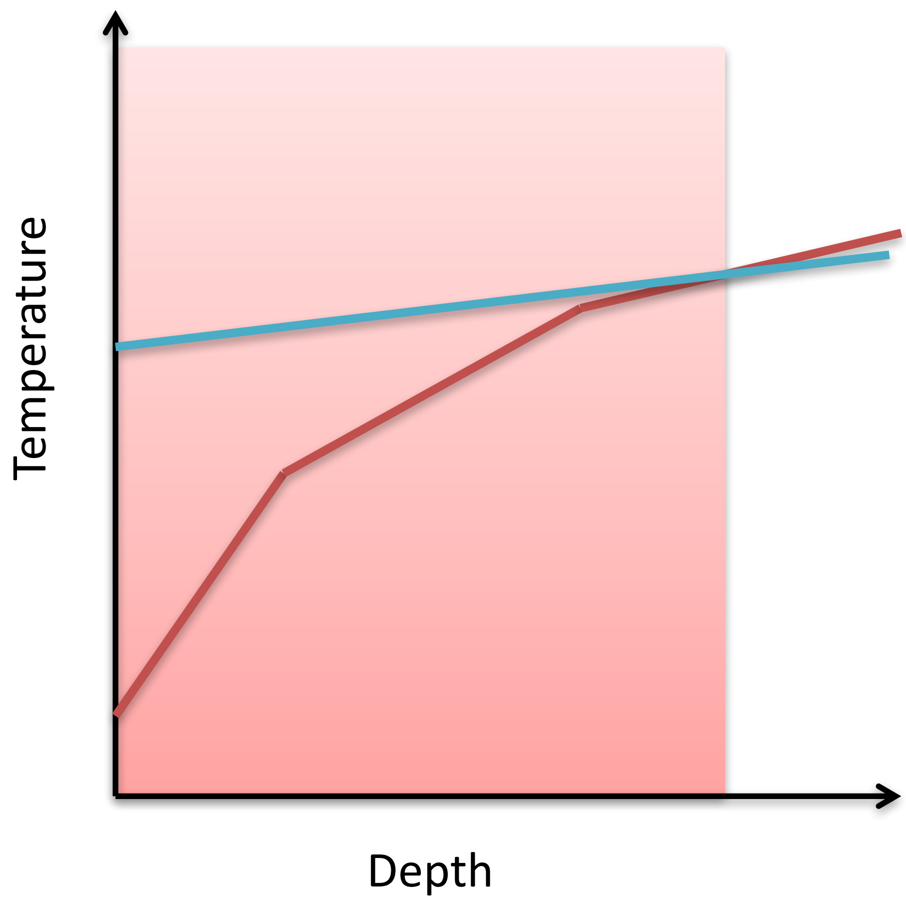
Partial melts denser than solids



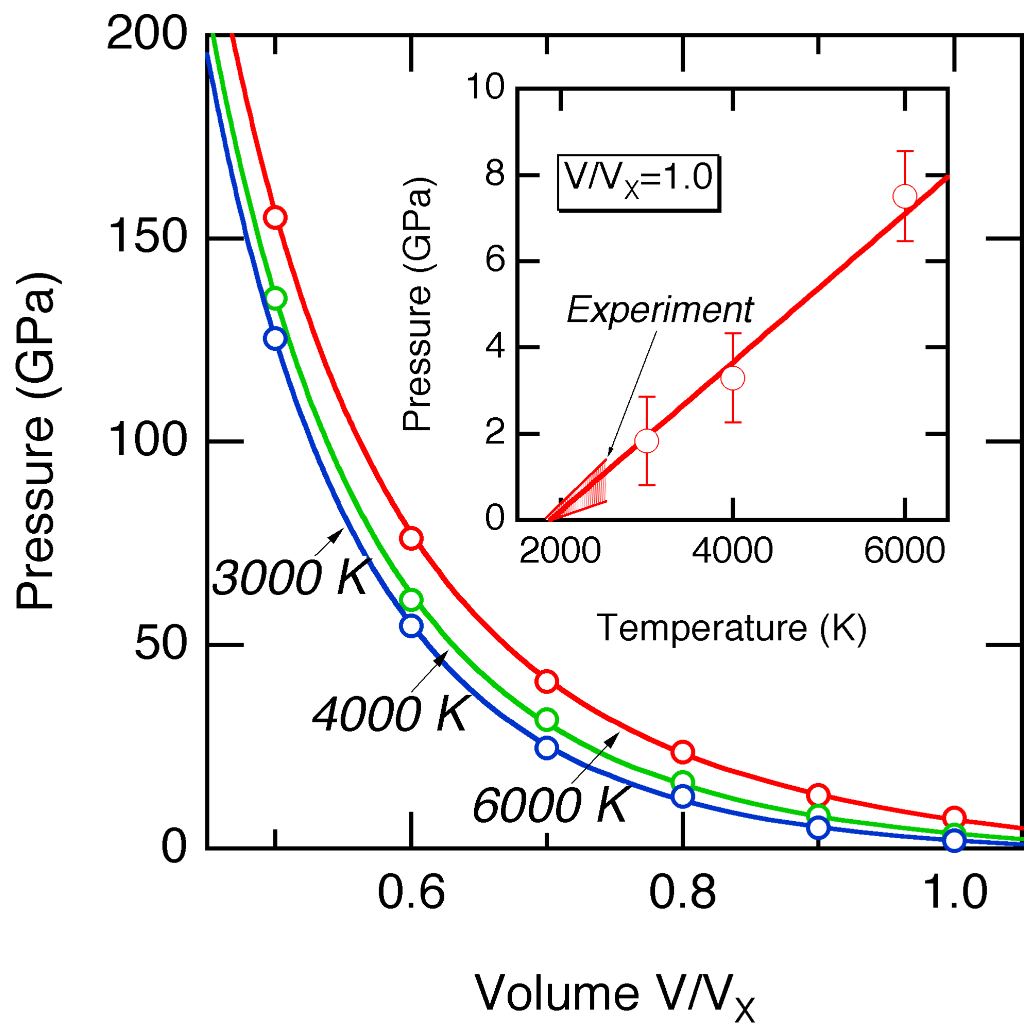
Muñoz Ramo & Stixrude (2014) *GRL*


Temperature
Depth

Melting in the Early Earth?



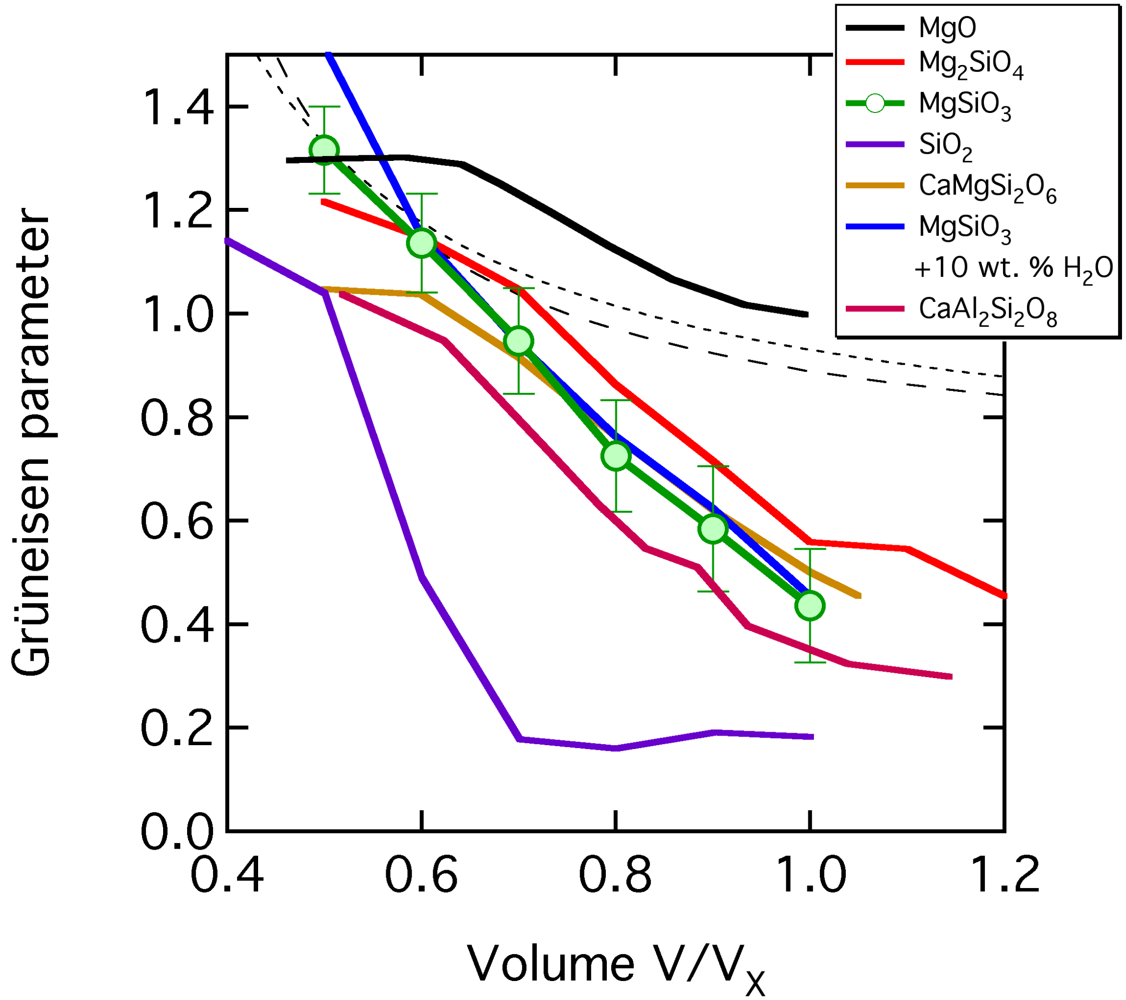
Equation of State



MgSiO$_3$

Stixrude & Karki (2005) *Science*

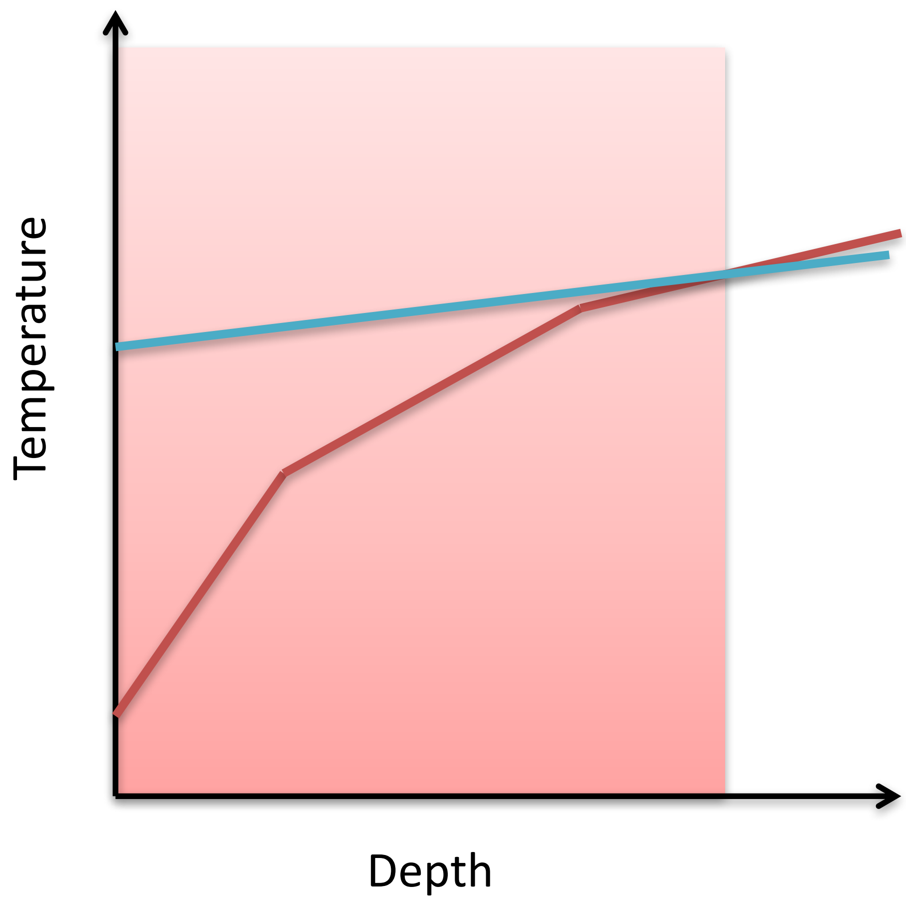
Grüneisen Parameter, γ

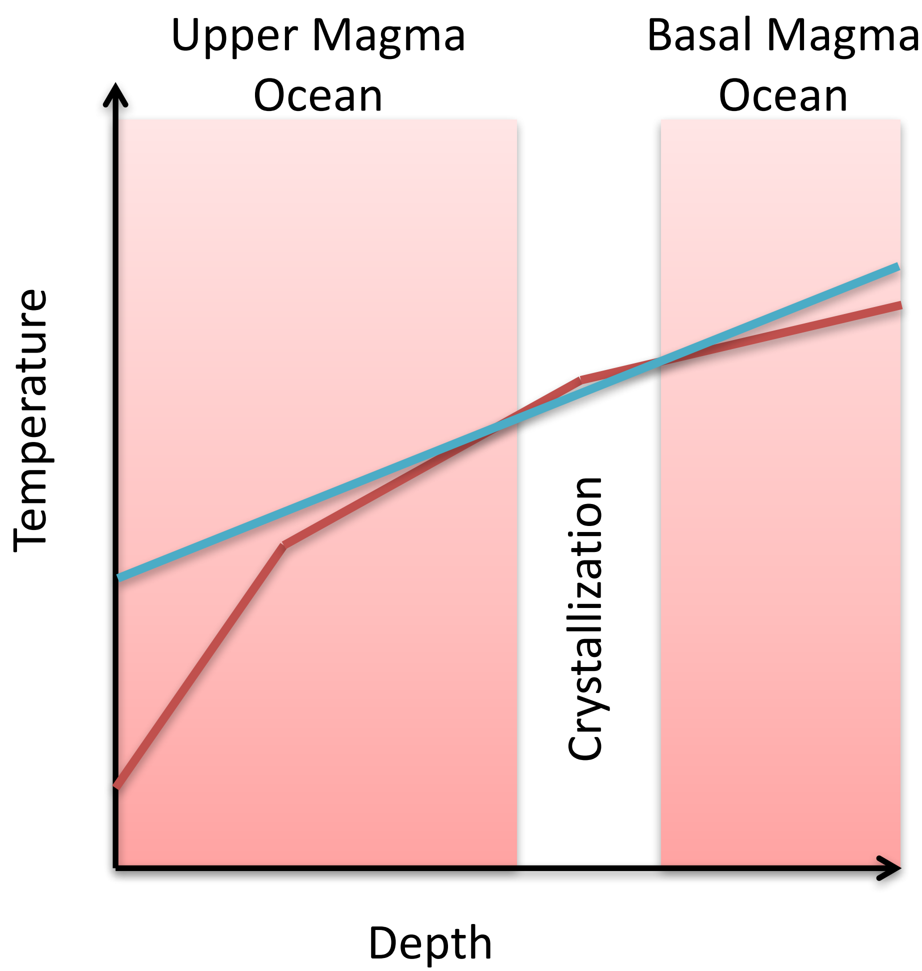


$$\left(\frac{\partial \ln T}{\partial P}\right)_S = \frac{\gamma}{K_S}$$

Stixrude & Karki (2005) Science; Karki et al. (2006) PRB; Karki et al. (2007) PRB; de Koker et al. (2008) GCA; Mookherjee et al. (2008) Nature; Sun et al. (2011) GCA; de Koker (2010) GCA

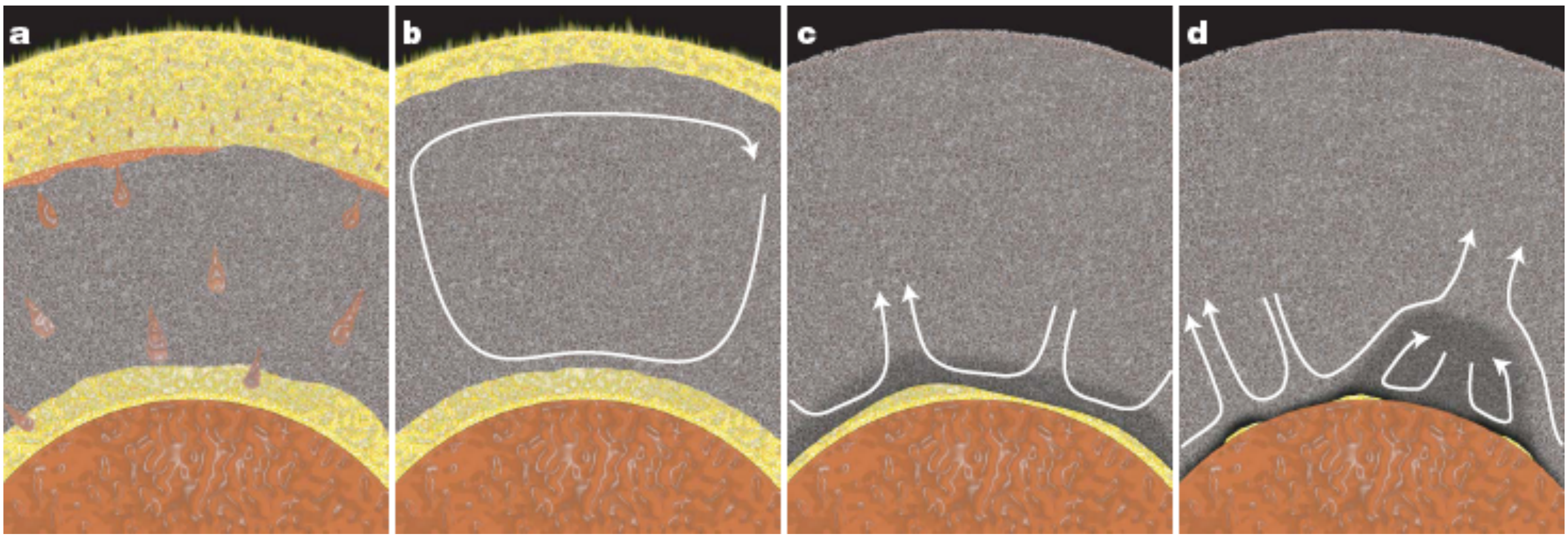
Melting in the Early Earth?





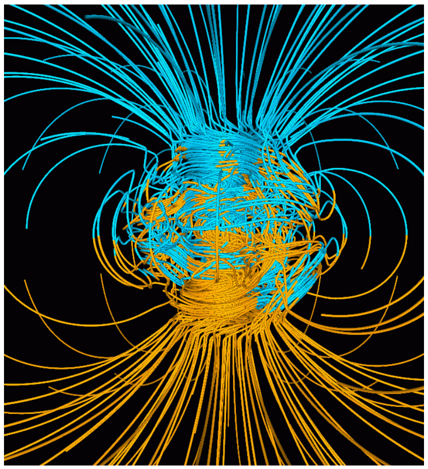
Upper Magma Ocean
Basal Magma Ocean
Temperature
Crystallization
Depth

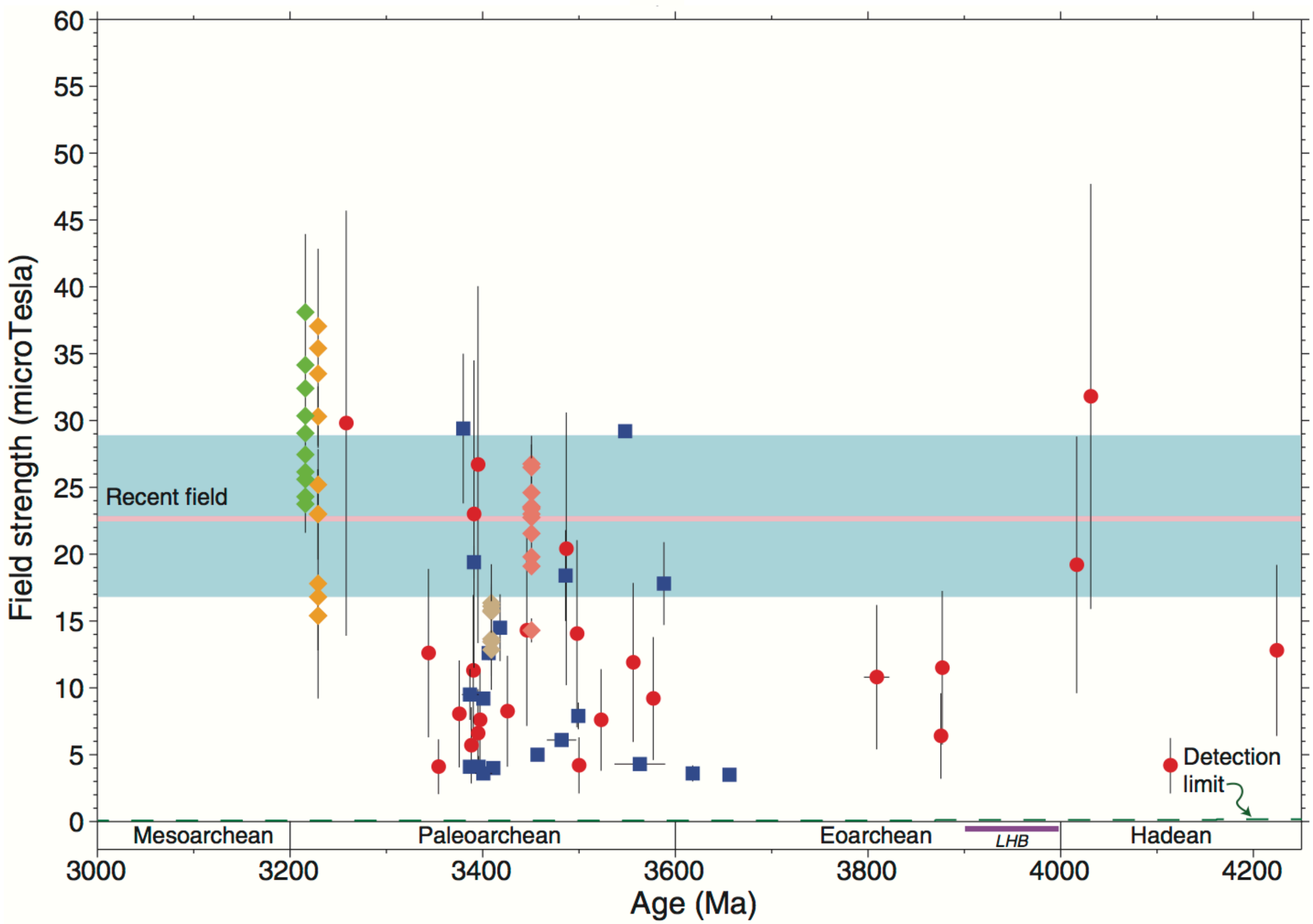
Basal Magma Ocean



Labrosse et al. (2007) Nature

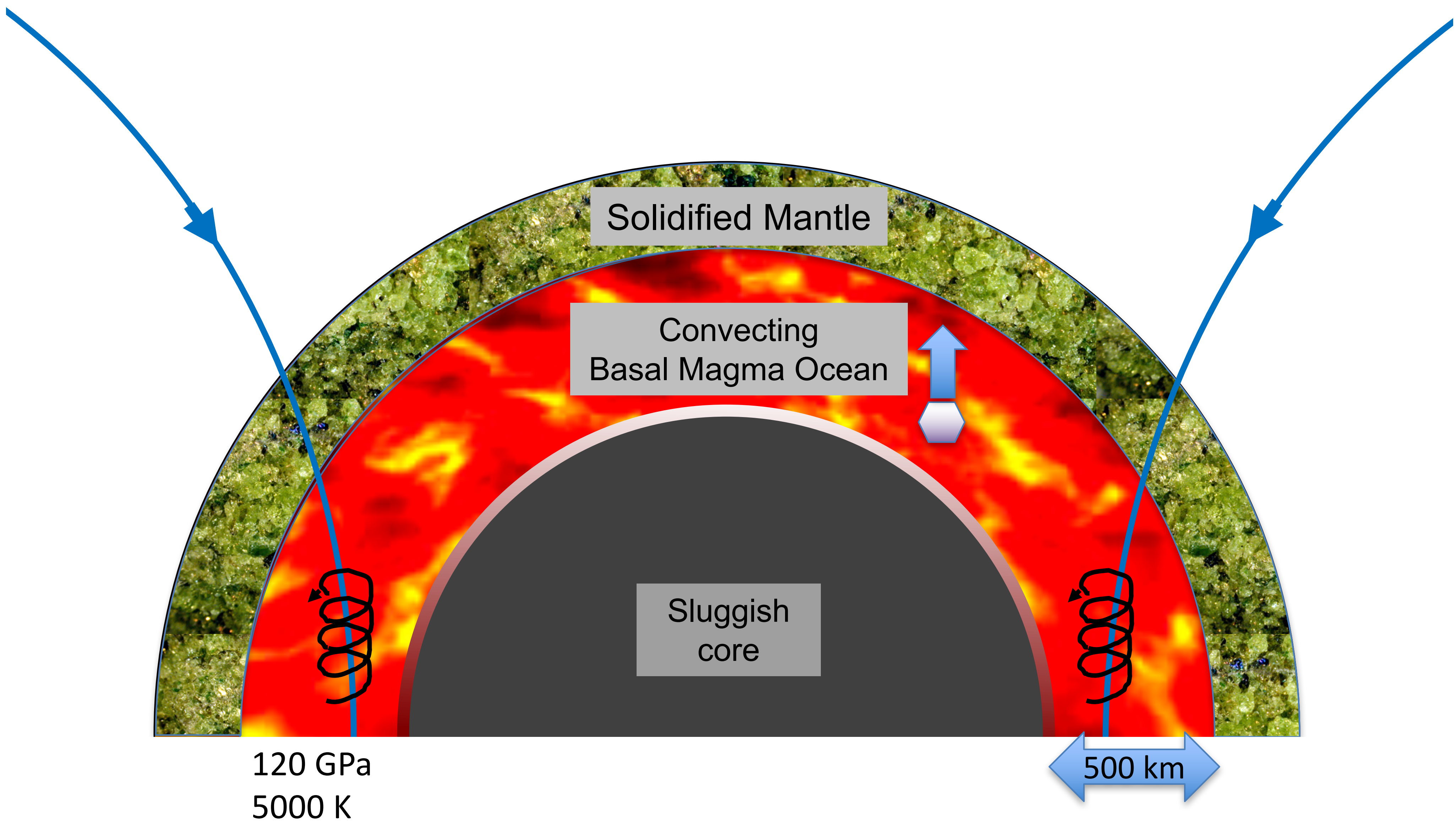
Earth's Ancient Magnetic Field





Glatzmaier & Roberts (1995) Nature
Tarduno et al. (2015) Science

Hypothesis: Silicate Dynamo



Ziegler & Stegman (2013) G³

Magnetic Reynolds Number

$$\frac{\partial \vec{B}}{\partial t} = \frac{1}{\mu_0 \sigma} \nabla^2 \vec{B} + \nabla \times (\vec{v} \times \vec{B})$$

$$R_m = v L \mu_0 \sigma$$

$$R_m = 10 \left(\frac{v}{1\ \mathrm{mm/s}}\right) \left(\frac{L}{500\ \mathrm{km}}\right) \left(\frac{\sigma}{10{,}000\ \mathrm{S/m}}\right)$$

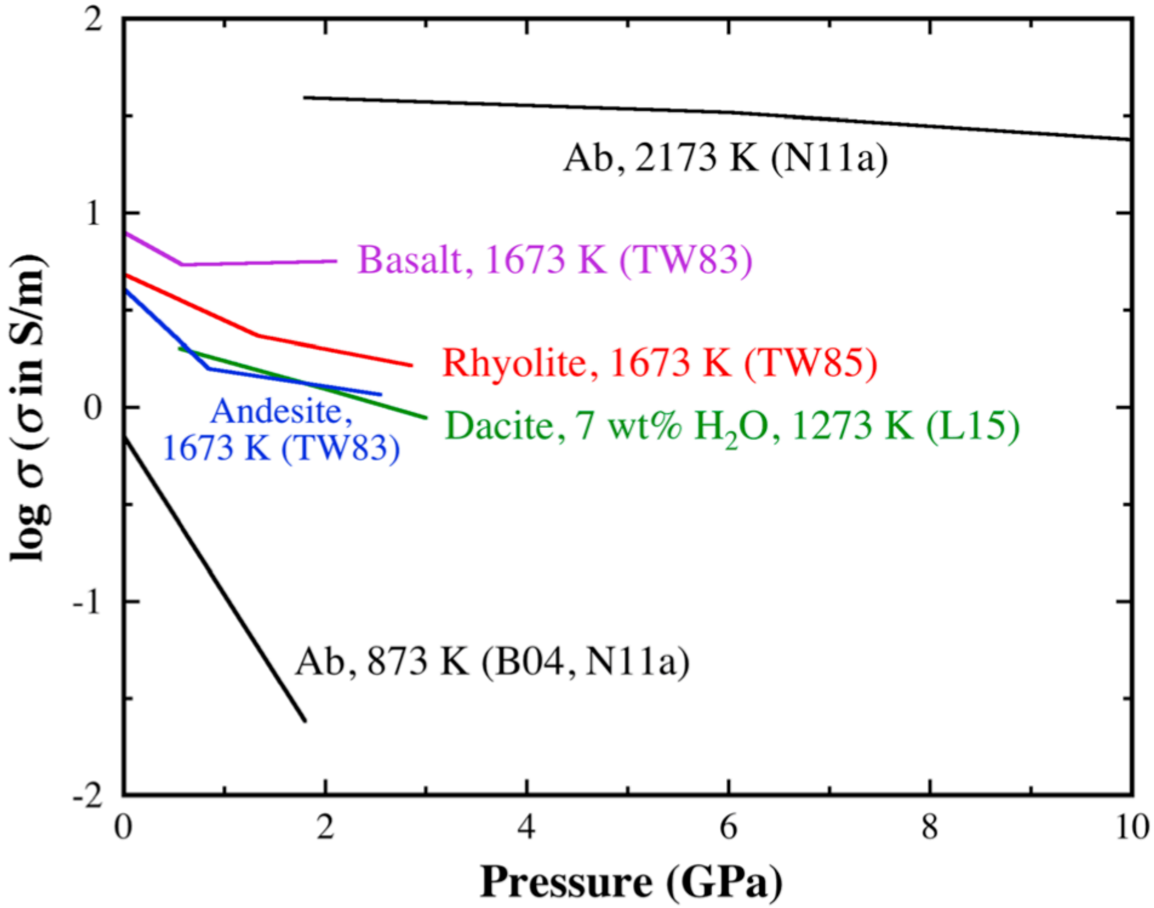
$$v = \left(\frac{Lq}{\rho H_T}\right)^{1/3}$$

$$\frac{B^2}{2\mu_0} = c f_{ohm} \rho v^2$$

Christensen (2010) Space Sci. Rev.

Electrical conductivity of silicate liquids

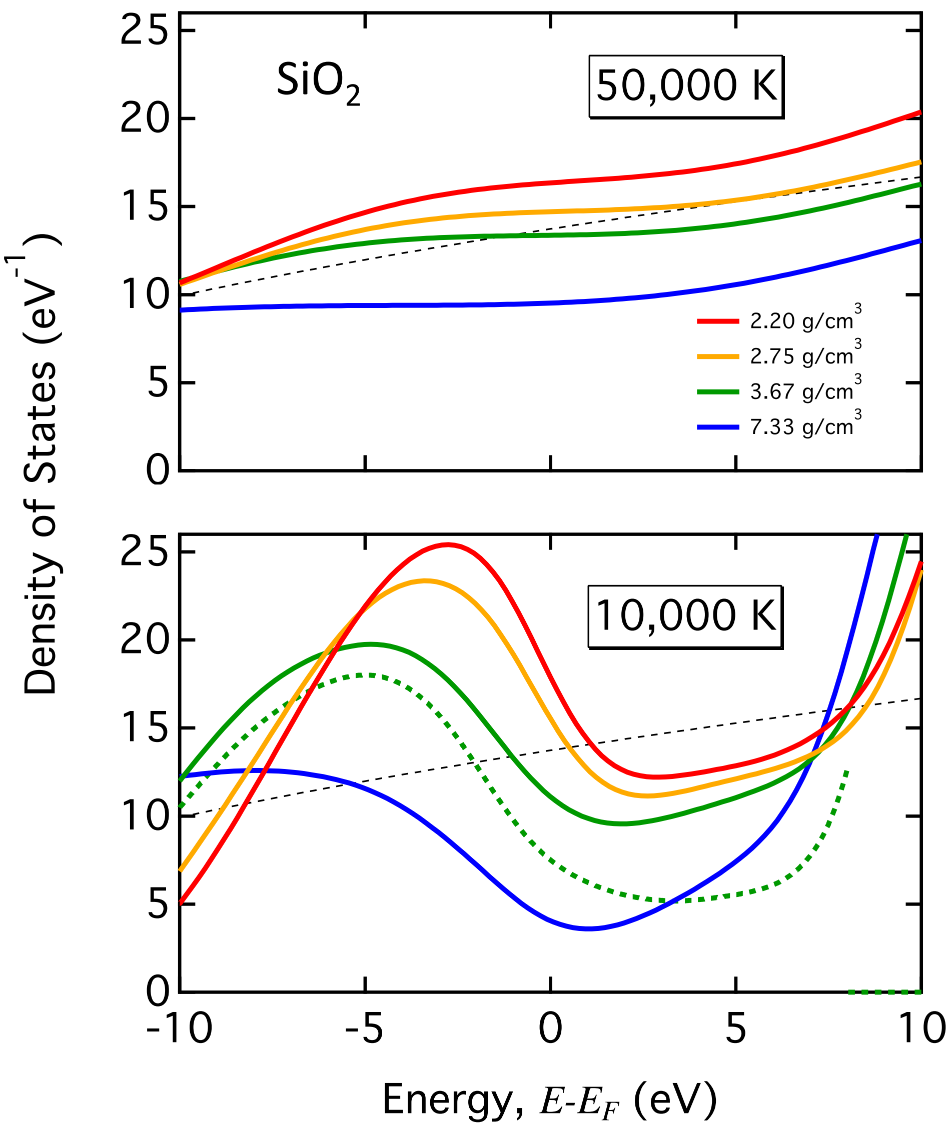
At low pressure and temperature:
small and *ionic*



Ni et al. (2015) Revs. Geophys.

Electrical conductivity of silicate liquids

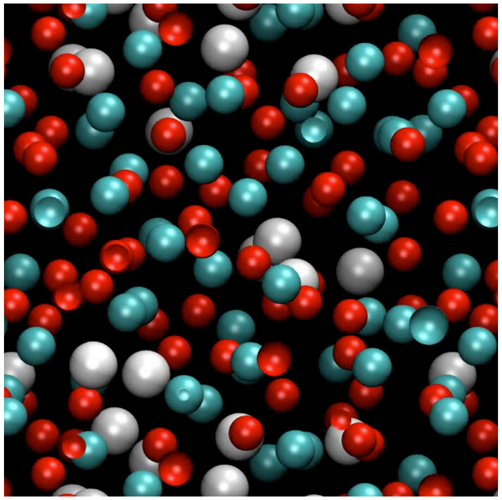
At high pressure and temperature:
large and *electronic*



Scipioni et al. (2017) PNAS

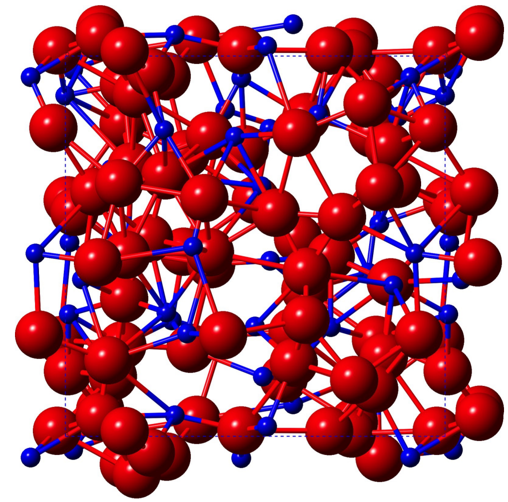
Systems

(Mg,Fe)O



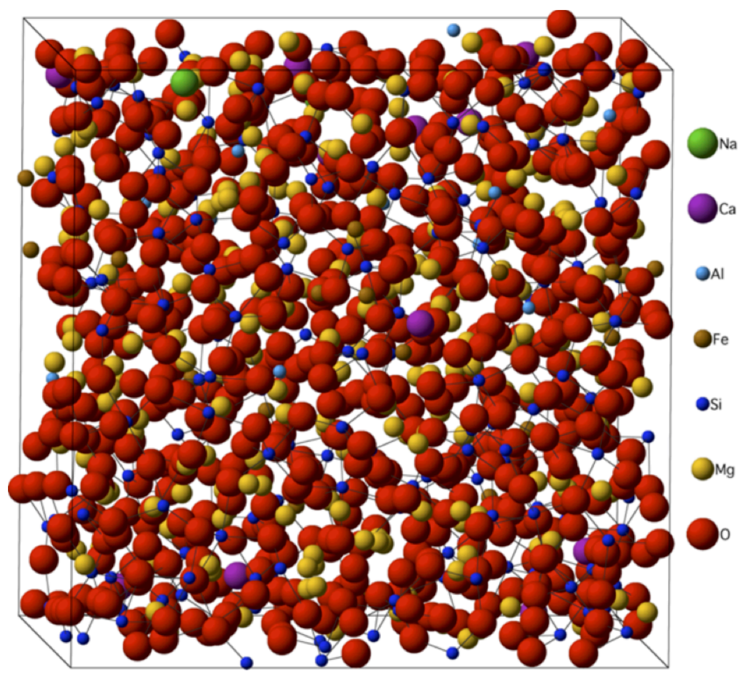
Holmstrom et al. (2018) EPSL

SiO_2



Scipioni et al. (2017) PNAS

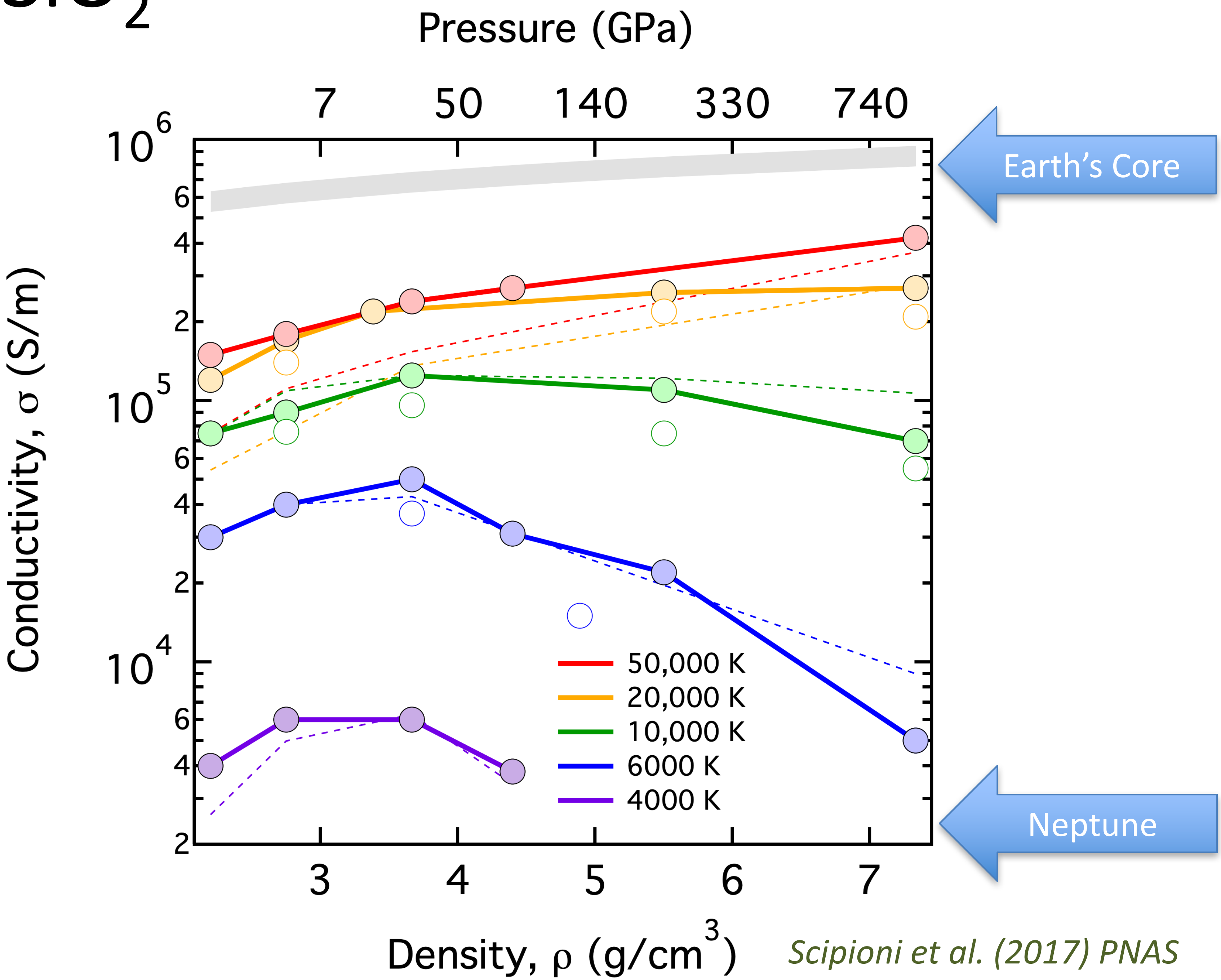
Atom	Number	Oxides	DMM
Si	178	44.93	44.93
Mg	229	38.78	38.82
Fe	28	8.45	8.56
Ca	14	3.30	3.18
Al	20	4.28	4.37
Na	2	0.26	0.13
O	658	-	-



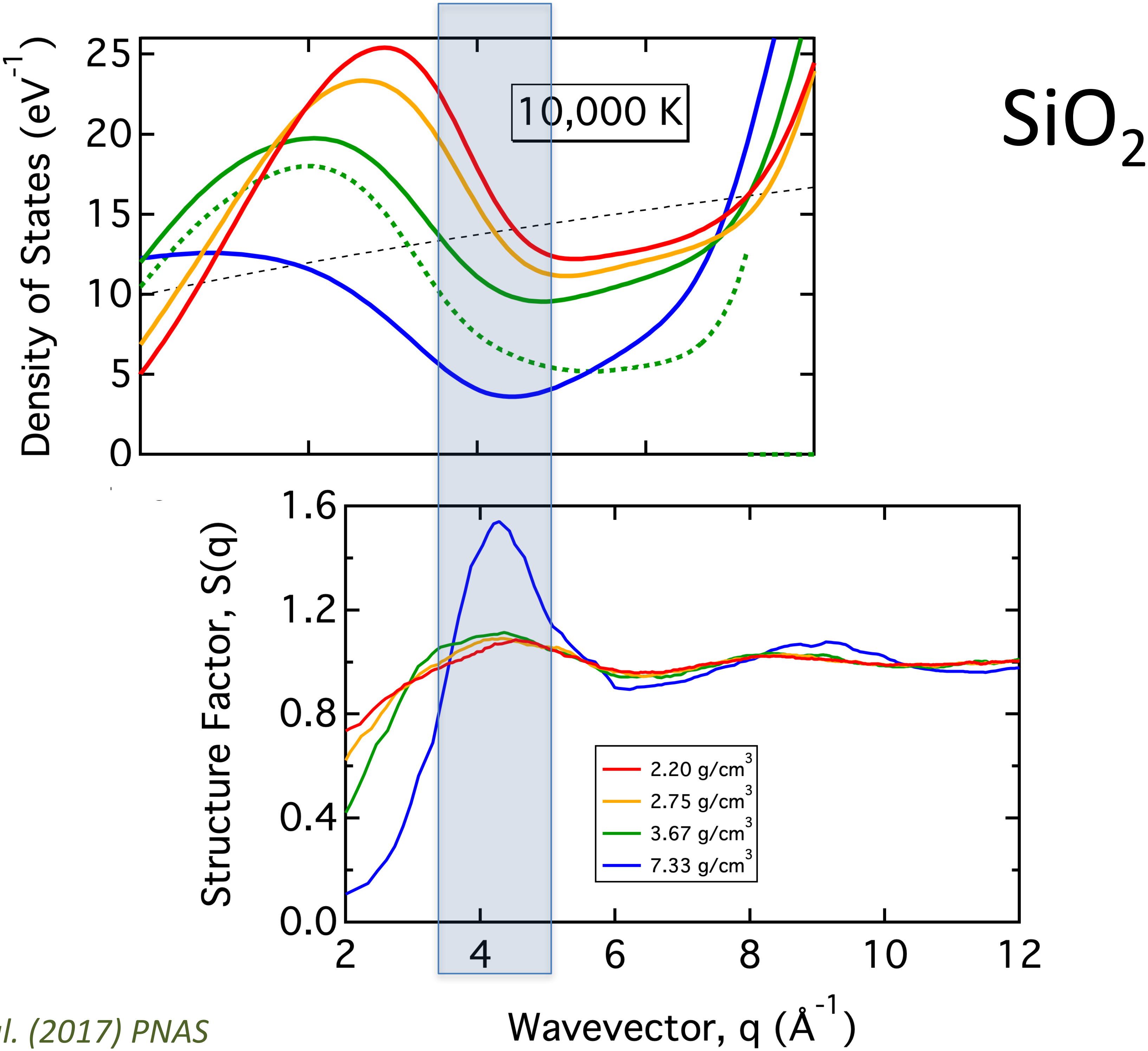
~Bulk silicate Earth

Scipioni et al. (2018) In Prep

SiO_2

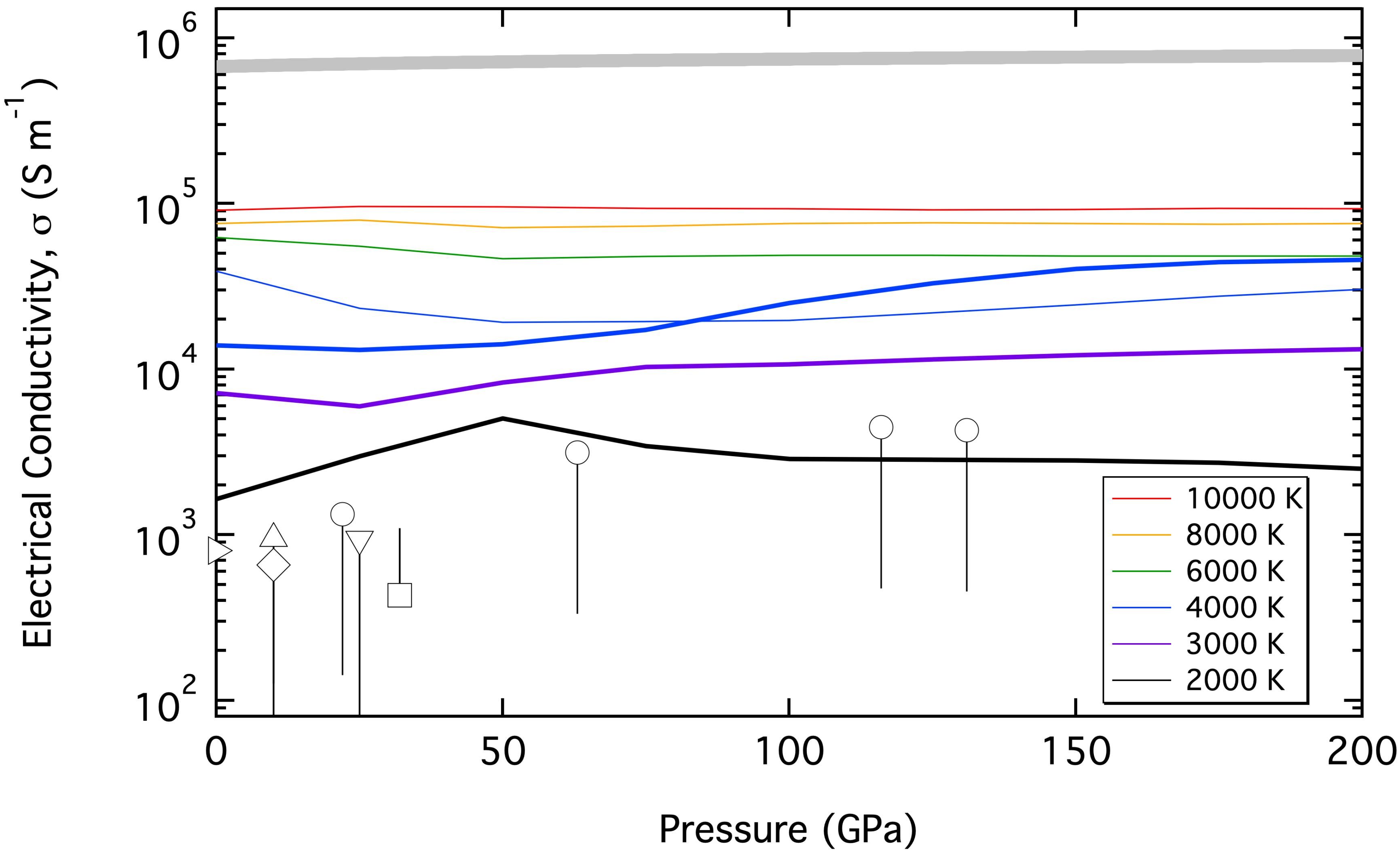


Scipioni et al. (2017) PNAS



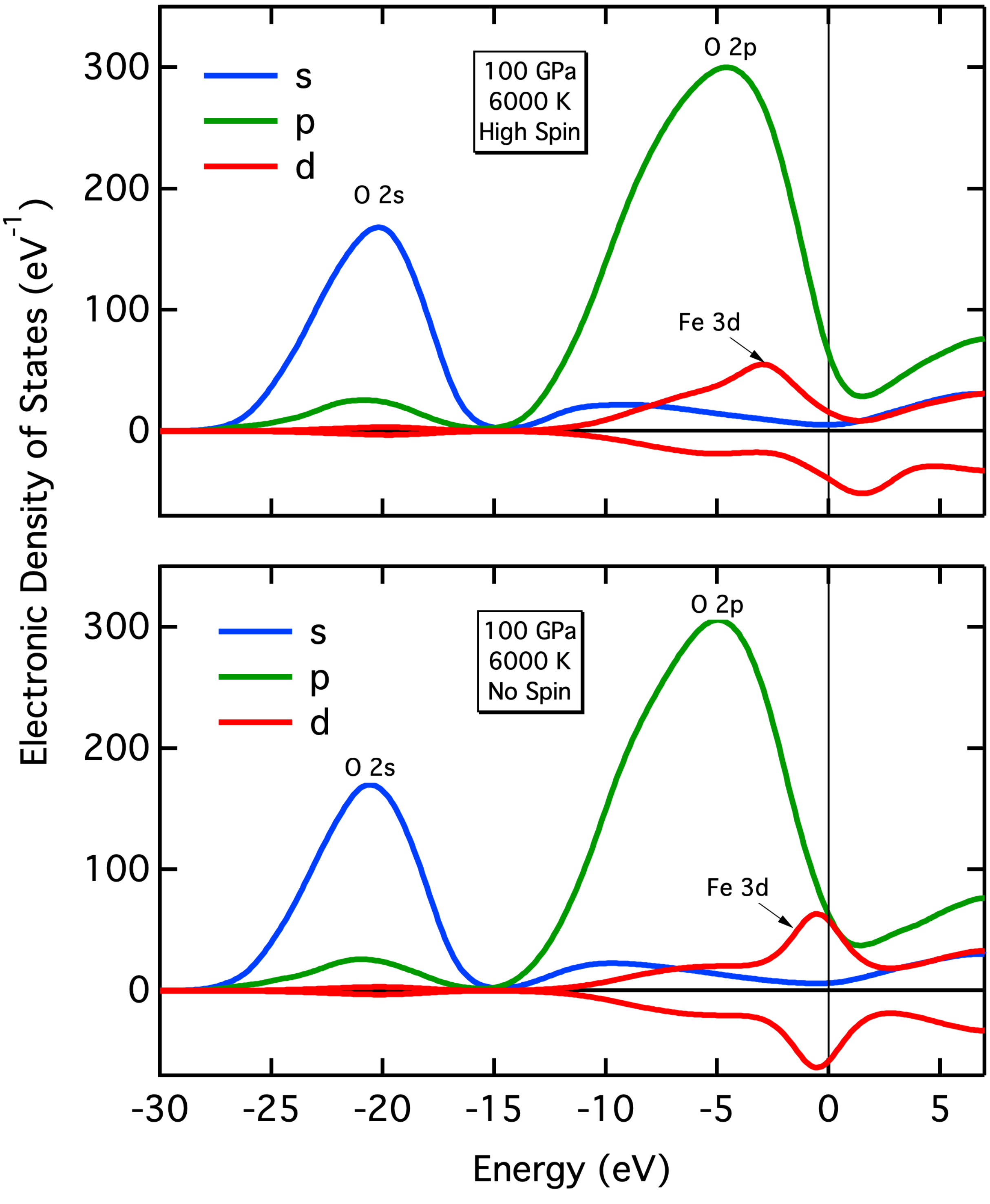
Scipioni et al. (2017) PNAS

(Mg,Fe)O

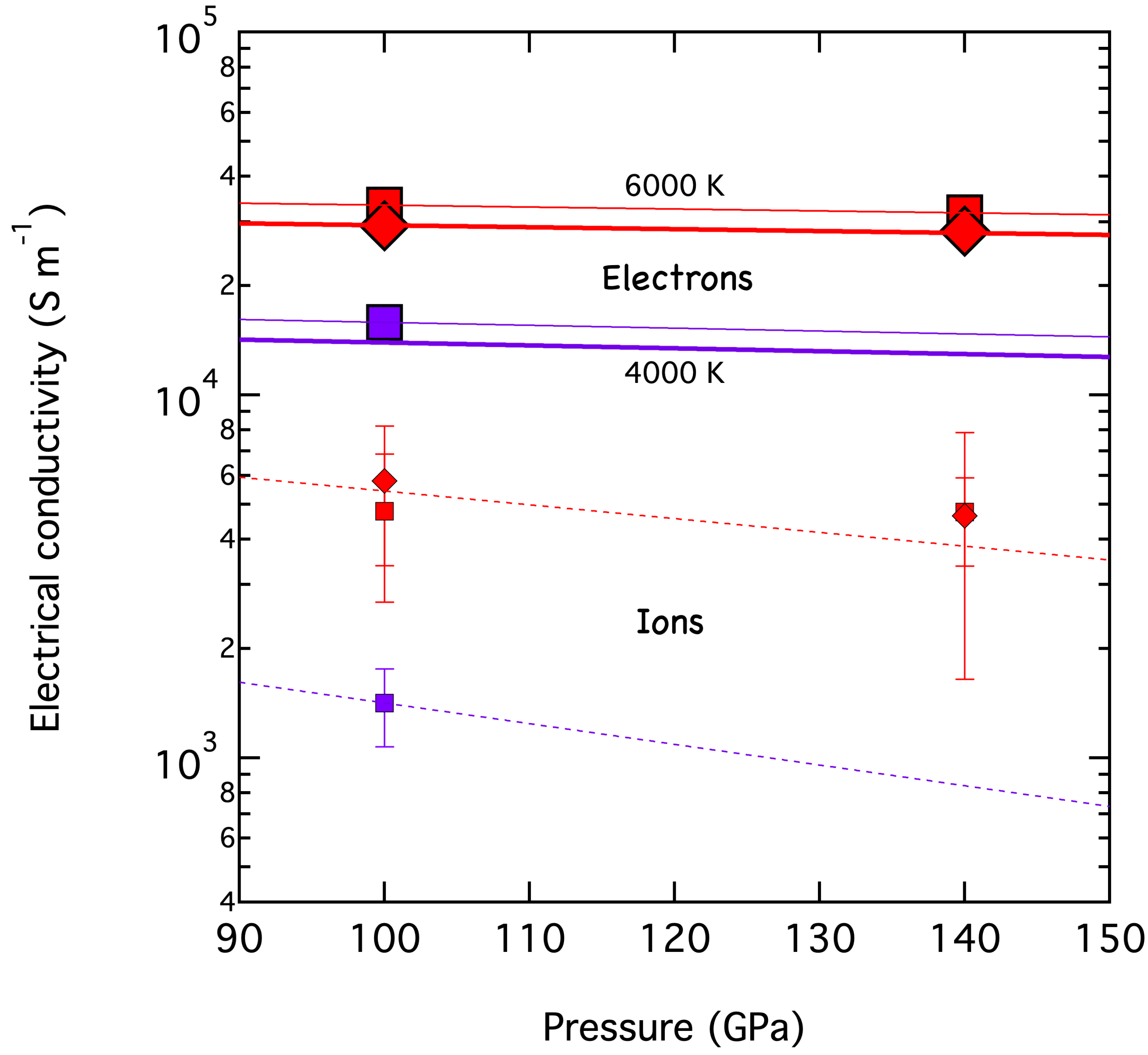


Holmström et al. (2018) EPSL

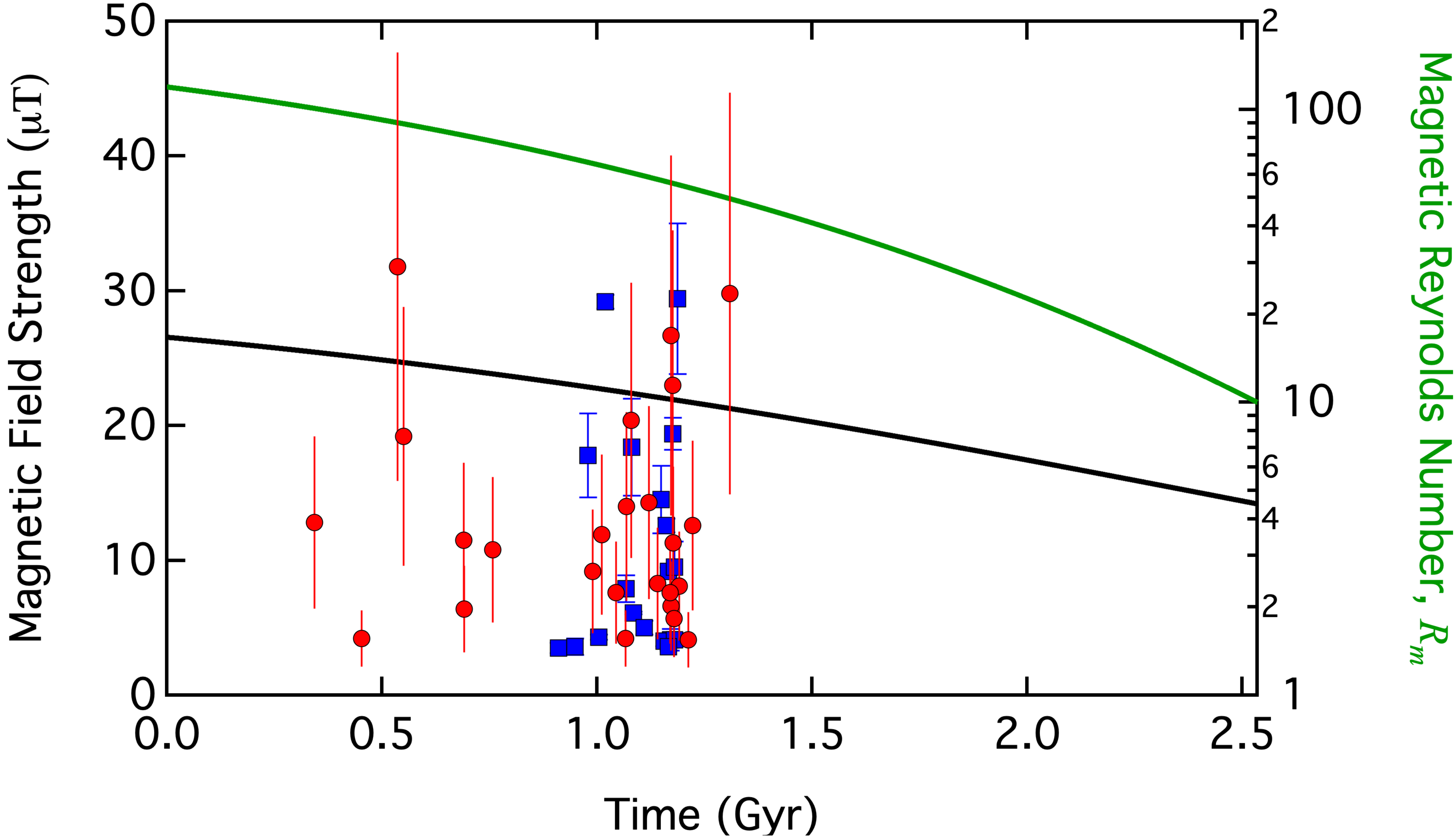
Bulk Silicate Earth

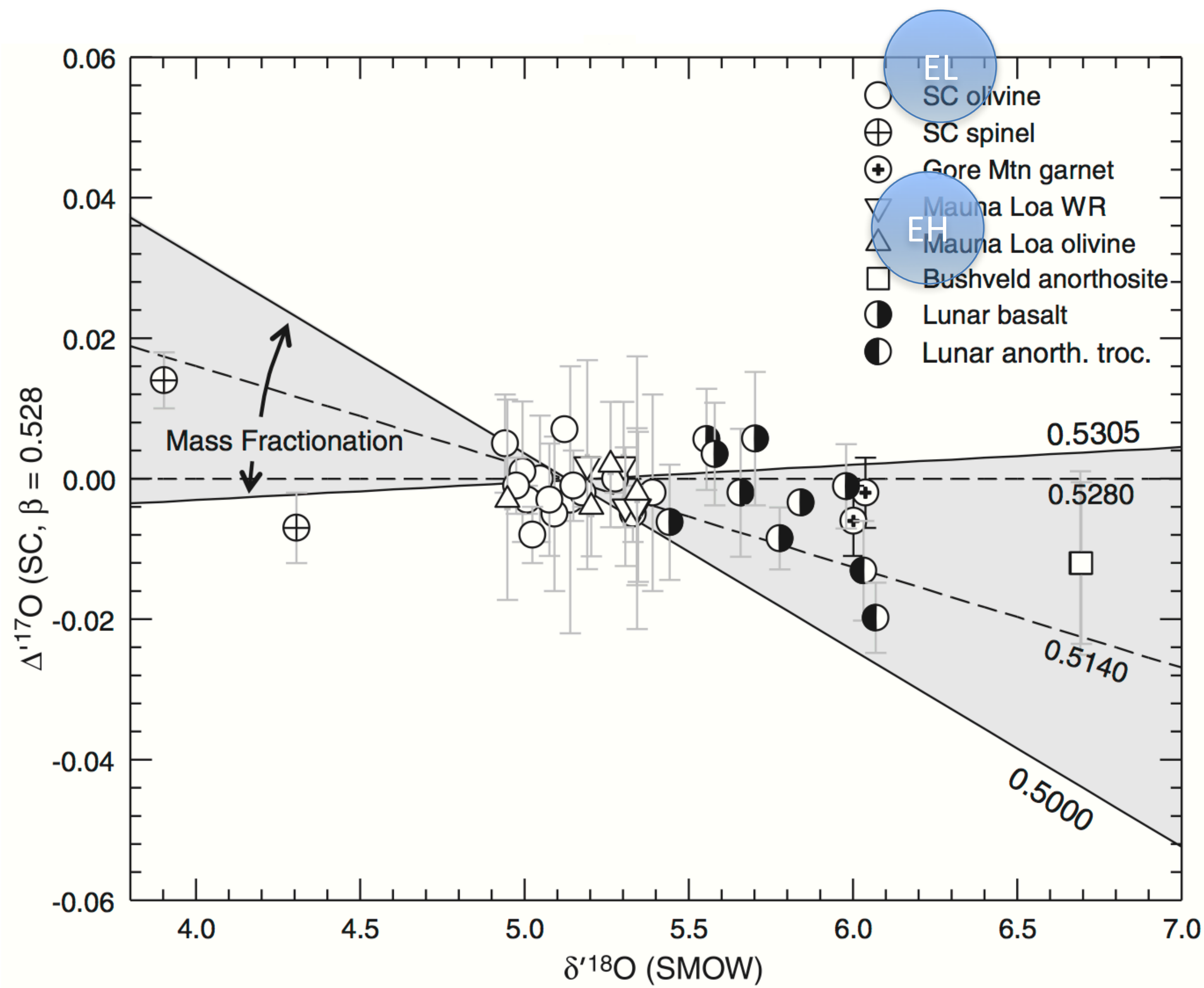


Bulk Silicate Earth



Silicate Dynamo



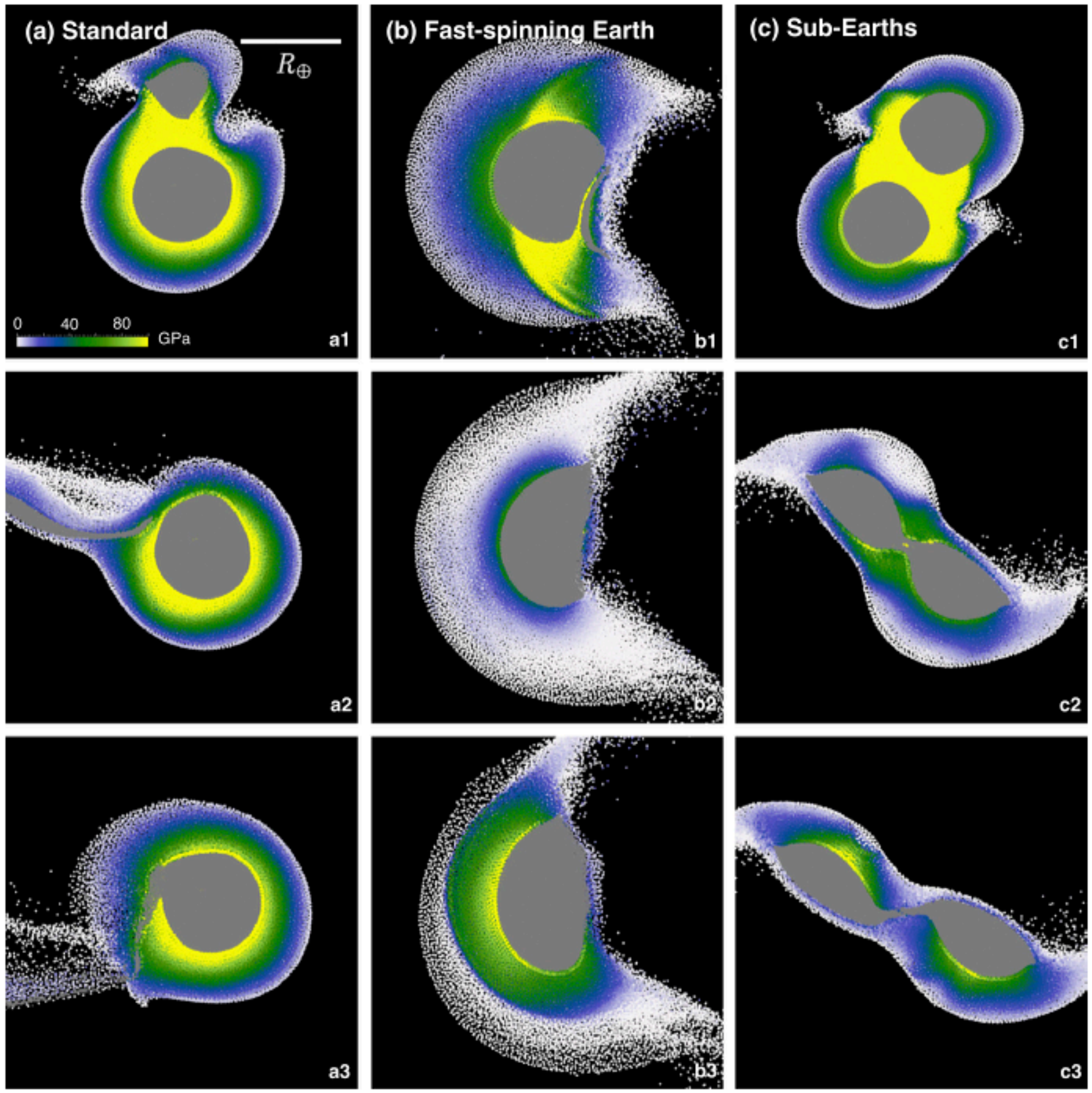


Young et al. (2016) Science

Canonical
Canup (2004)

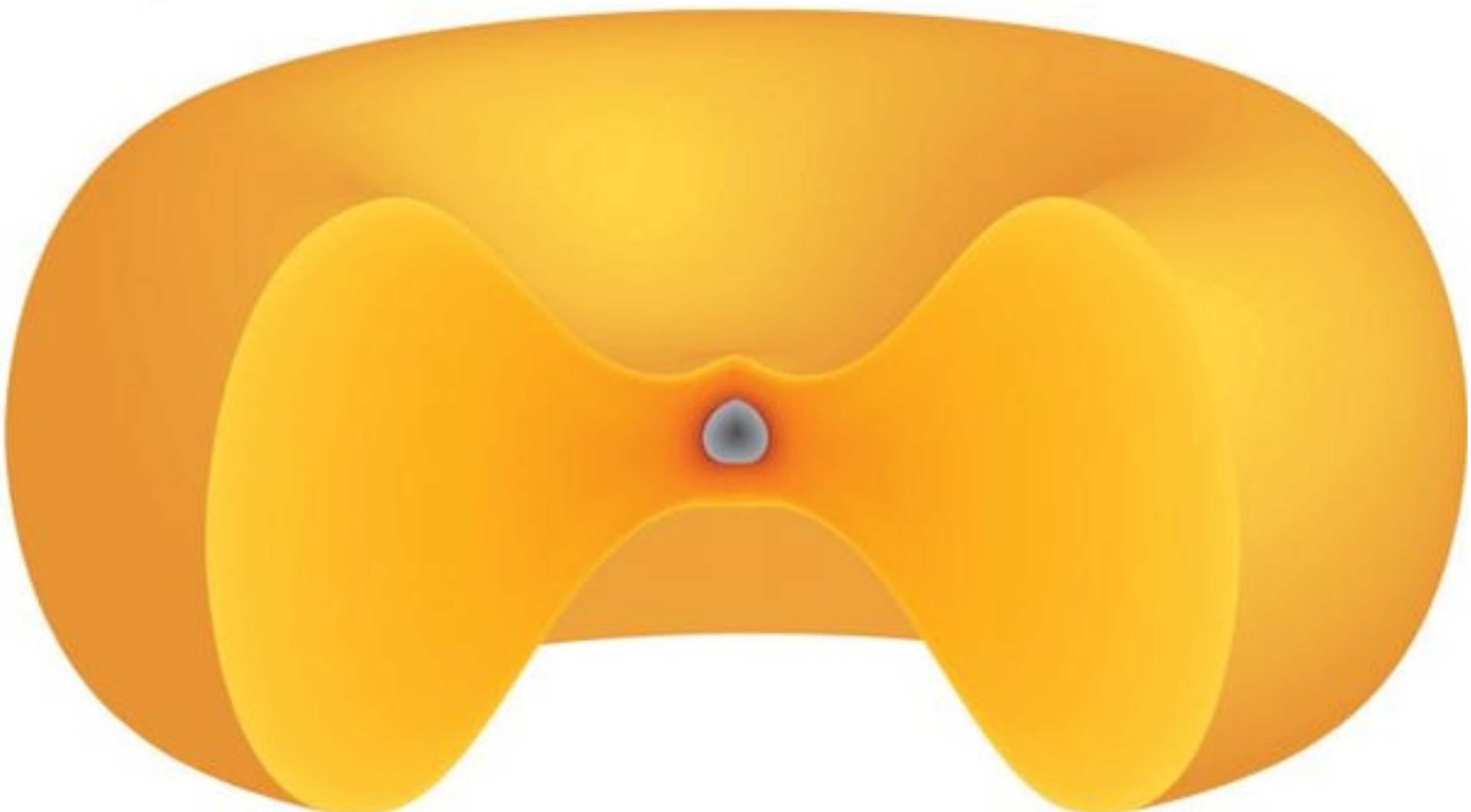
Fast-Spin
Cuk & Stewart
(2012)

Sub-Earths
Canup (2012)

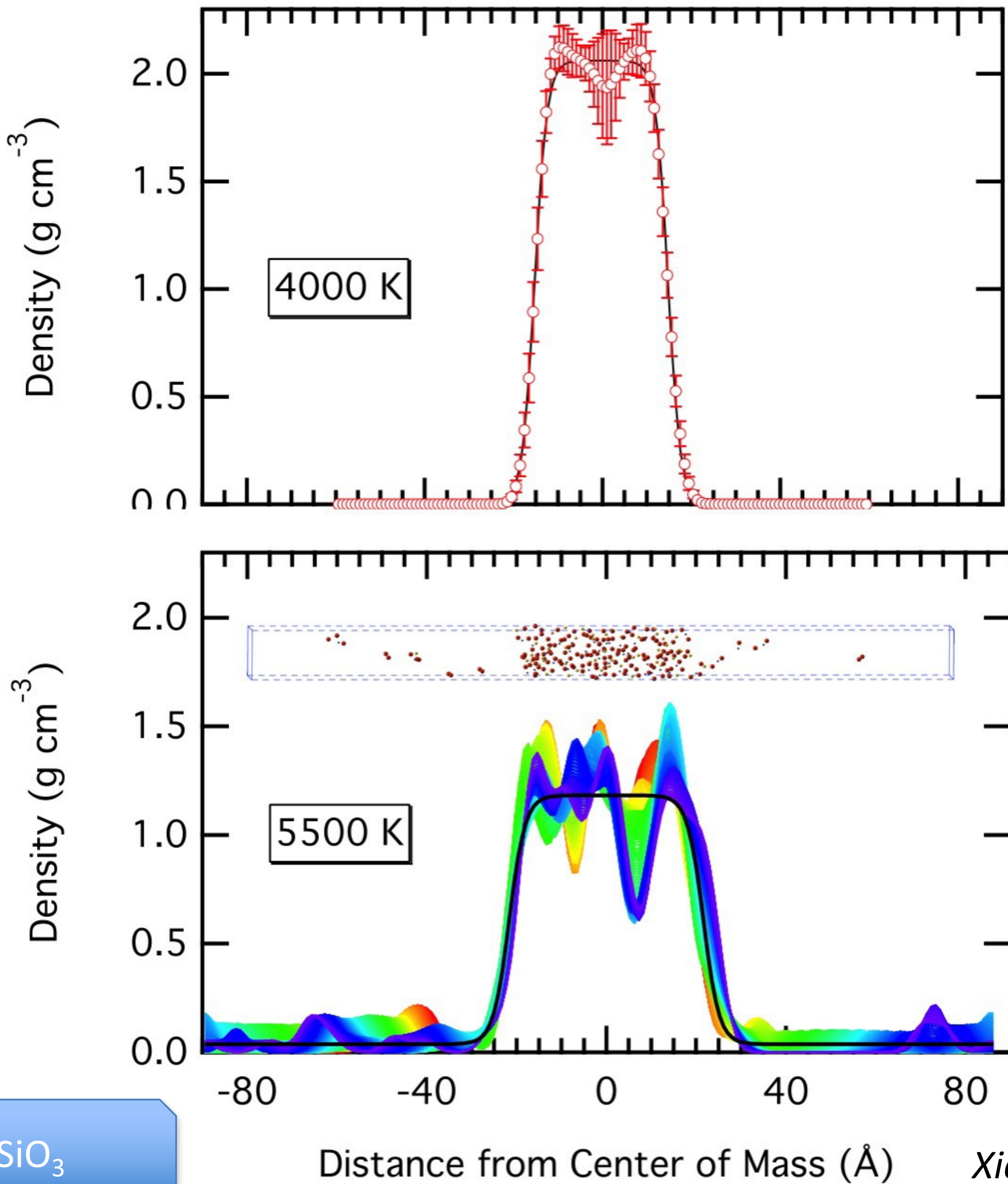


Nakajima & Stevenson (2015) EPSL

Synestia

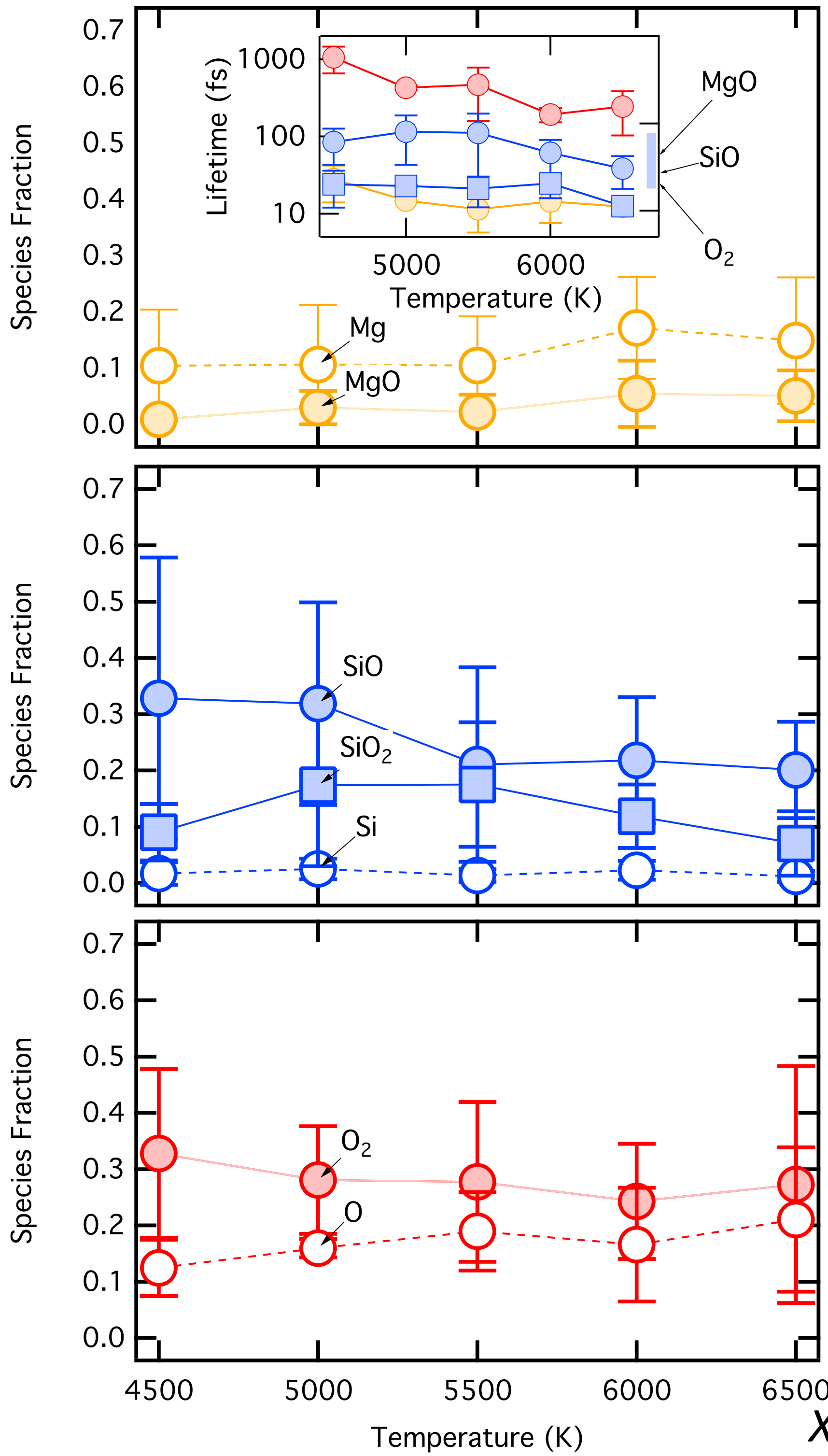


Lock and Stewart (2017) JGR

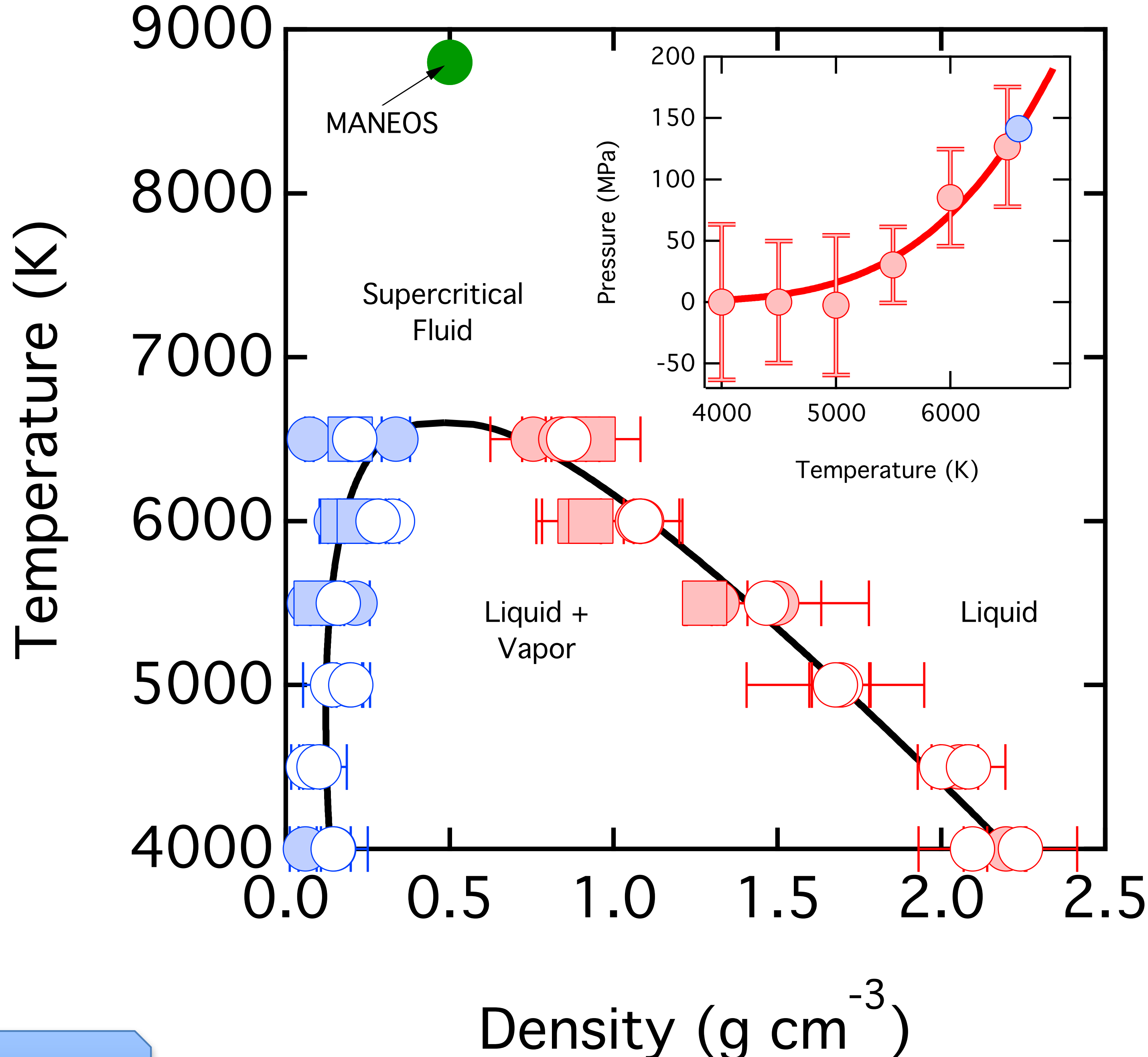


$MgSiO_3$

Xiao and Stixrude (2018) PNAS



Xiao and Stixrude (2018) PNAS



$MgSiO_3$

Xiao and Stixrude (2018) PNAS

Conclusions

- Partial melts sink at the bottom of the mantle
- Much easier to melt the whole Earth than previously thought
- Magma ocean starts crystallizing from the middle
- Crystals may float in the magma ocean
- Silicate dynamos are possible
- Silicate vaporization is much easier than we thought