



Toward Real Rocky Planet Interiors with Ideal Multicomponent Mixing

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Two Approaches to Exoplanet Interiors

Physics/Geology

- Material Properties
- Miscibility
- Temperature Gradients
- Gibbs Free Energy Solvers
- Evolution
- Differentiation
- Magma and Crystallization



Astronomy

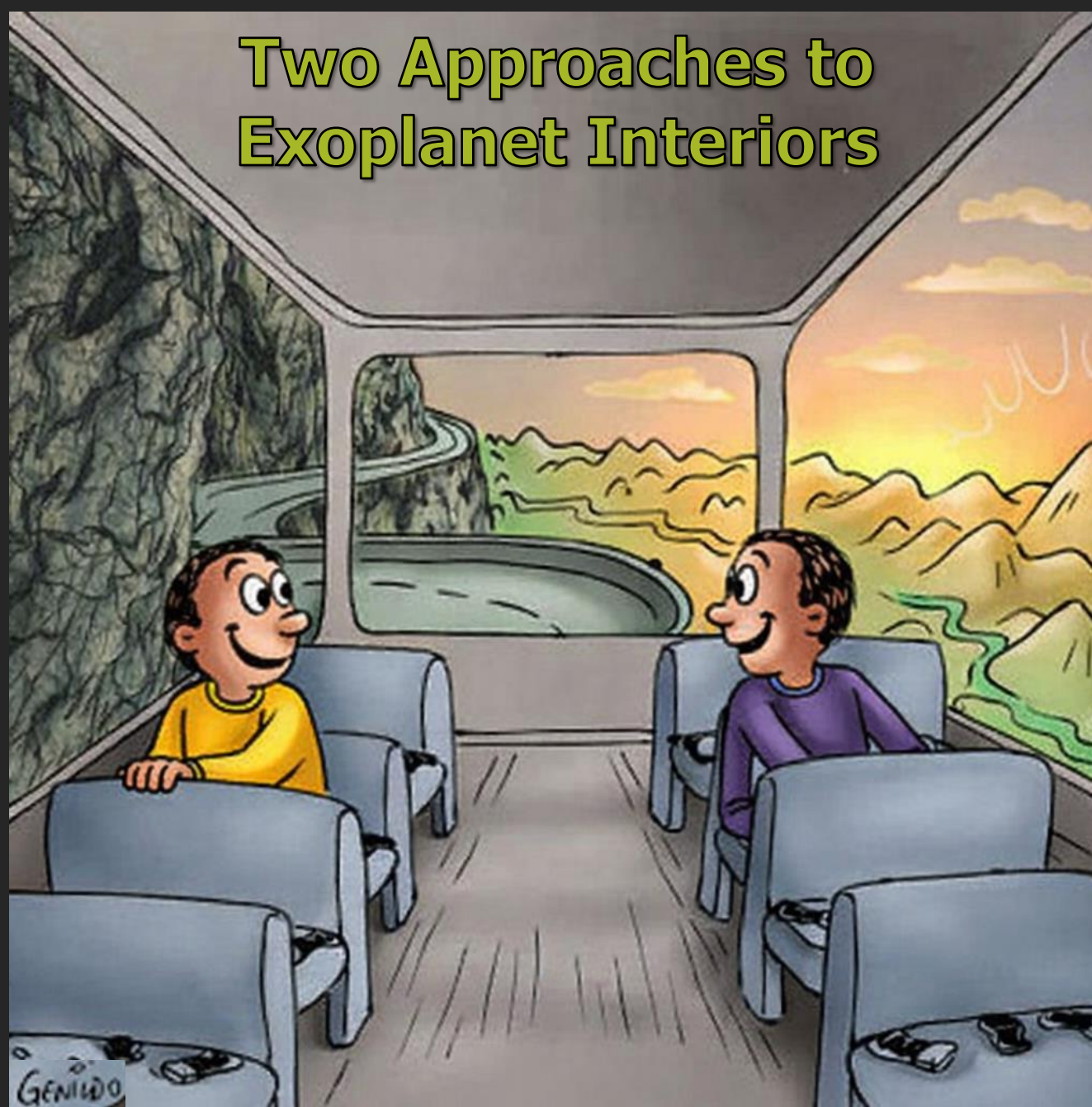
- Observables
- M-R Diagrams
- Polytropic EOS
- Demographics
- Bulk chemical properties
- Star-Planet
- Galactic context
- Fast Inference

Art: Genildo Ronchi (2013).
Two Guys on a Bus

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Two Guys on a Bus

Open Source
Planet Interior Platform



MAGRATHEA

v1 Huang, Rice, Steffen '22

v2 Rice et al. '25

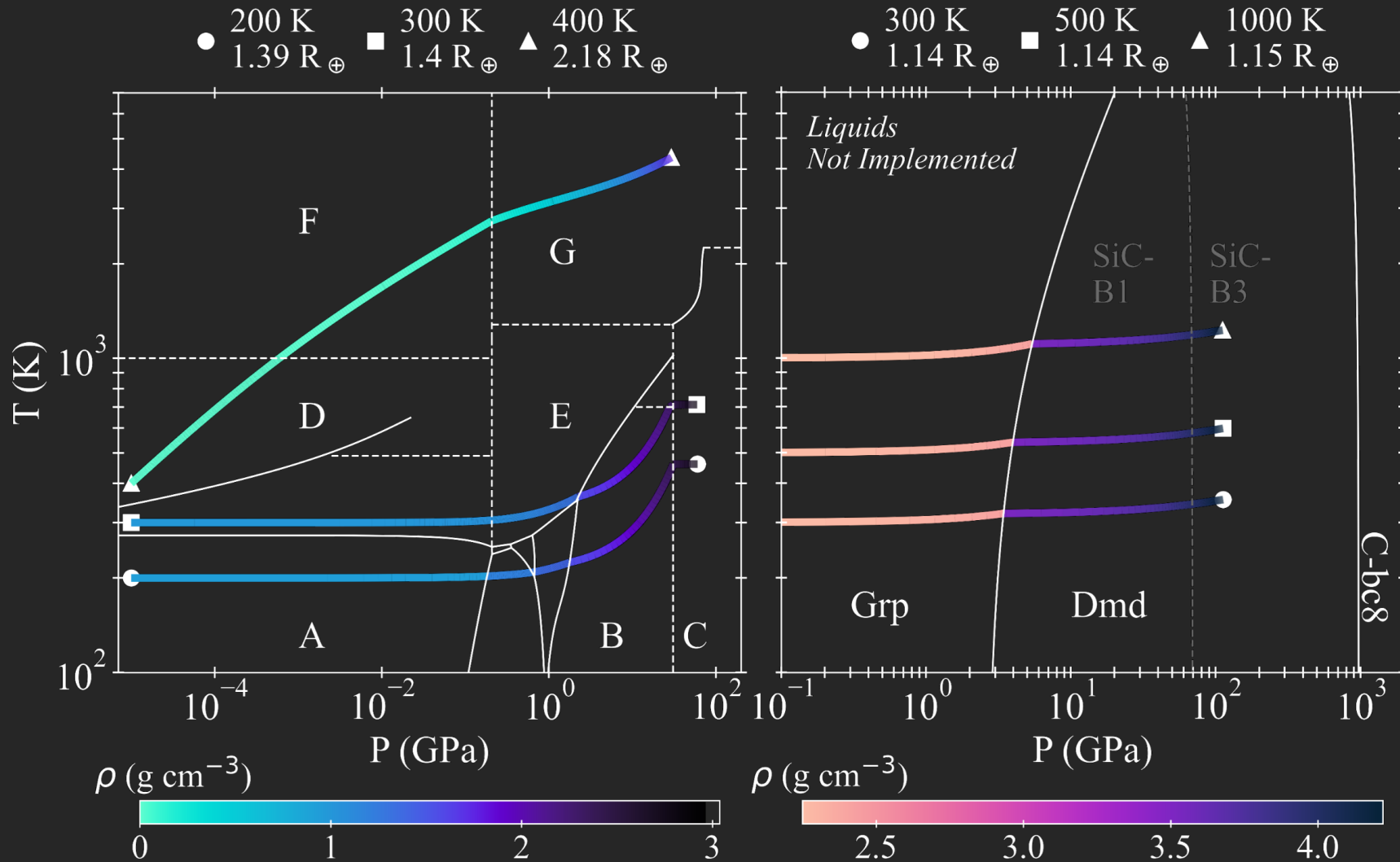
Used in ~12 publications

C++
Shoot to a Fitting Point
~0.5 seconds/run*
*w/o mixing

Extensible
Terrestrial++

**Modular Library of
Phase Diagrams
& EOS**

v2.0 New Phase Diagrams



Hydrosphere

- Solid, liquid, gas, supercritical
- Inspired by AQUA: Haldemann+ 20
- AQUA table available too!

Carbon

- Graphite, diamond, BC8
- Bo Royer at Las Vegas

v3.0

Real planet interiors are
multicomponent.

Sotin et al. 07: mixed two minerals and two end members per mantle layer.

Ideal Mixing

Additive Volume Law:

Total volume equals sum of each pure component

$$V_{\text{mix}} = \sum_i n_i V_i(P, T),$$
$$V_i(P, T) = m_i / \rho_i(P, T)$$

Mixture Density:

Mass-weighted harmonic mean

$$\rho_{\text{mix}} = \left(\sum_i \frac{x_i}{\rho_i(P, T)} \right)^{-1}$$

Adiabat:

Pure molar entropy adds

$$\sum_i \frac{x_i}{m_i} dS_i^{\text{pure}} = 0$$

Mixture adiabat –
weighted harmonic mean
of pure adiabats weighted
by thermal expansion

$$\left(\frac{dT}{dP} \right)_{S, \text{mix}} = \frac{\sum_i \frac{x_i}{\rho_i^2} \cdot \frac{(\partial P_i / \partial T)_{\rho_i}}{(\partial P_i / \partial \rho_i)_T}}{\sum_i \frac{1}{\left(\frac{dT}{dP} \right)_{S, i}} \cdot \frac{x_i}{\rho_i^2} \cdot \frac{(\partial P_i / \partial T)_{\rho_i}}{(\partial P_i / \partial \rho_i)_T}}$$

Robust Implementation of Mixtures

- Mixtures of N-components
- All EOS formulations work within mixture
- Mixtures behave as EOS objects chosen in phase diagrams

```
// ----- Rock-Water Mix -----  
static vector<EOS*> comps_RockWatMix{Fo, H2O_AQUA};  
static vector<double> x_RockWatMix{0.9269, 0.0731};  
DEFINE_IDEAL_MIX_WRAPPERS(RockWatMix)
```

BM3 and Tabulated

mass fractions

Mixing Rocks

Mantle Mineralogy

MgO, FeO, SiO₂, CaO, Al₂O₃

Perple_X

Stixrude & Lithgow-Bertelloni 11 & 22, Connolly 09

Self-consistent phase equilibria and assemblage properties via Gibbs free-energy minimization.

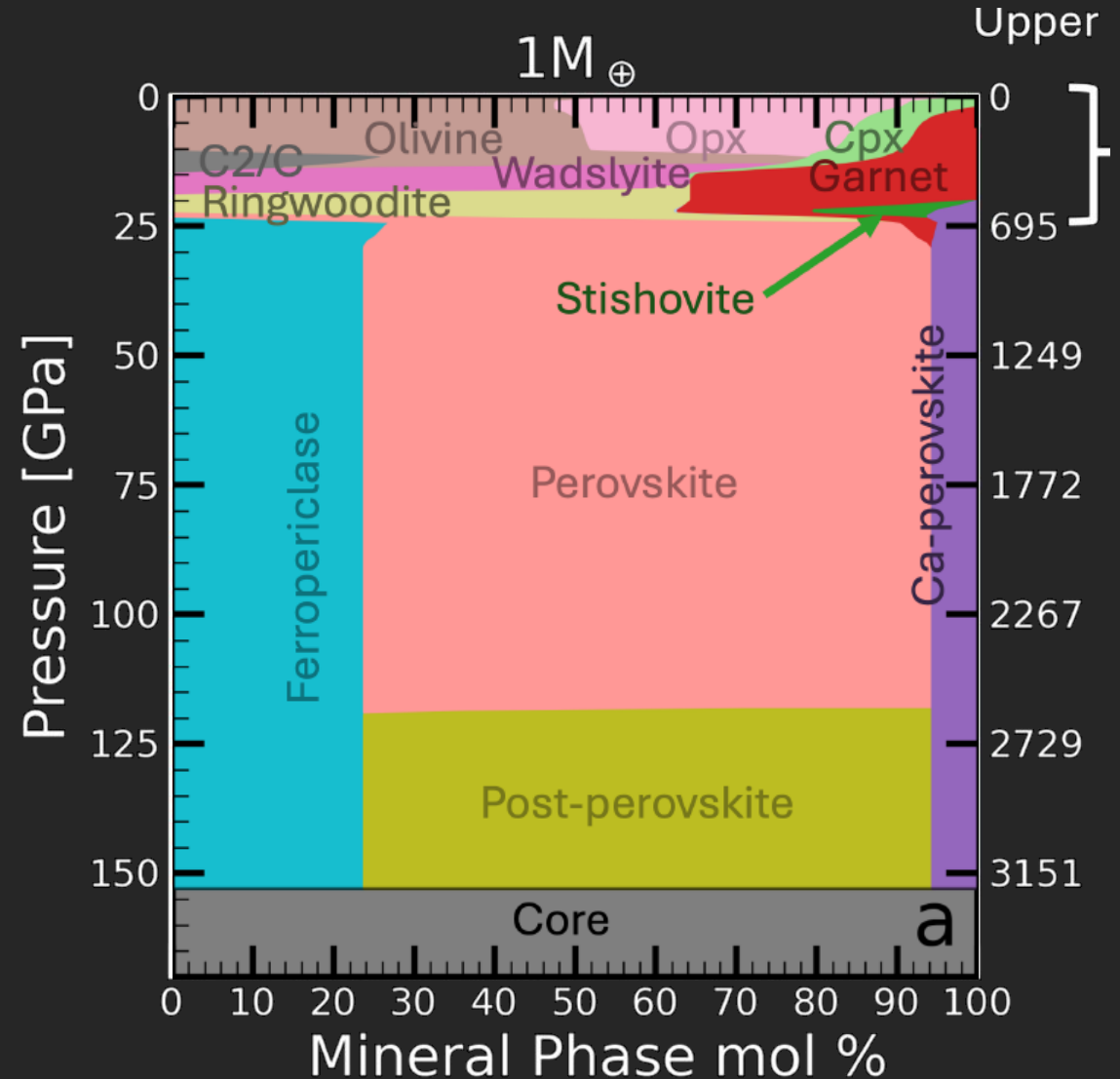
Used in MRCode, ExoPlex, BICEPS, and more

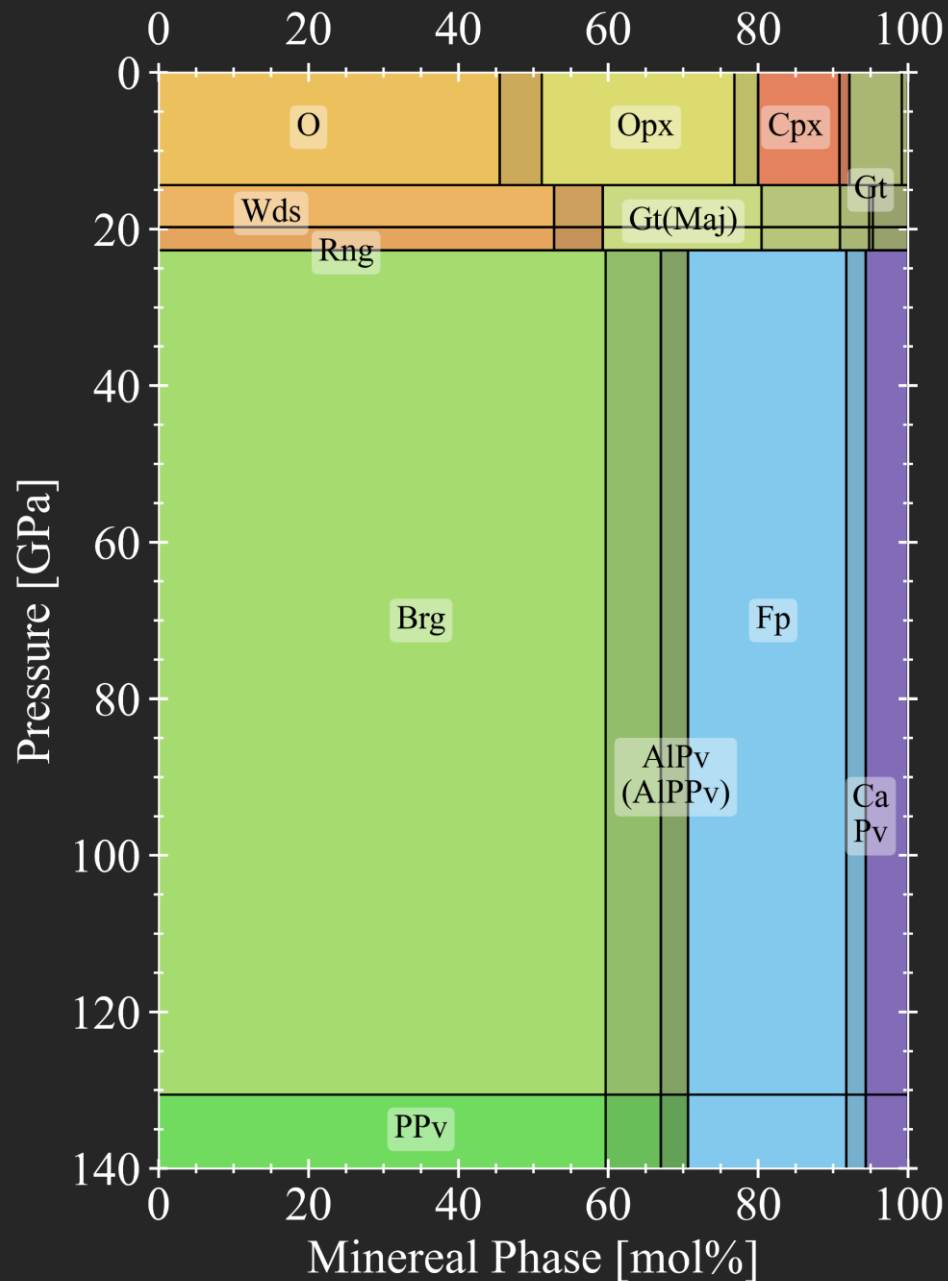
Limitations:

Intended for Earth-like conditions

EOS not modular in planet solution

Long runtimes or large tabulated files





Fully Stoichiometric Mantle

Phase proportions determined by elemental ratios:
Si/Mg, Fe/Mg, Al/Mg, Ca/Mg

Entire mantle in chemical equilibrium with mixtures calculated before the run.

Split into 5 regions based on Mg-Si phases.

In each layer:

- One phase eats Ca
- One phase eats Al
- Two phases vary Si/Mg ratio
- Endmembers set by $Mg\# = Mg/(Mg+Fe)$

Mixes

Olivine Region:

Forsterite, Fayalite, Enstatite, Ferrosilite, Diopside, Hedenbergite, Pyrope, Almandine, SiO_2 , MgO, FeO

Wadsleyite (Rwd) Region:

Wadsleyite, Fe_Wadsleyite, Majorite, Akimotoite, Pyrope, Almandine, Grossular, SiO_2 , MgO, FeO

Perovskite (PPv) Region:

Bridgmanite, Fe_Perovskite, Al_Perovskite, Periclase, Wustite, Ca_Perovskite, SiO_2

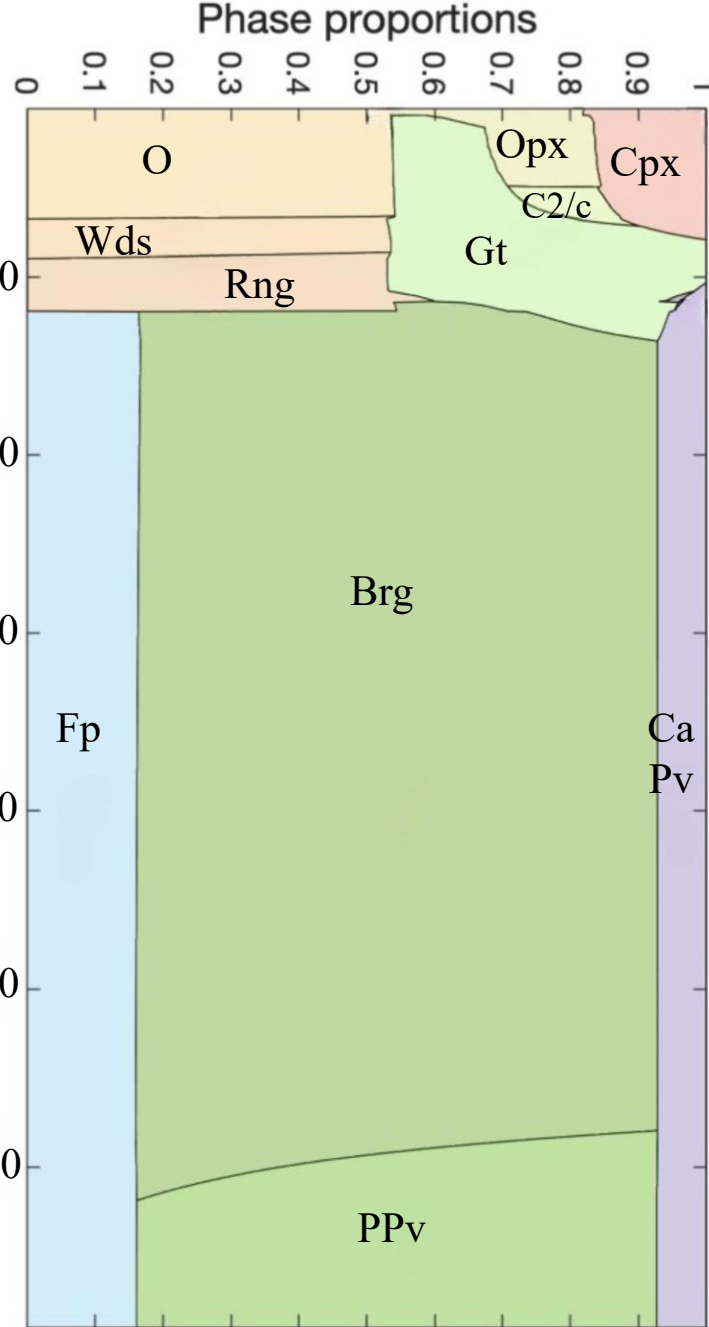
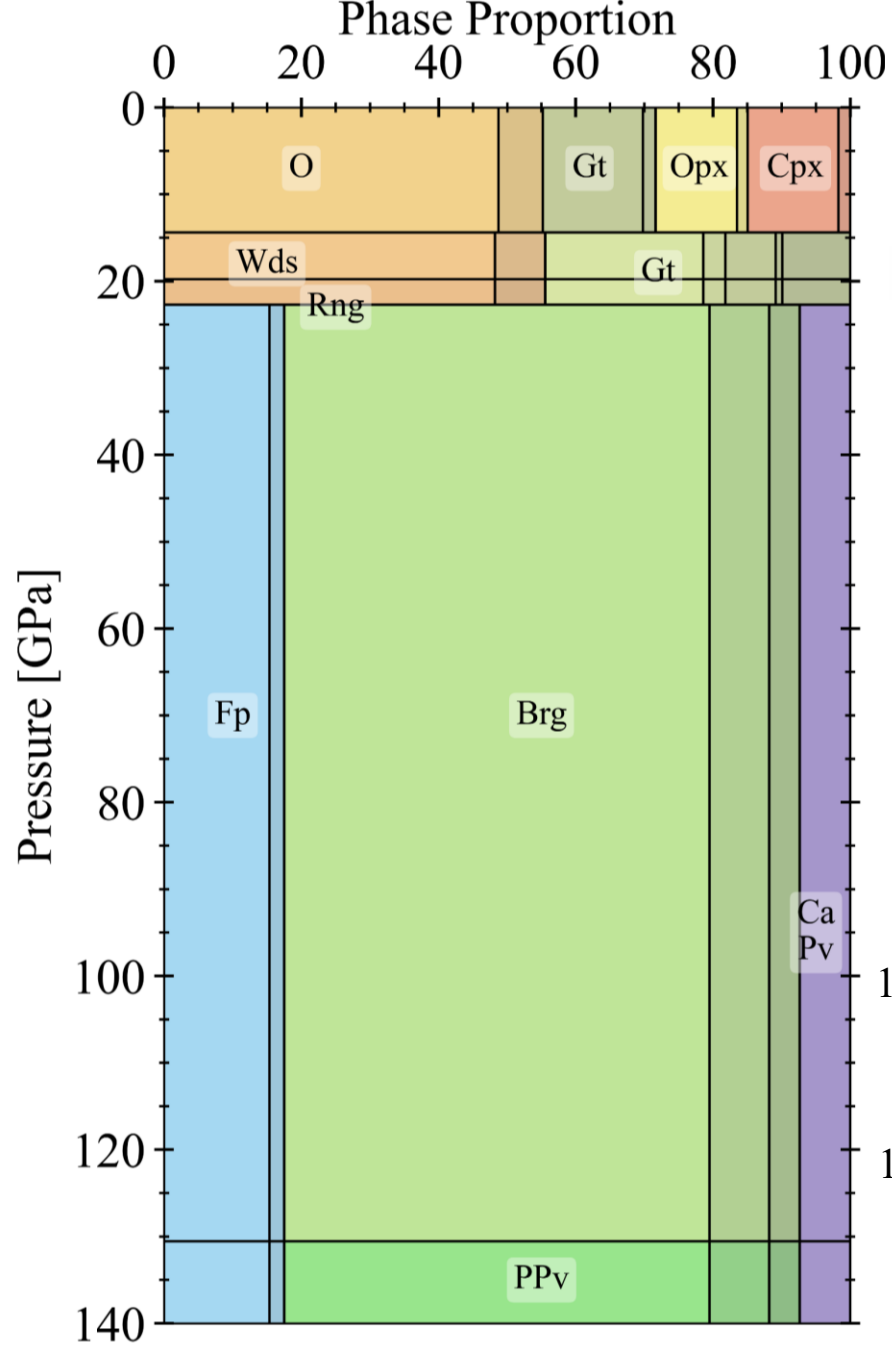
Limitations

- $R_{\text{Al}} > 2/3 R_{\text{Ca}}$ (Grossular Garnet)
- $R_{\text{Si}} > 2 R_{\text{Ca}} + 3/2 R_{\text{Al}}$

Assumptions

- Shared Mg#
- Hard Phase Boundaries
- Ignored minor phases
- Na, K, Ti, Cr, Ni ignored

New



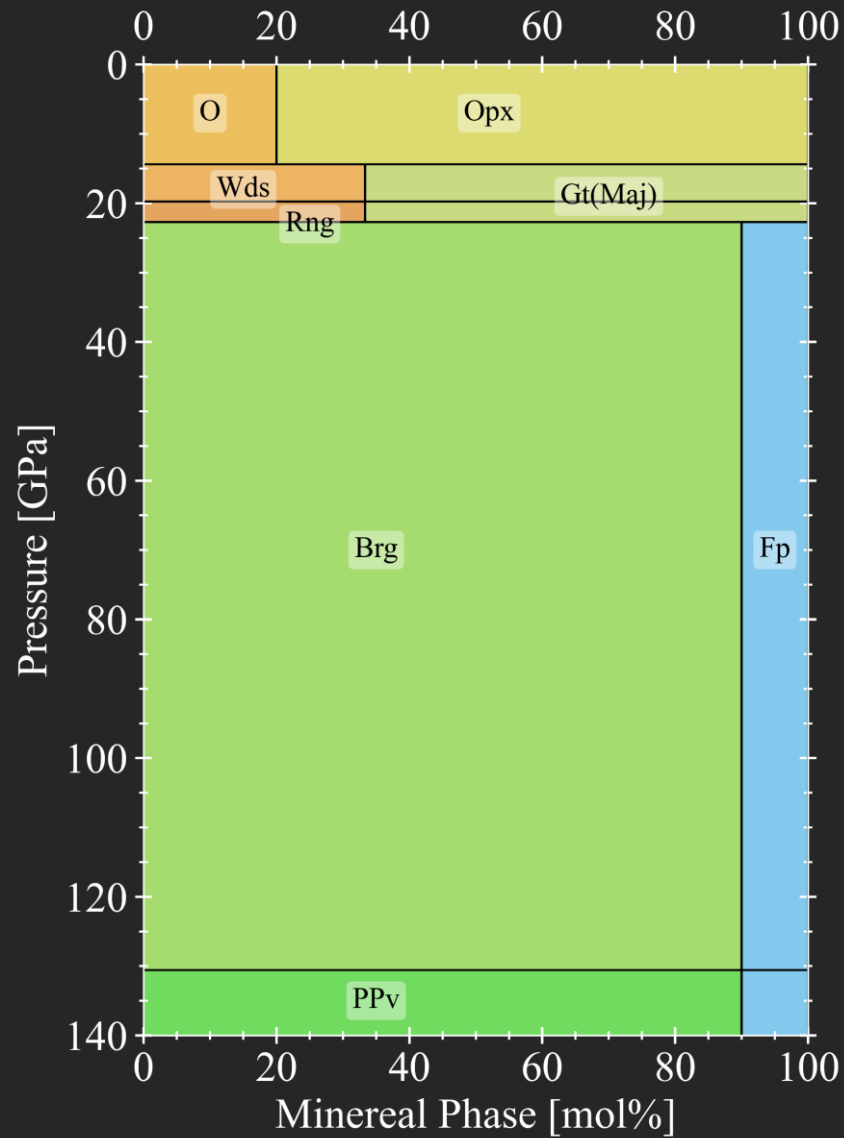
Perple_X

Ca/Mg=0.07,
Al/Mg=0.09,
Si/Mg=0.8,
Mg#=0.89.

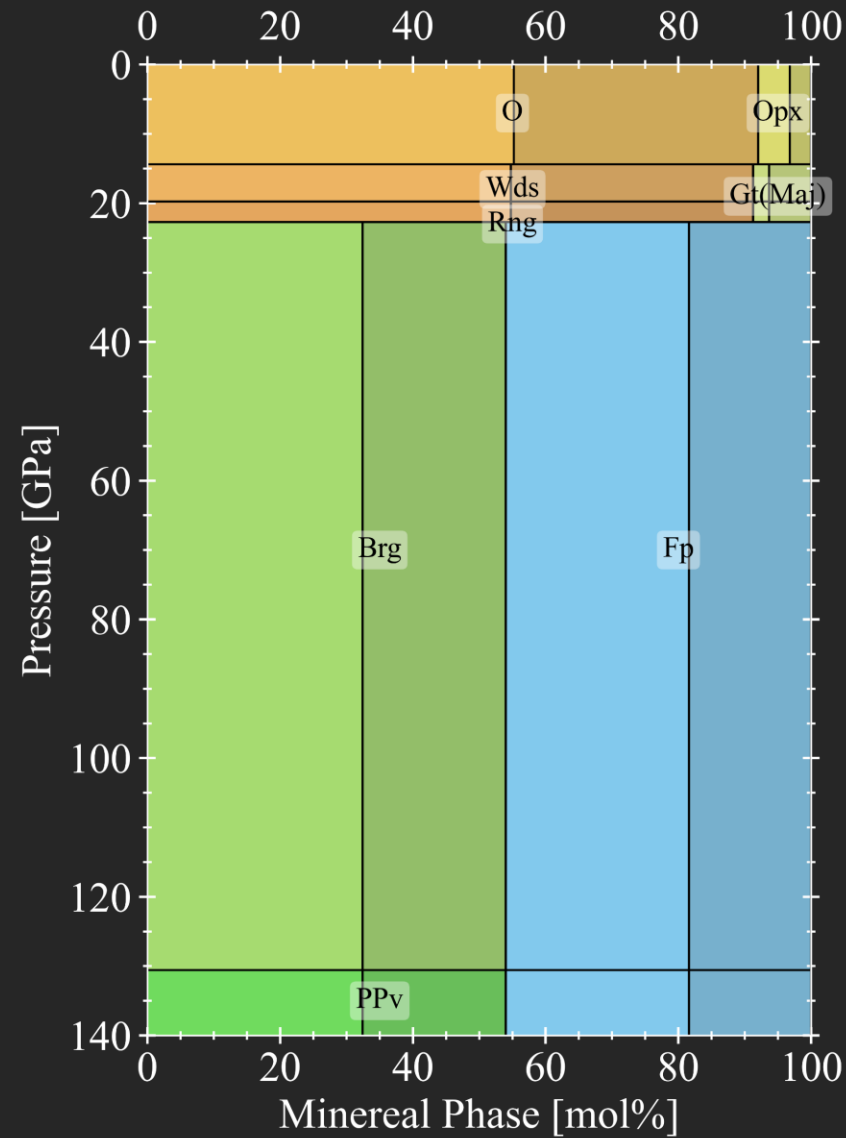
Dark regions are the end members



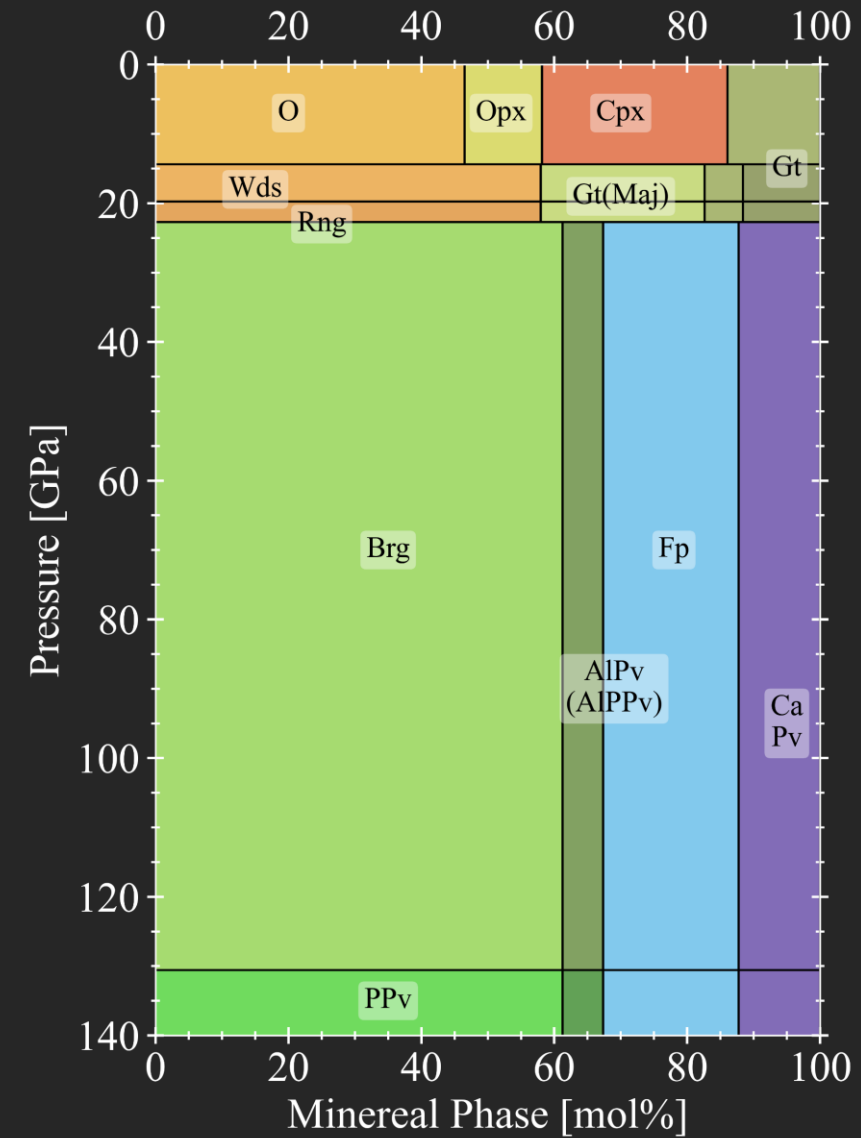
No Fe, No Minor

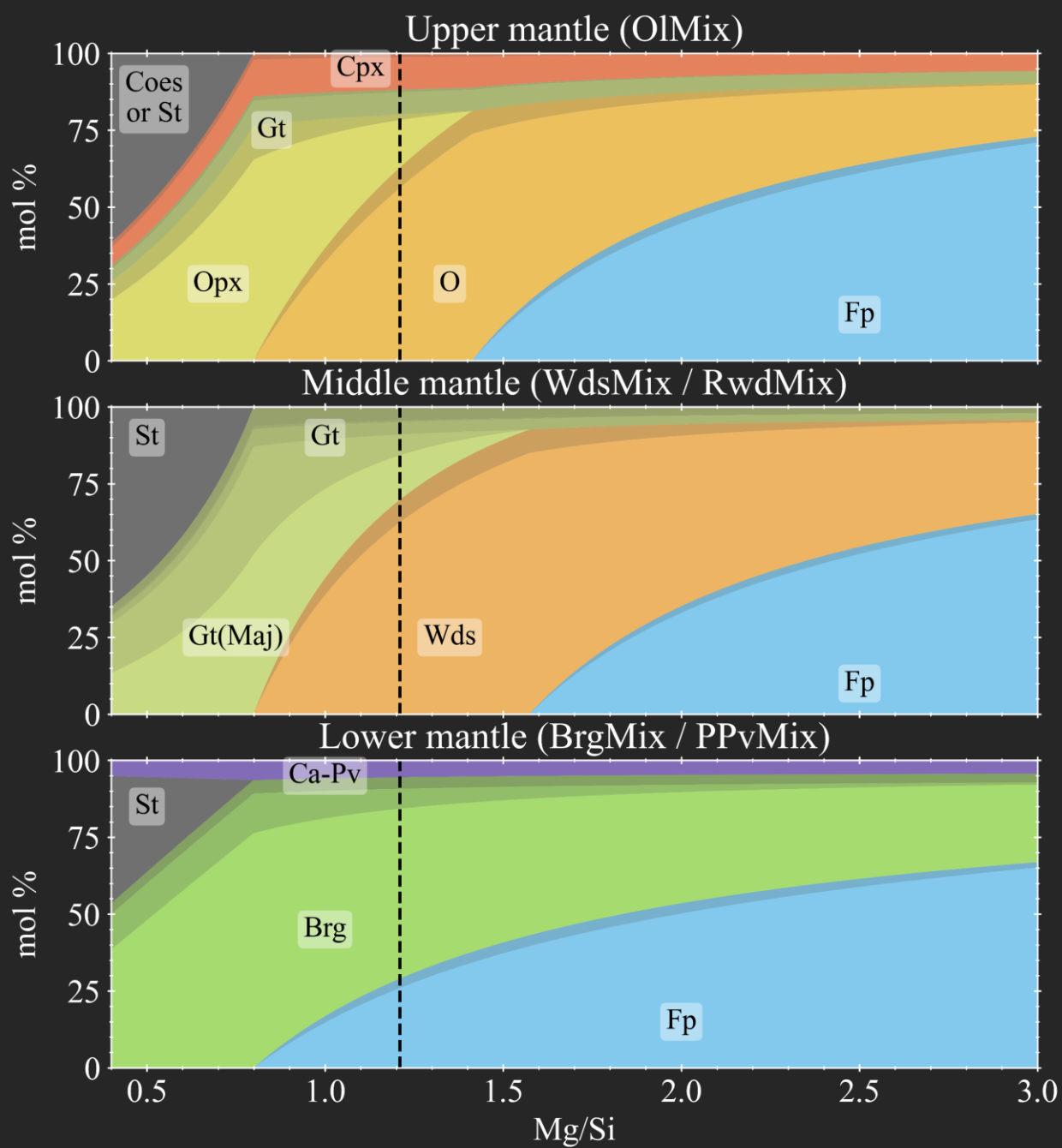


High Fe, No Minor



No Fe, High Minor





Varying Mg/Si

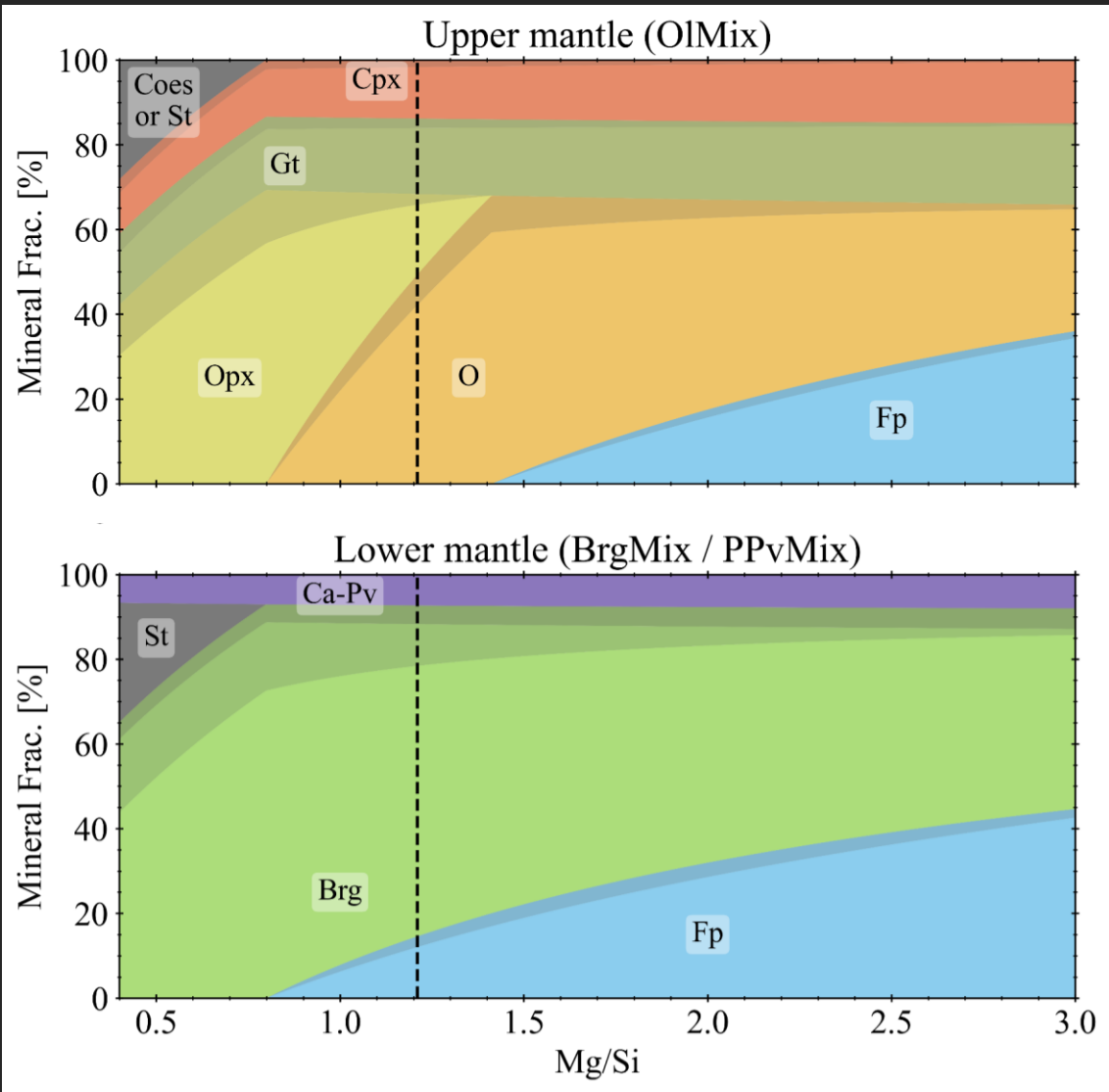
O : Mg/Si = 2

Opx : Mg/Si = 1

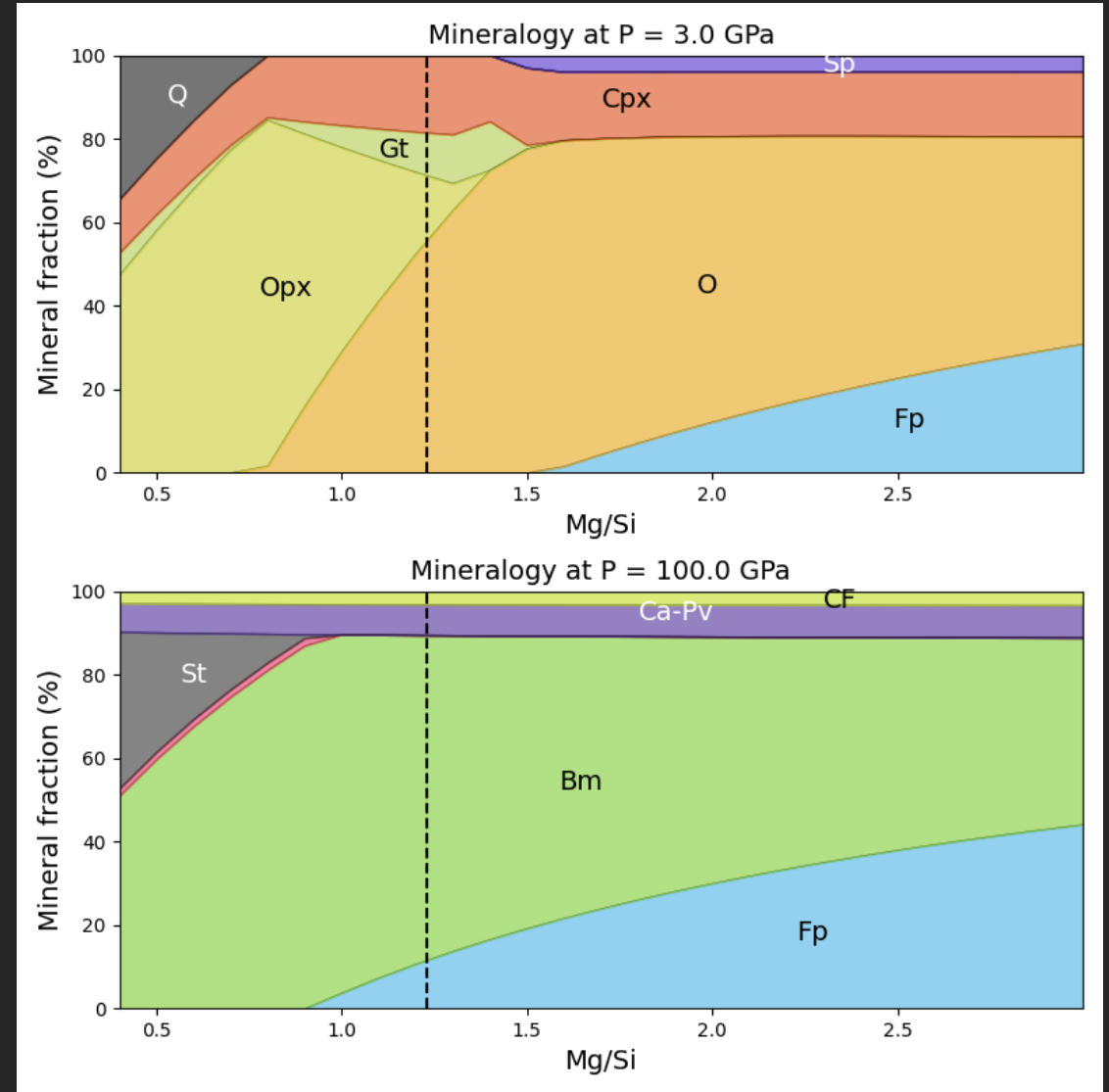
St : SiO₂

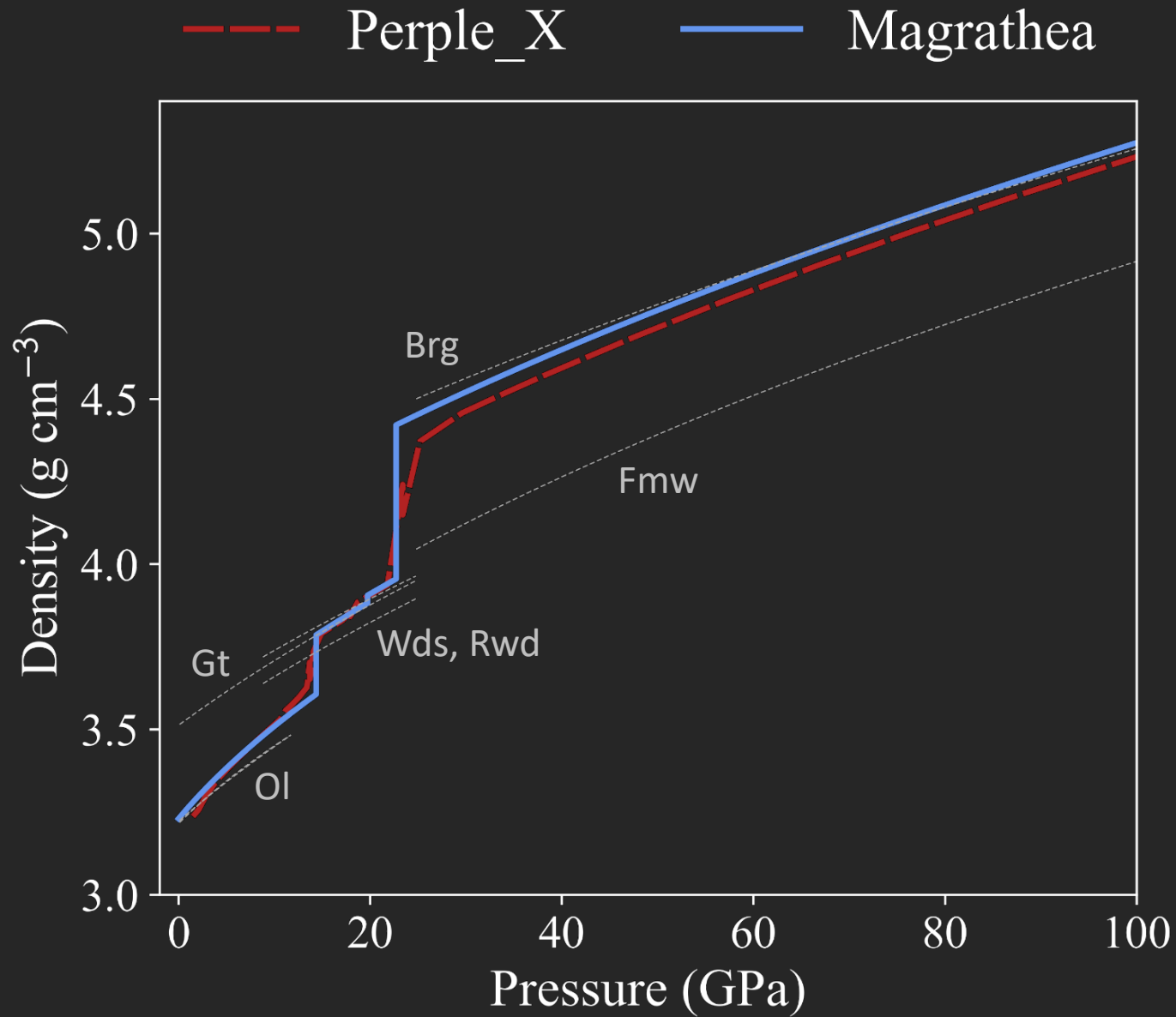
Fp : MgO

Stoichiometric

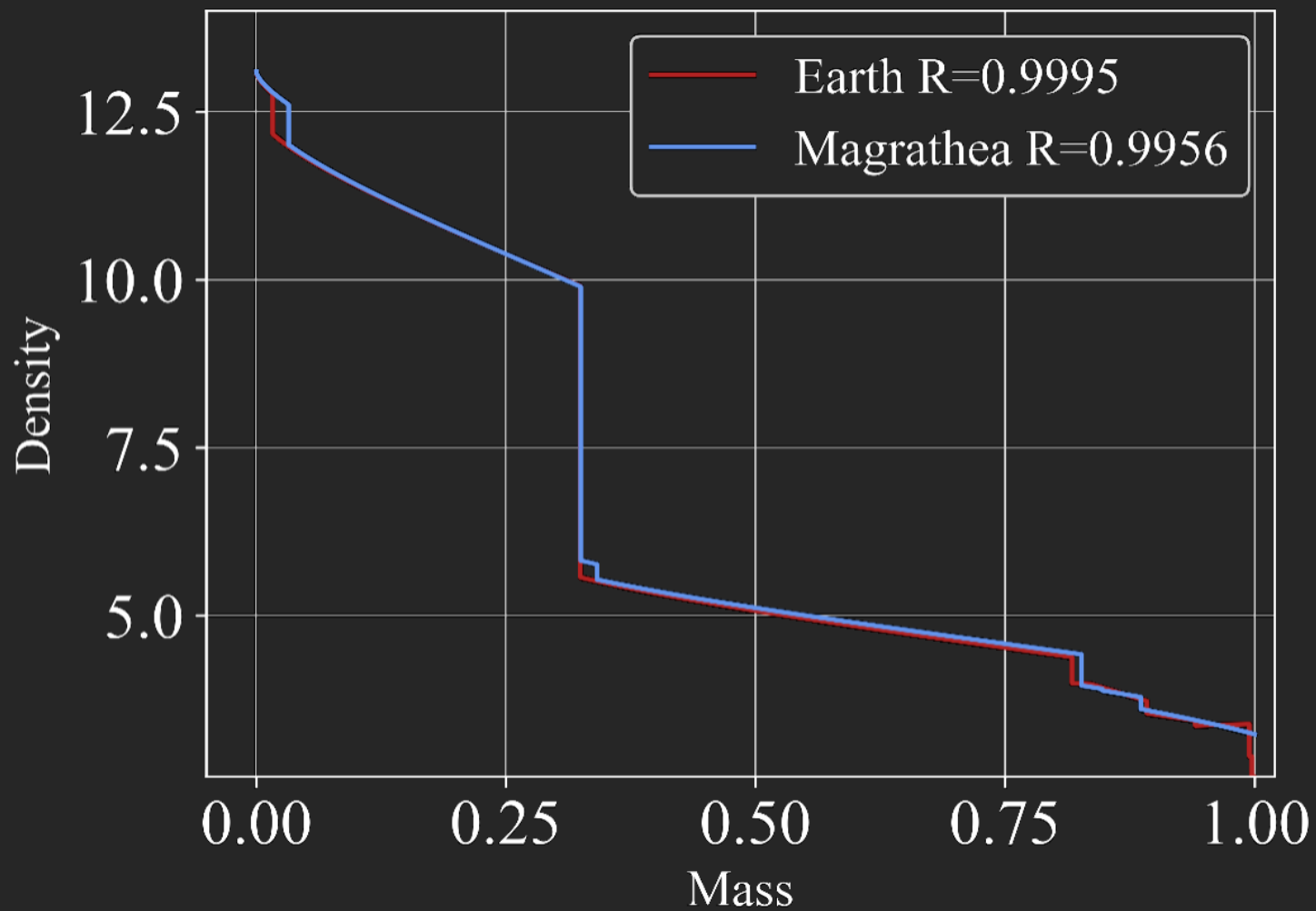


Perple_X



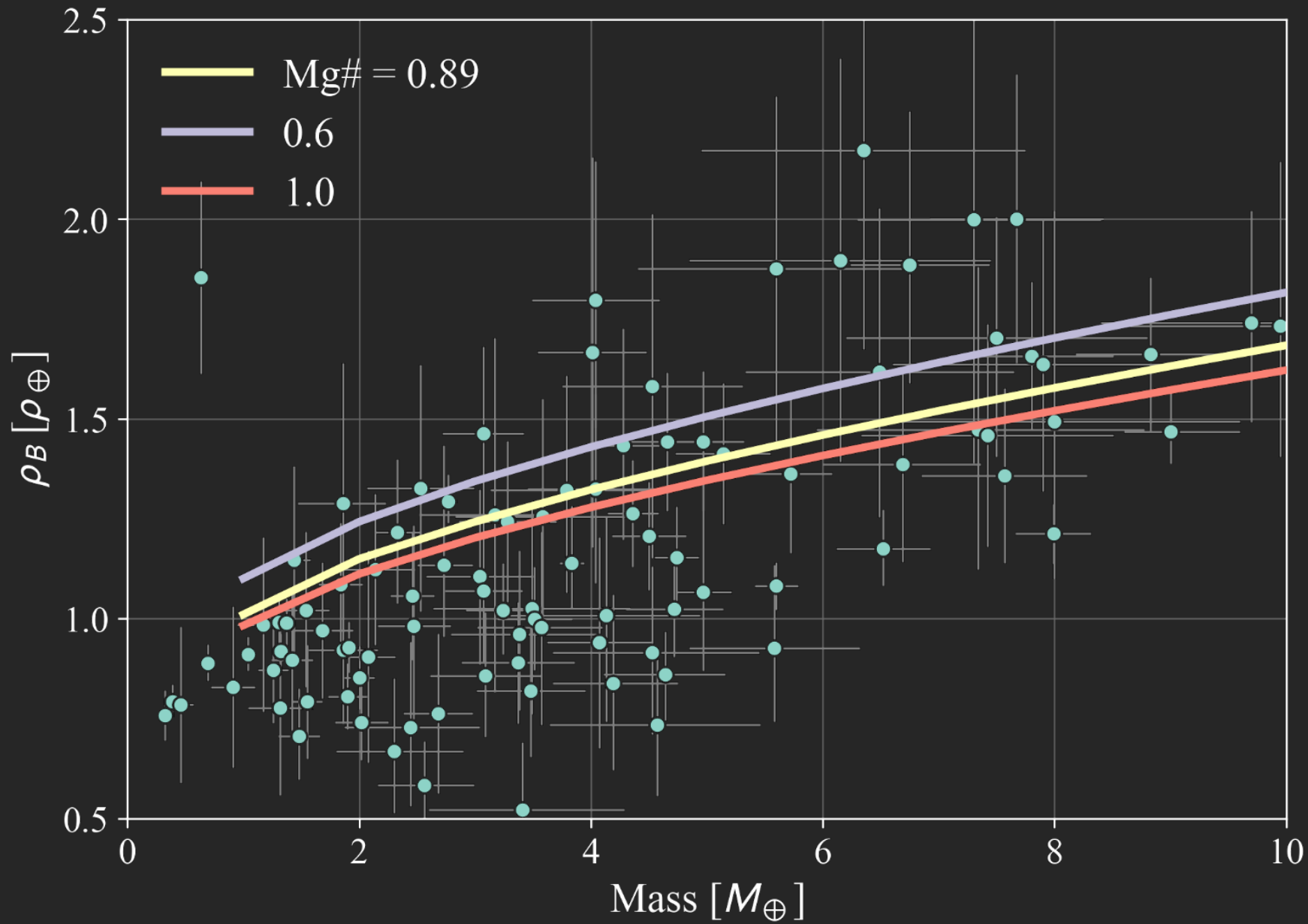


Comparing
Densities
<2% Difference



Earth

Calibrated to Earth,
but immediately tunable

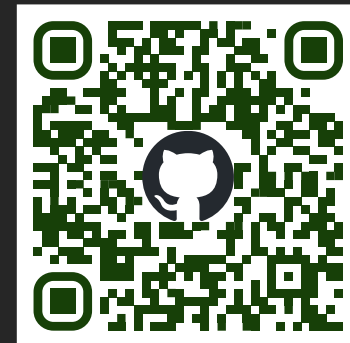


Reasonable ranges of FeO in the mantle change radii by 2.5%.

Toward Real Rocky Planet Interiors

- Rocky-planet materials are multicomponent
- Mixtures can be treated as EOS objects
- Stoichiometric mantles make composition explicit
- Standardization should not mean shared blind spots

Build planet models that are both physically richer and astronomically testable.



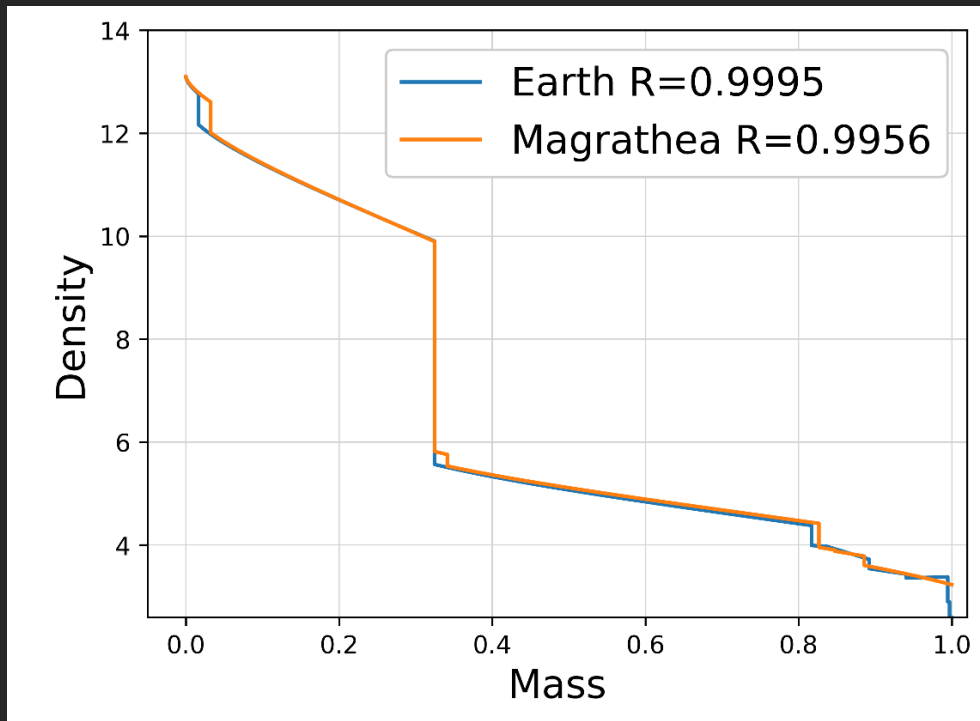




```

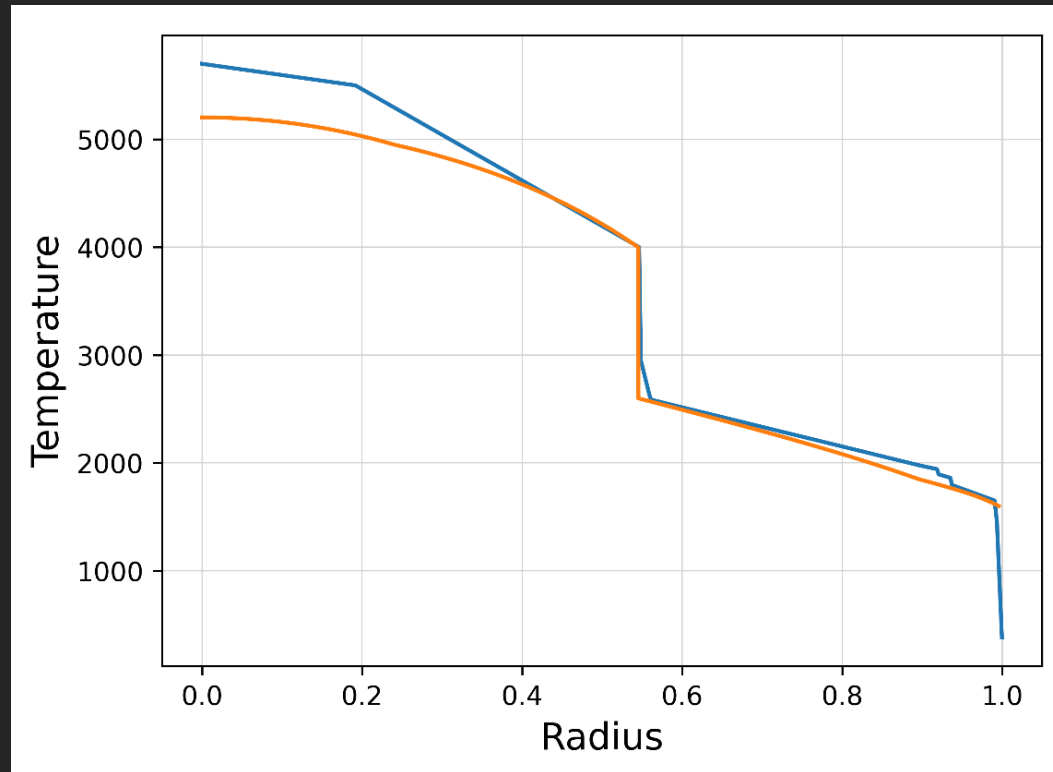
#Welcome to MAGRATHEA (\/)
#Authors: Huang C., Rice D.R., Steffen J.H. (•_•)
#Planet interior structure code for astronomers, planetary scientists, mice, and more. / < \
#=====
#Input Mode 9
#Full Solver with Chemistry
#Solve the interior properties of a planet
#Requires mass of each differentiated layer, surface temperature, and discontinuities
#-----
#Input Mode 9 inputs
input_mode=9
total_mass=1.0 # Earth masses total (mass of core and mantle will be calculated with elemental ratios)
mass_of_hydro=0.0 # Earth masses in hydrosphere
mass_of_atm=0.0 # Earth masses in atmosphere
CaMg = 0.07 #Ca/Mg ratio. Earth: 0.07
SiMg = 0.9 #Si/Mg ratio. Earth: 0.9
AlMg = 0.09 #Al/Mg ratio. Earth: 0.09
#Three Coupled knobs for determining location of Fe, Set 2 and comment out the 3rd, all 3 will be calculated and reported
#FeMg = 0.95 #Bulk Fe/Mg ratio. Earth: 0.9
mantle_Mg_num = 0.89 #Mg# of the mantle. Earth: 0.89
RCMF = 0.325 #CMF of the rocky portion of planet (CMF/(MMF+CMF) #Earth: 0.325
#wt fractions of non-Fe elements in core: Earth: 0.05-0.1 (excluding Ni)
wt_fract_S_core = 0.02 #wt. frac. of sulfur in core, affects core density.
wt_fract_O_core = 0.01 #wt. frac. of oxygen in core
wt_fract_H_core = 0.00 #wt. frac. of hydrogen in core
wt_fract_C_core = 0.00 #wt. frac. of carbon in core
wt_fract_Si_core = 0.06 #wt. frac. of silicon in core. Ignored in mantle's SiMg balance
wt_fract_Ni_core = 0.05 #wt fraction of Ni in core. Earth: 0.05
core_partition_flag = true #partitions LE between solid/liquid core, increases run time
surface_temp=1600 # K, top of planet where enclosed mass equals total mass, #Earth mantle temp ~1600 K
#Temperature of the outer boundary of the inner layer minus the inner boundary of the outer layer. A positive number indicates temperature increases inward.
temp_jump_1=0 # Atmosphere to hydrosphere discontinuity in K
temp_jump_2=0 # Hydrosphere to mantle discontinuity in K
temp_jump_3=1400 # Mantle to core discontinuity in K #Earth ~1400 K
output_file="./result/Structure_Earthmatch1.txt" # Output file name & location
..

```



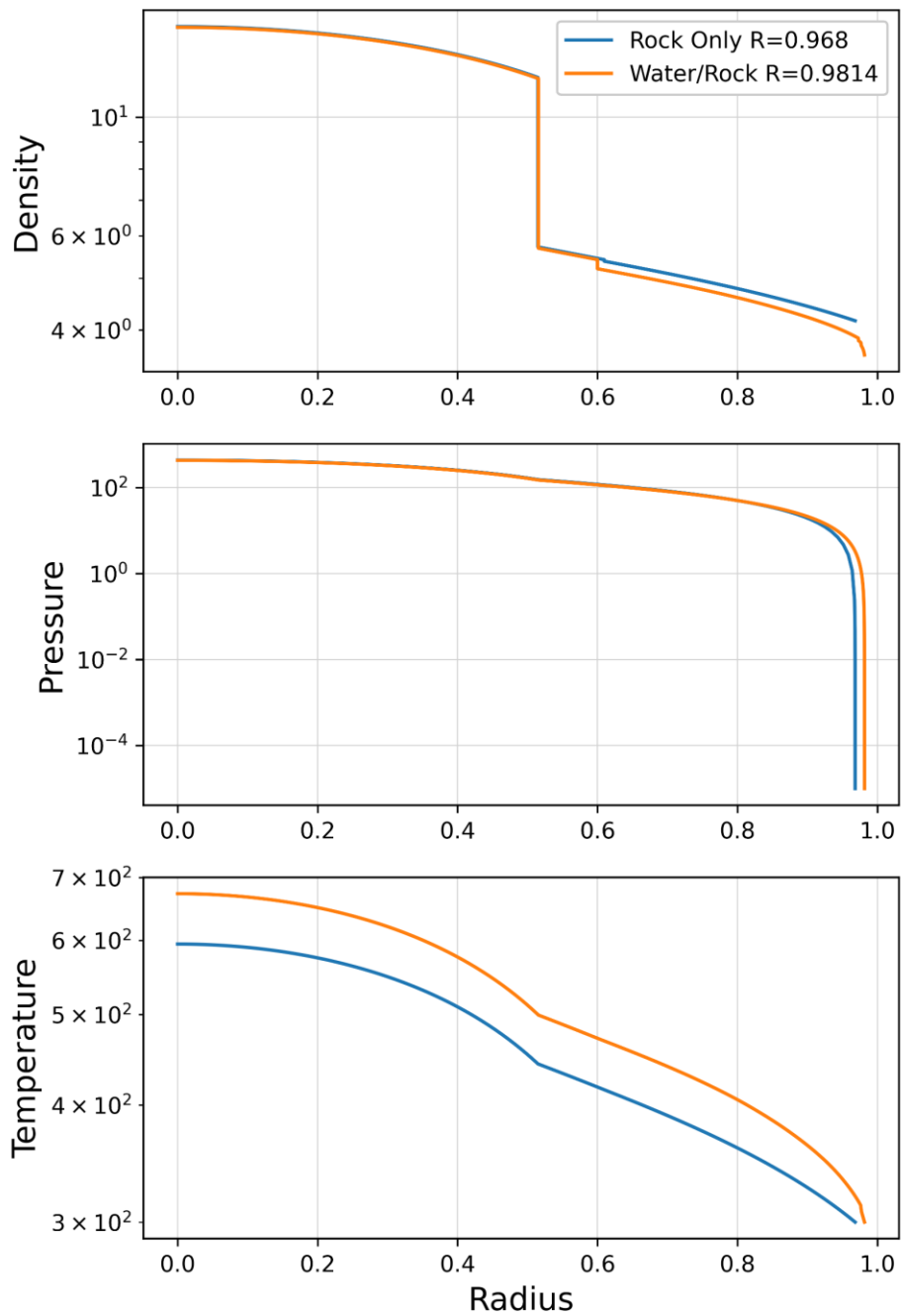
Earth

Calibrated to Earth,
but immediately
tunable

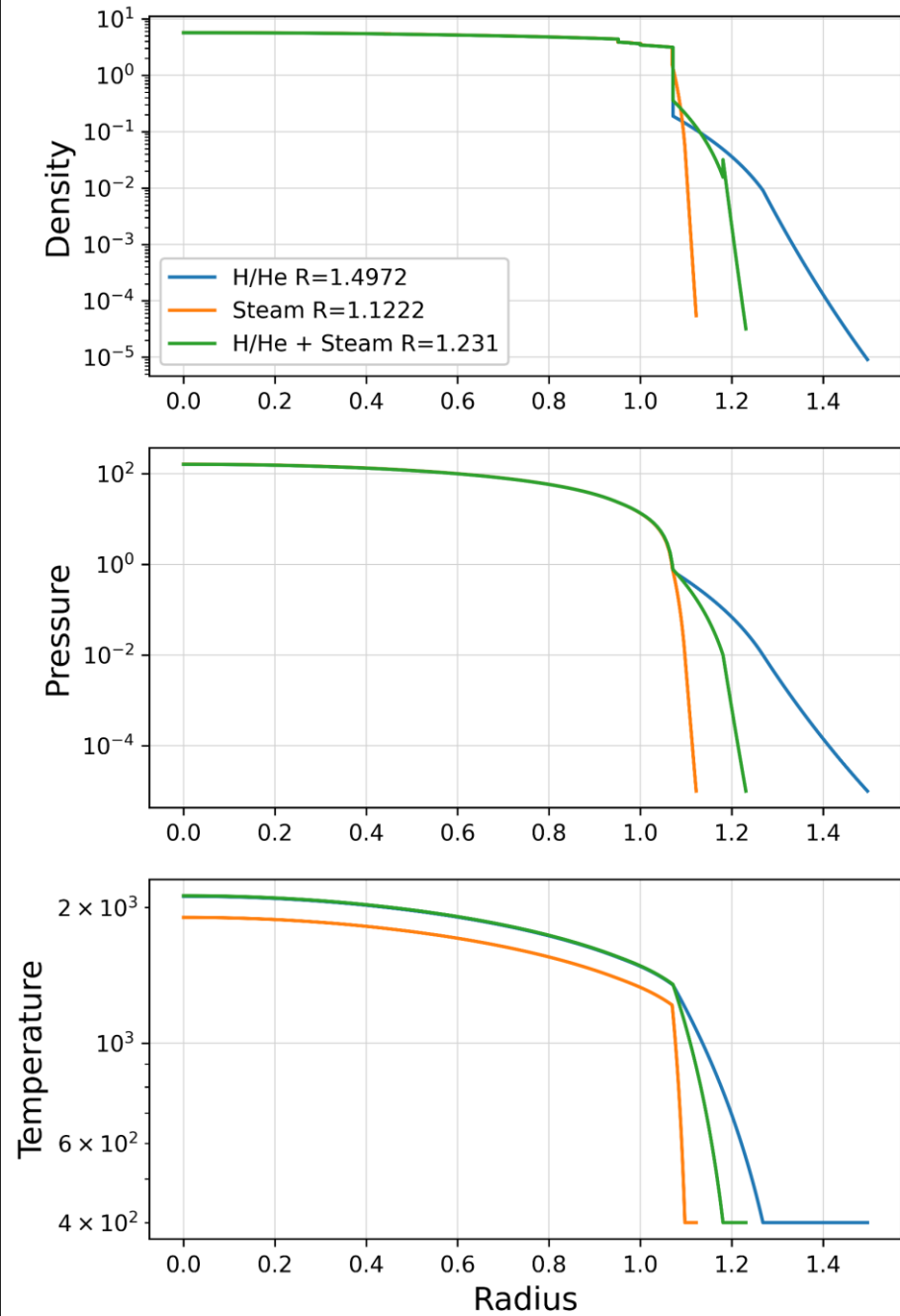


Mixing Fun

5 wt%
Water in
Mantle



0.5% H/He
0.5% Steam
0.5% Mix



MAGRATHEA

Planet Interior Structure Solver

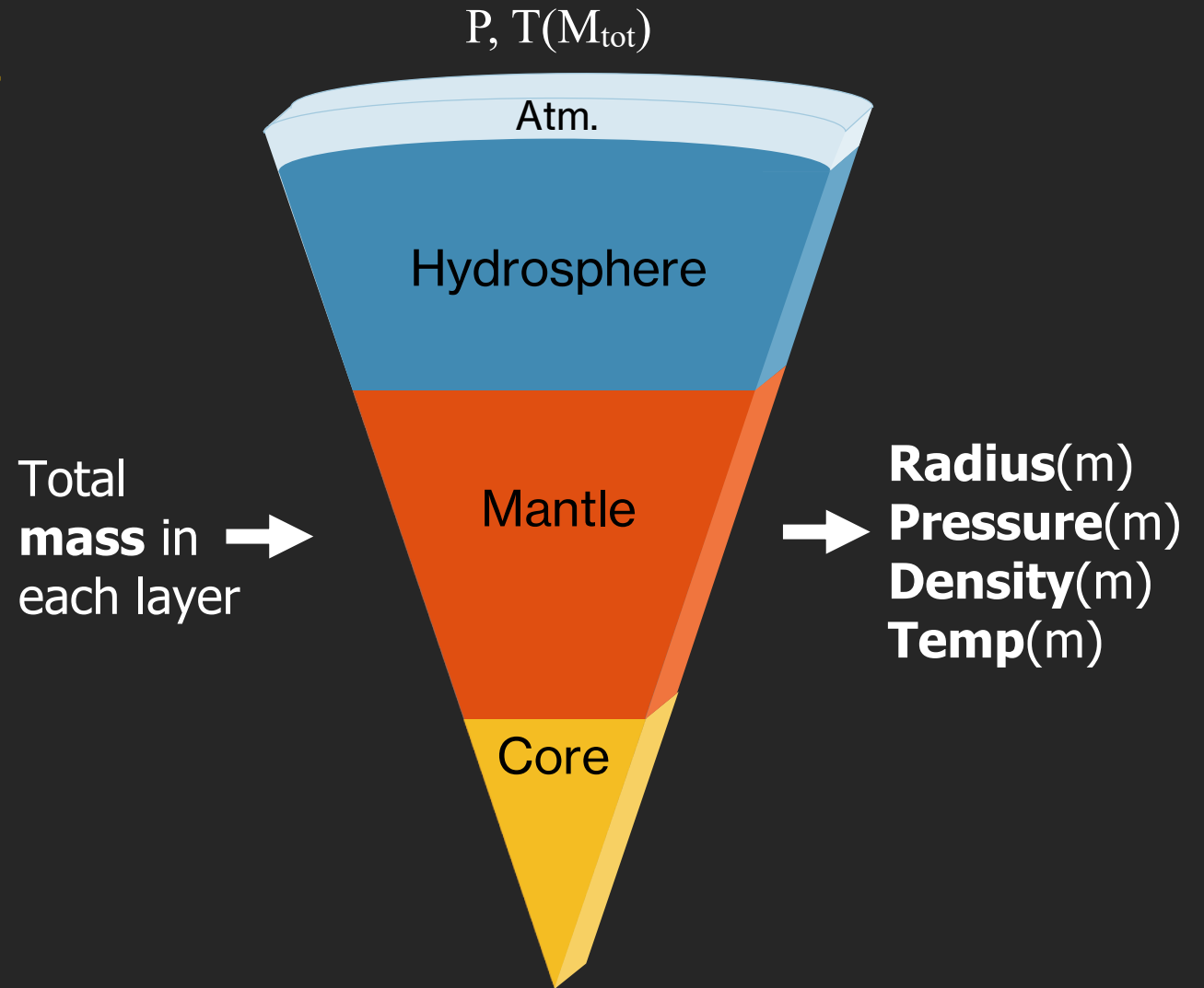
1D spherically-symmetric fully-differentiated **shell model**

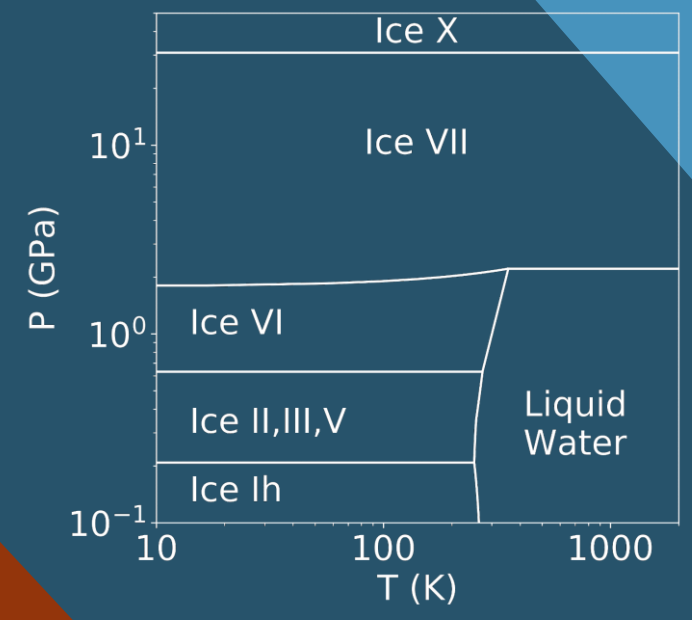
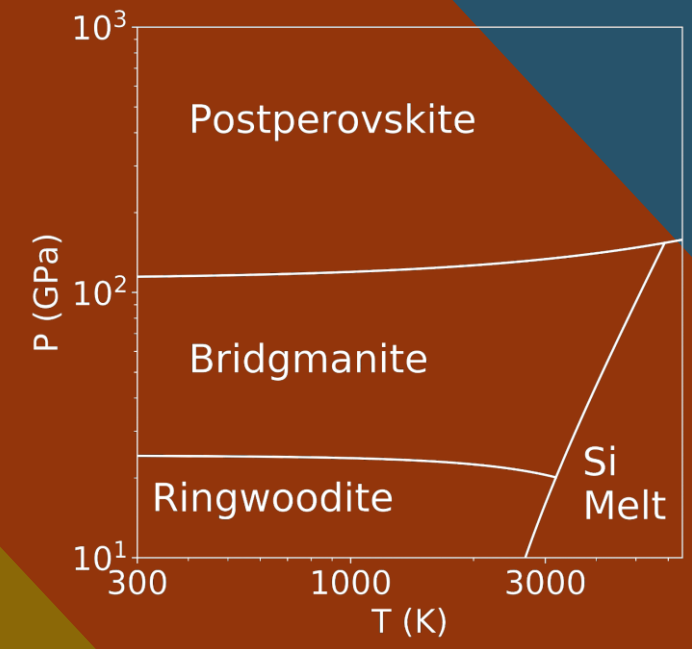
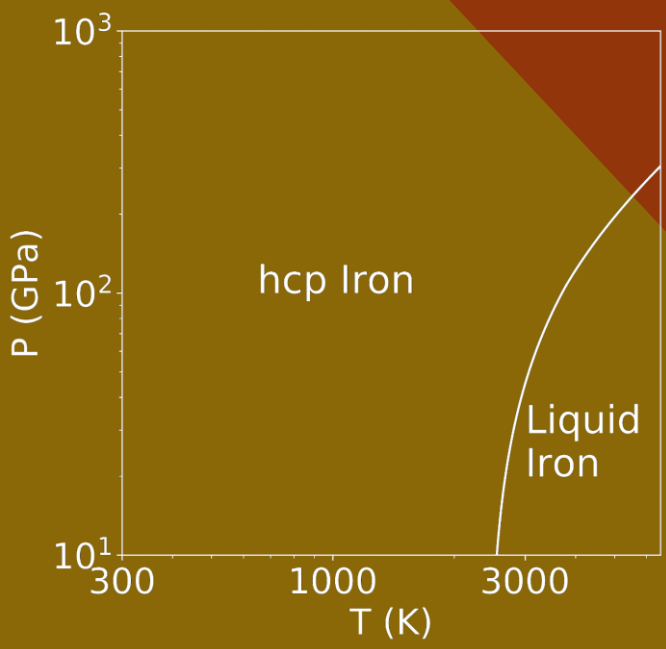
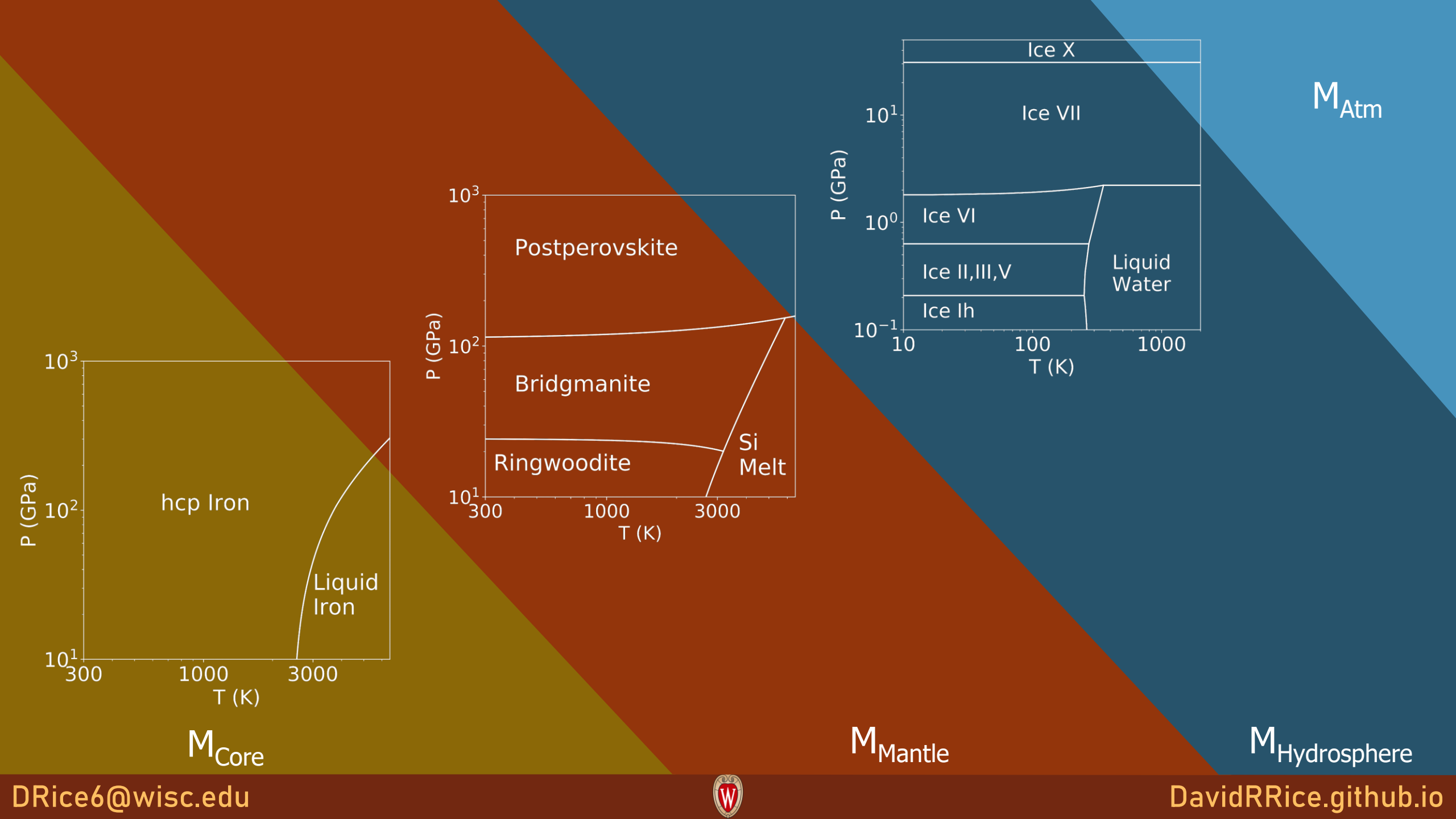
$$\frac{dr(m)}{dm} = \frac{1}{4\pi r^2 \rho(m)}$$

$$\frac{dP(m)}{dm} = -\frac{Gm}{4\pi r^4}$$

$$\frac{dT(m)}{dm} = \text{Isentropic}$$

Equation of State: $P(m) = P(\rho(m), T(m))$





M_{Core}

M_{Mantle}

$M_{\text{Hydrosphere}}$

M_{Atm}



Equations of State

Birch Murnaghan 3rd order

$$P(V) = \frac{3B_0}{2} \left[\left(\frac{V_0}{V} \right)^{\frac{7}{3}} - \left(\frac{V_0}{V} \right)^{\frac{5}{3}} \right] \left\{ 1 + \frac{3}{4} (B'_0 - 4) \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \right\}$$

Bulk Modulus
Resistance to Compression

Reference Volume

$\frac{\partial B_0}{\partial P}$

+ 6 formulations

Debye Thermal Pressure

$$P_{th}(T) = \frac{\gamma}{V} E_{th}(T)$$

Grüneisen

+ 3 formulations

Equations of State

Birch Murnaghan 3rd order

$$P(V) = \frac{3B_0}{2} \left[\left(\frac{V_0}{V} \right)^{\frac{7}{3}} - \left(\frac{V_0}{V} \right)^{\frac{5}{3}} \right] \left\{ 1 + \frac{3}{2} (B' - 4) \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \right\}$$

Bulk Modulus
Resistance to Compression

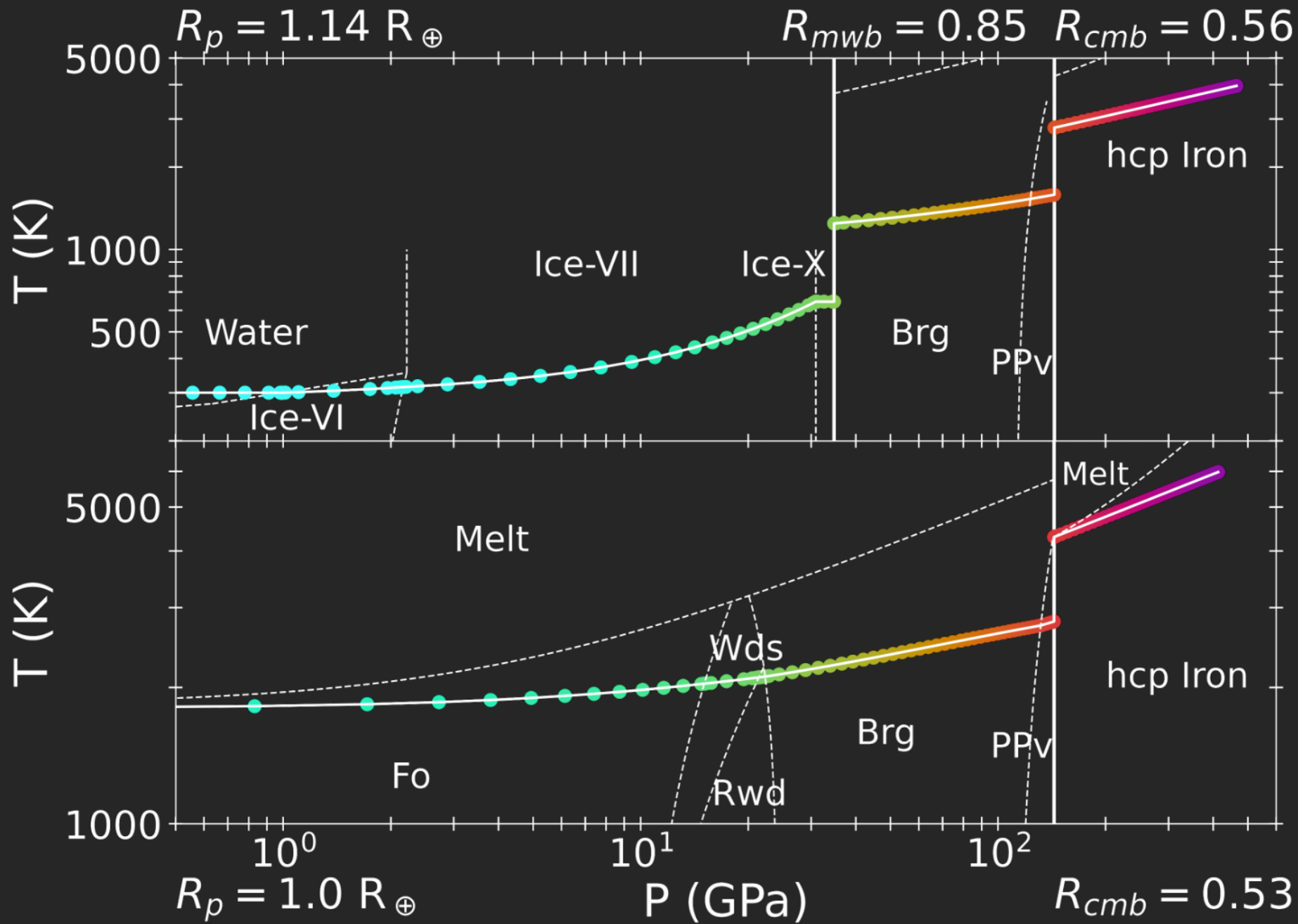
**Library of 60+ materials
and measurements.**

+ 6 formulations

$$P_{th}(T) = \frac{1}{V} E_{th}(T)$$

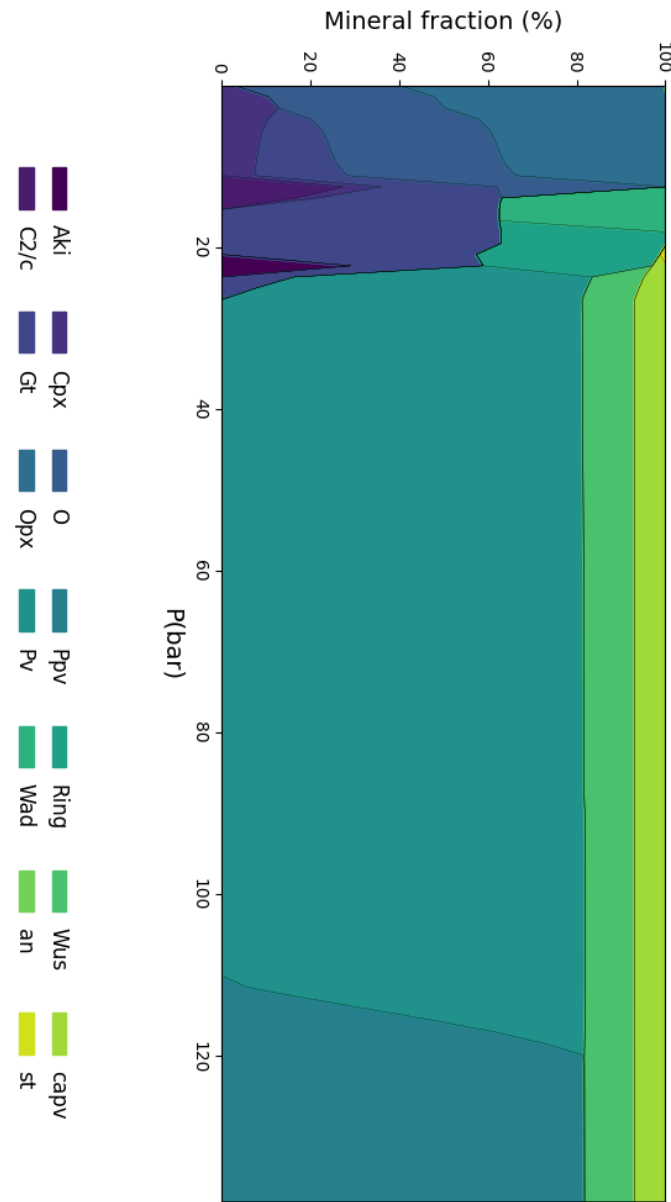
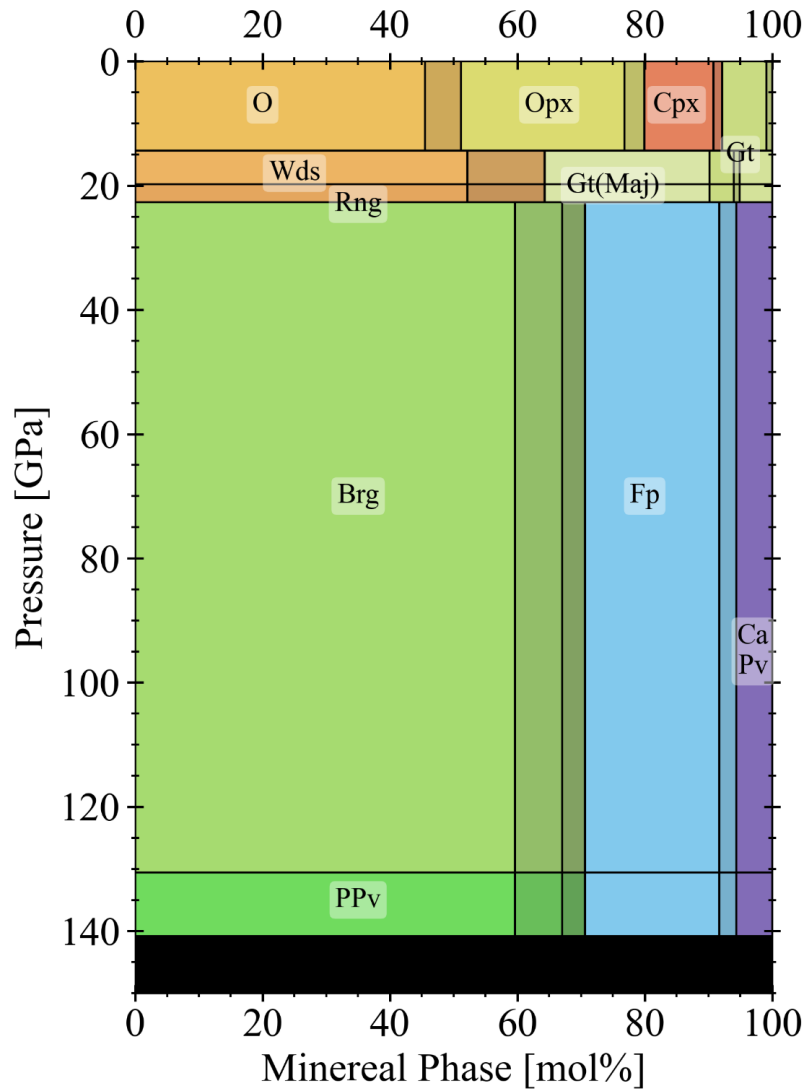
Grüneisen

+ 3 formulations



M_\oplus	Planet 1	Planet 2
1.1	1.1 M_\oplus	1.0 M_\oplus
0.4	0.4 C	0.33 C
0.4	0.4 M	0.67 M
0.3	0.3 W	



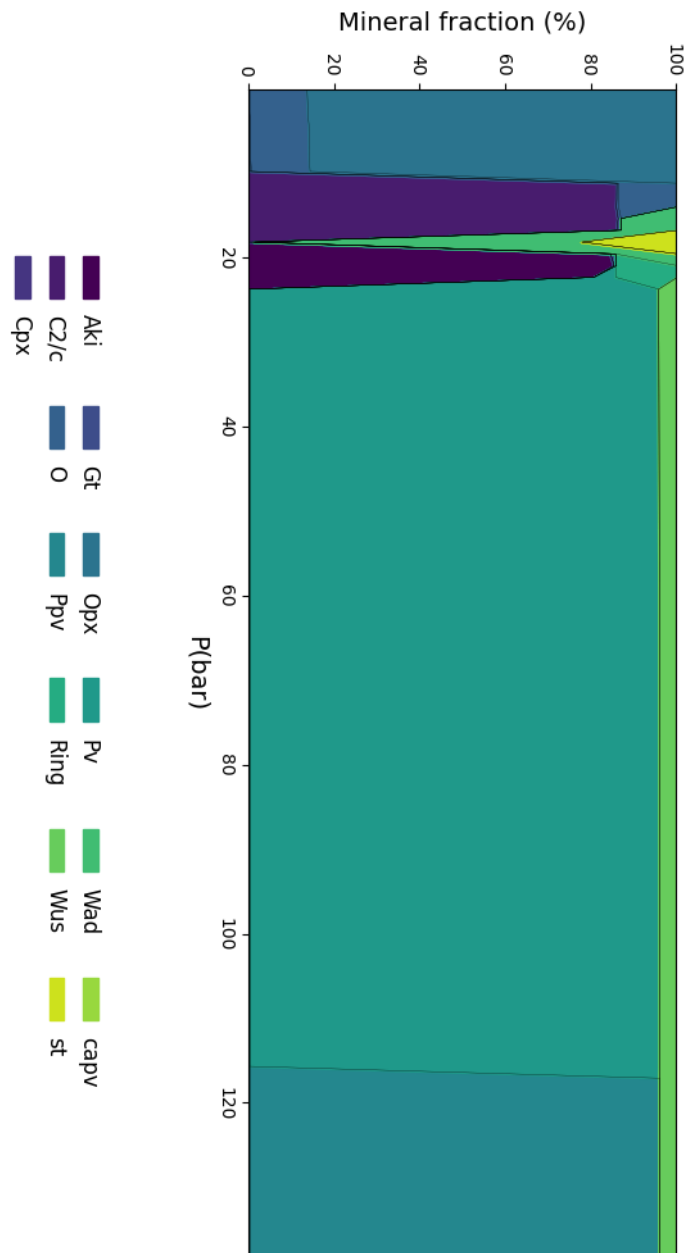
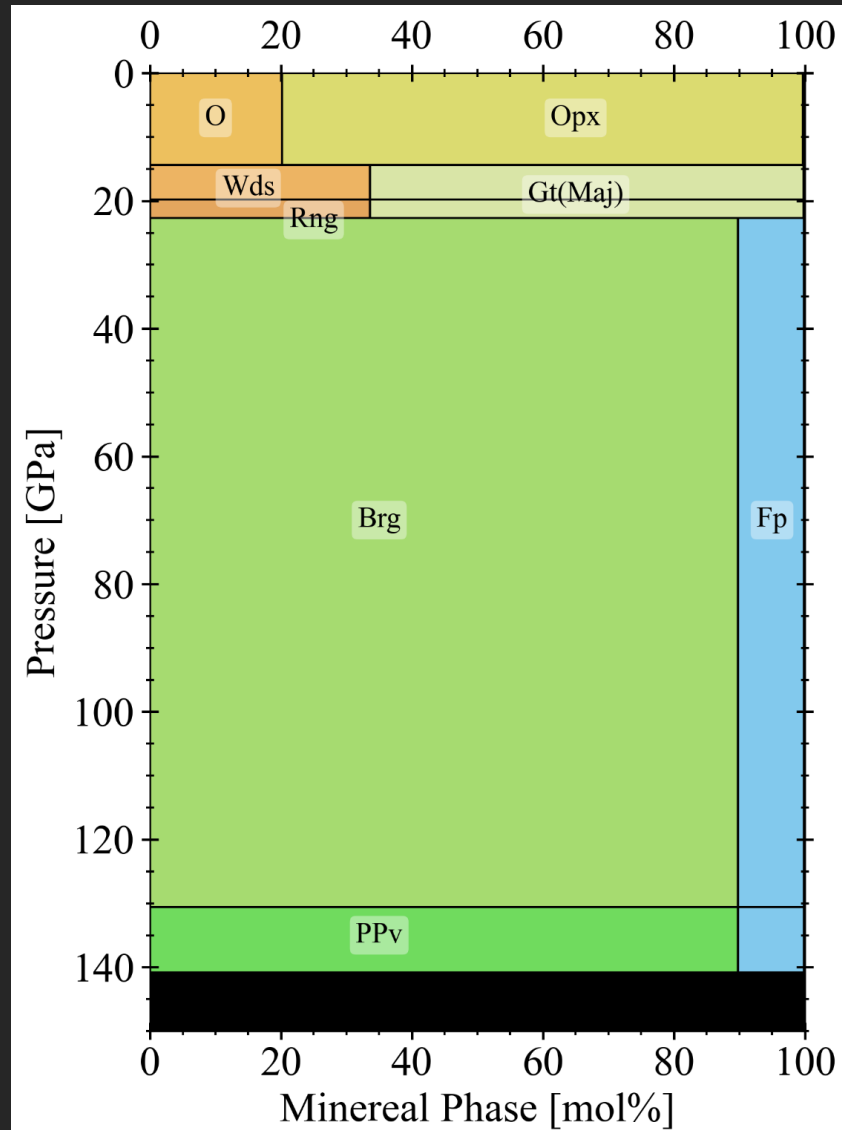


Upper: Mag: Stx:
 Olivine 50% 35-40%
 Cpx 12% 10%
 Gt 8% 12%
 Opx 30% 35-40%

Middle:
 Gt 35% 60%
 Rng 65% 40%
 (we need iron in gt would even out some)

Lower:
 Pv 70% 80%
 Wus 25% 15%
 Ca Pv 5% 5%

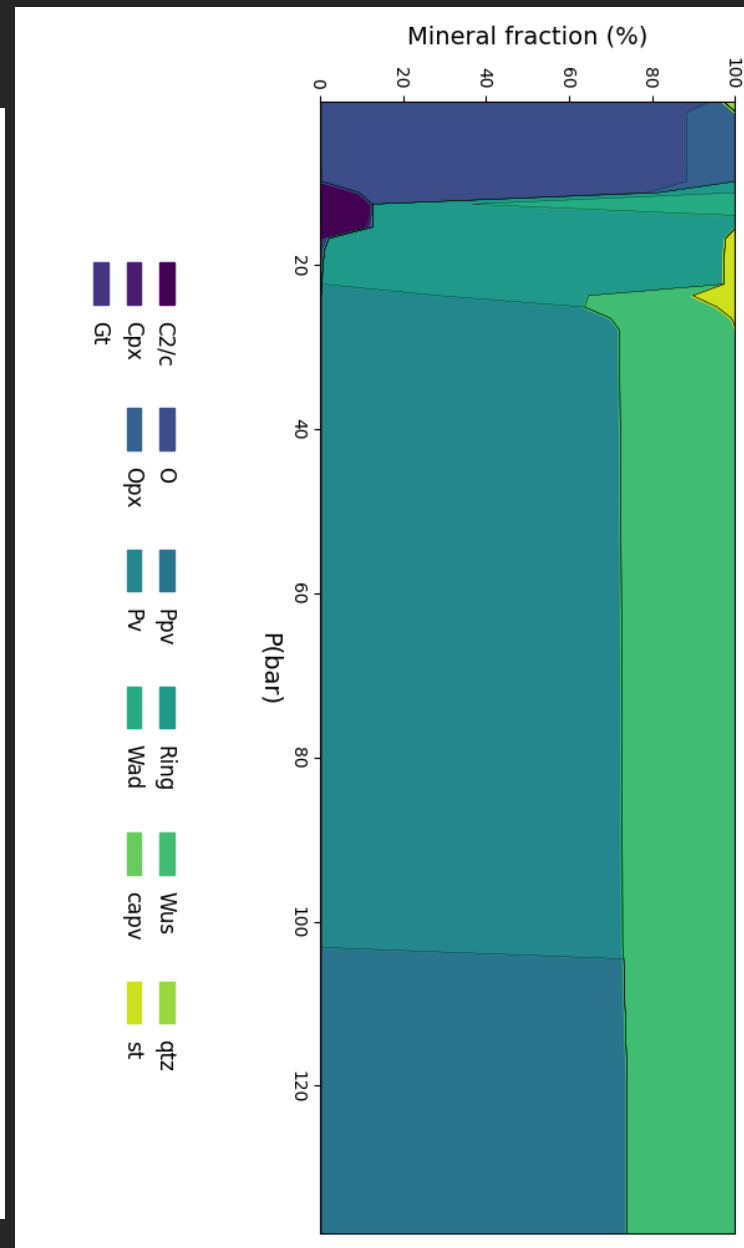
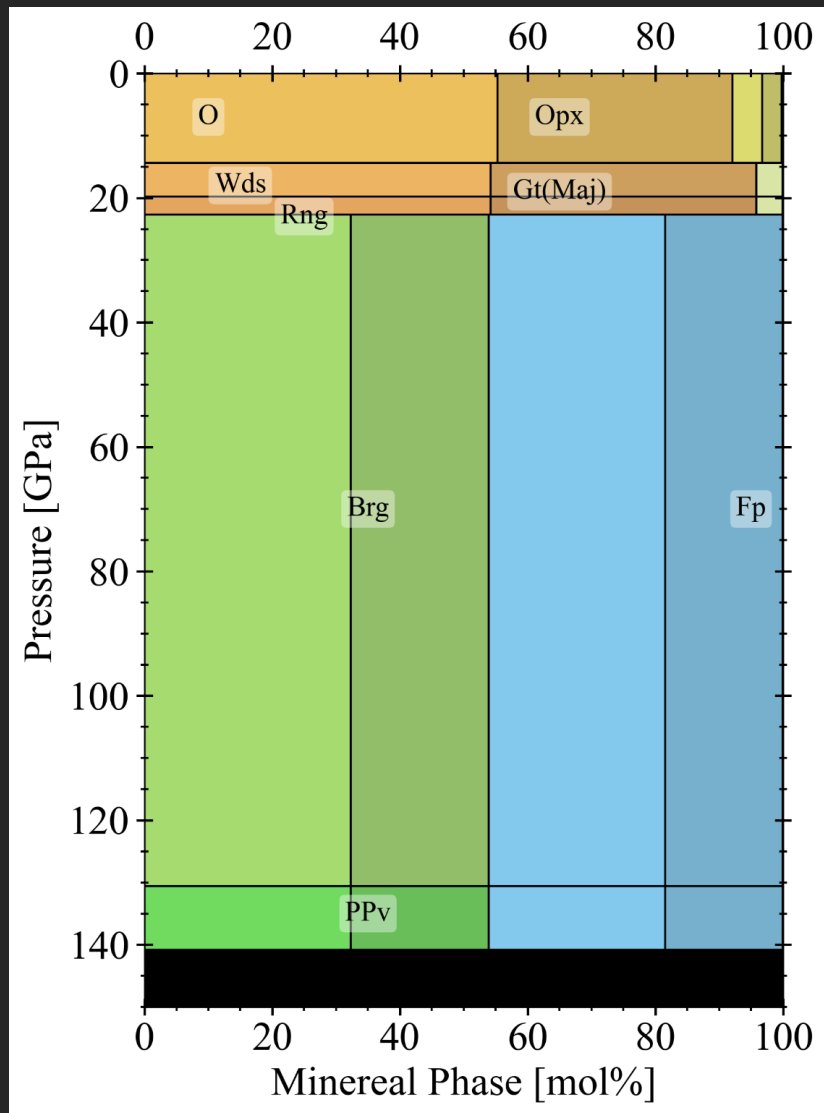




Upper: Mag: Stx:
 Olivine 20% 15%
 Opx 80% 75%

Middle:
 All kinds of weirdness

Lower:
 Pv 90% 95%
 Wus 10% 5%

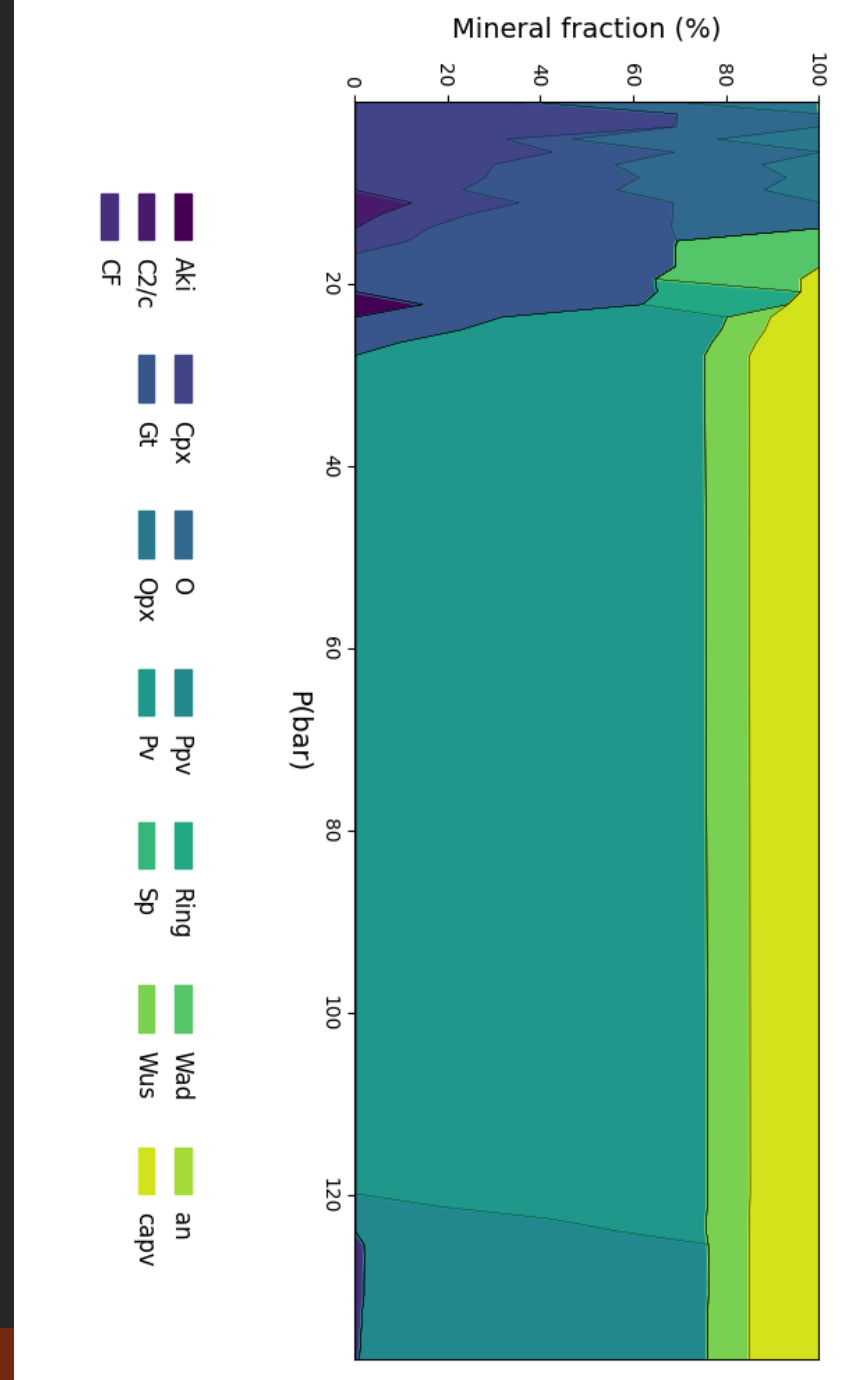
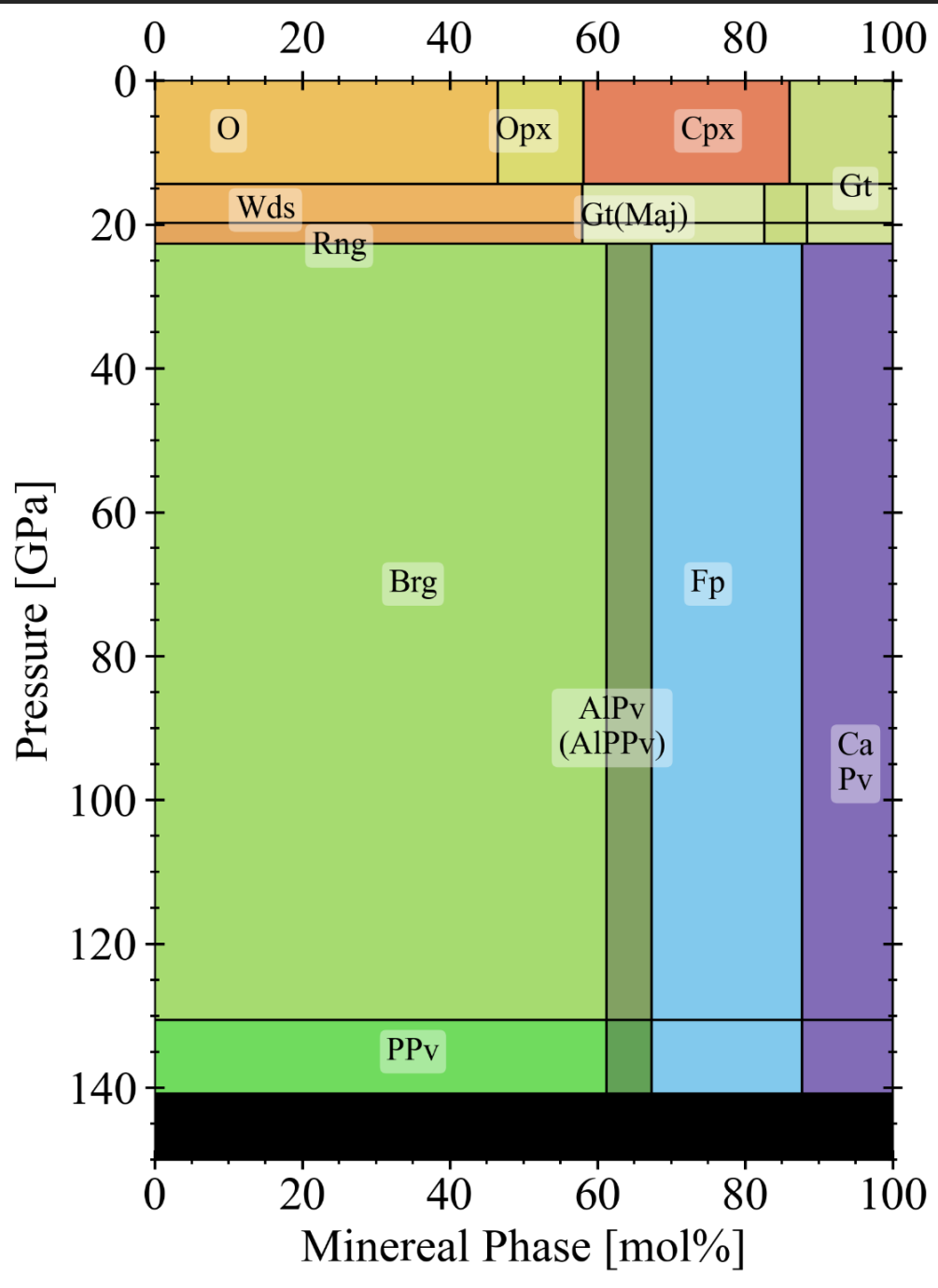


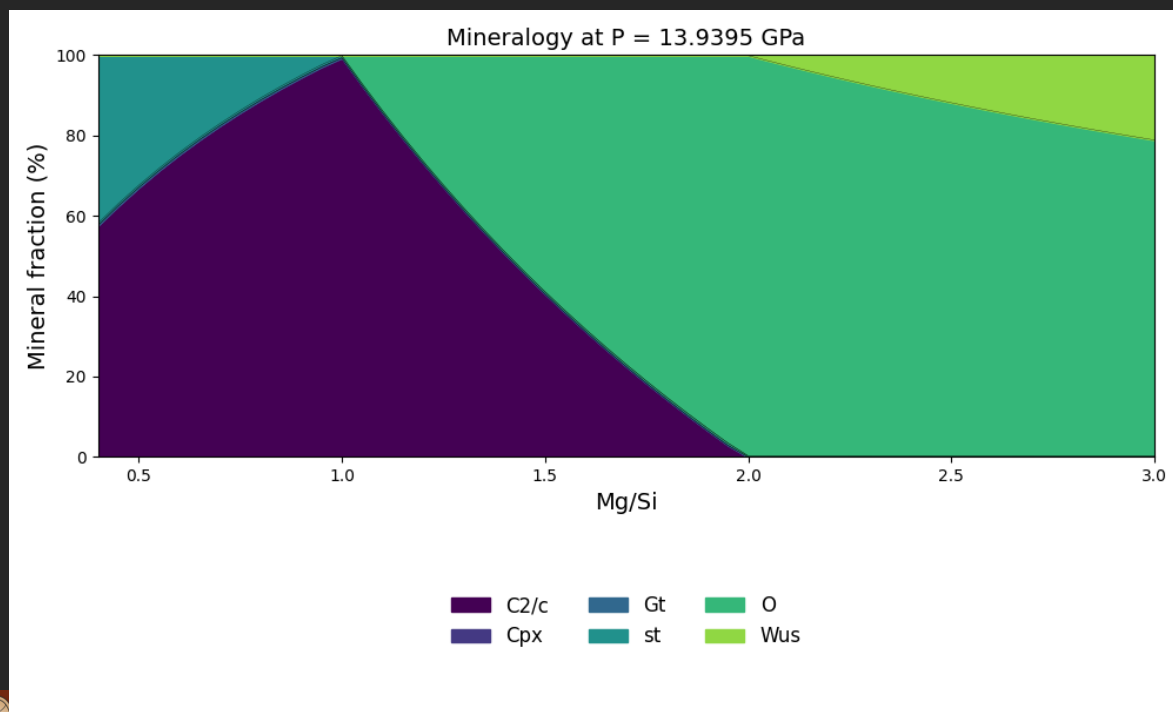
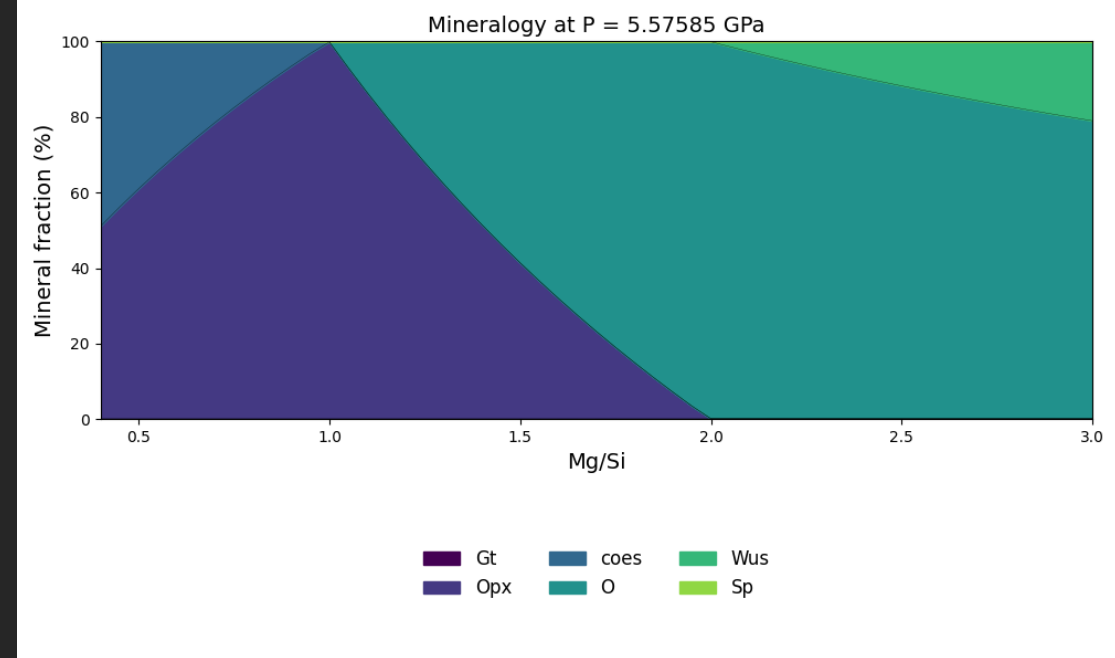
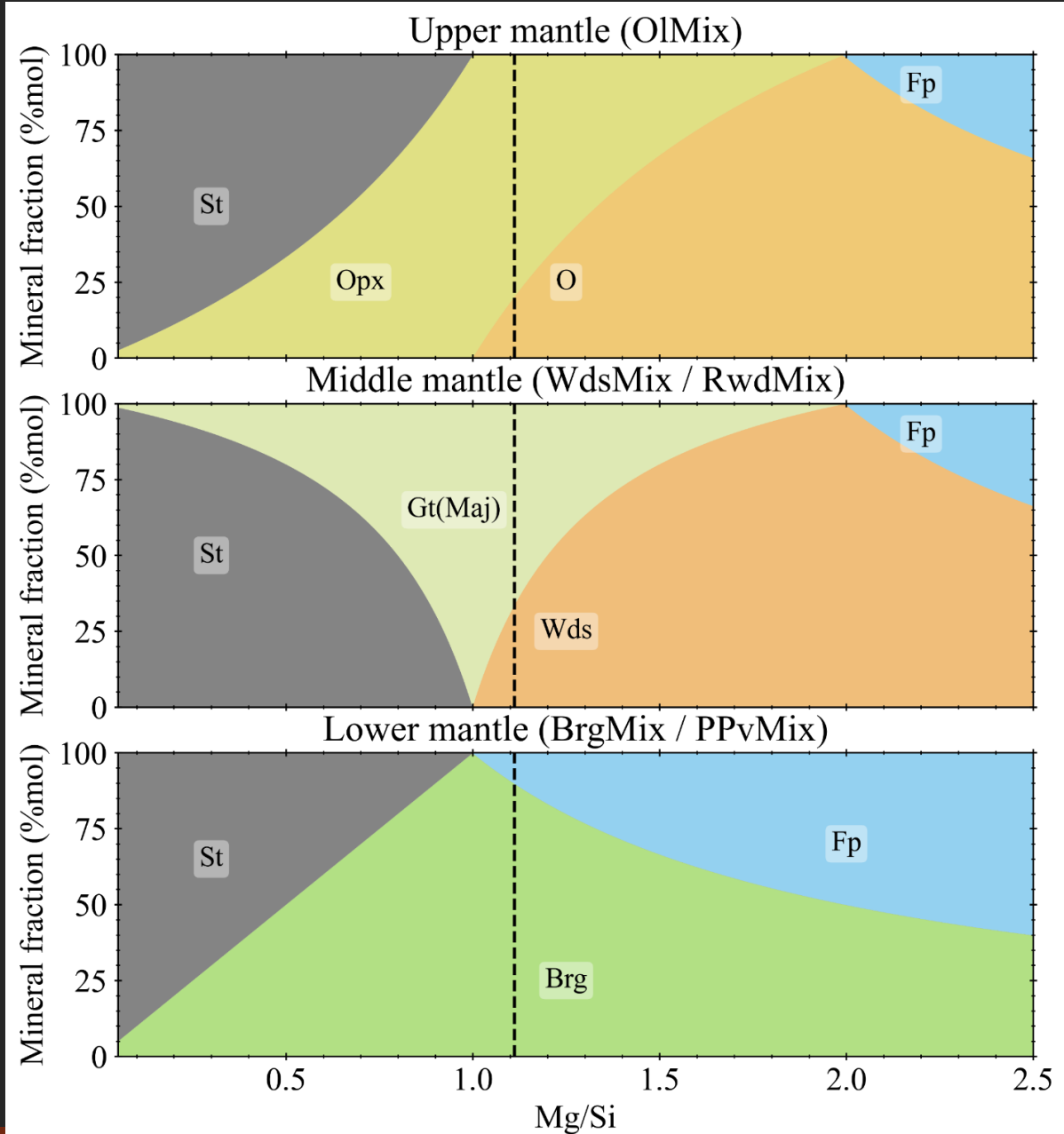
Upper: Mag: Stx:
Olivine 92% 90%
Opx 8% 10%

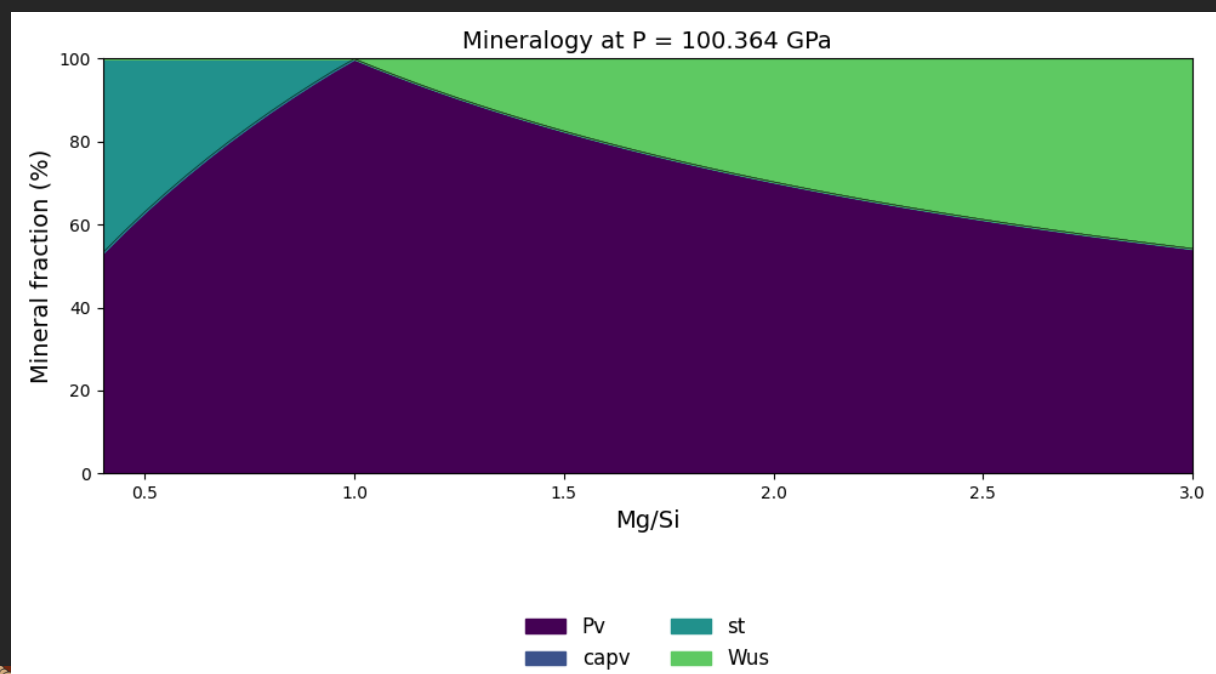
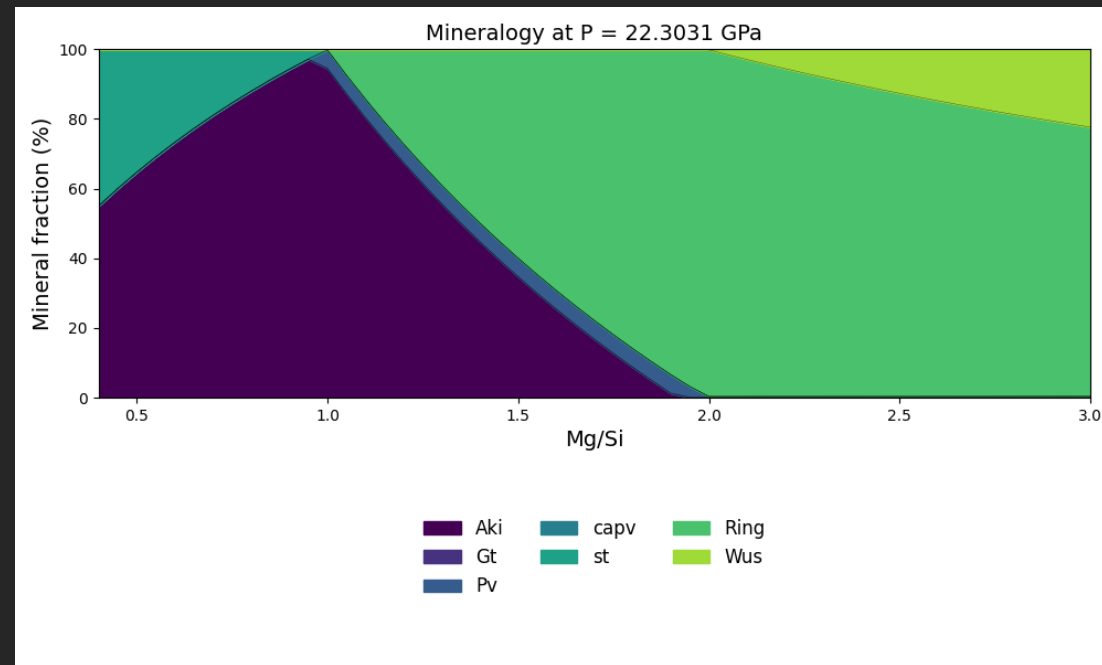
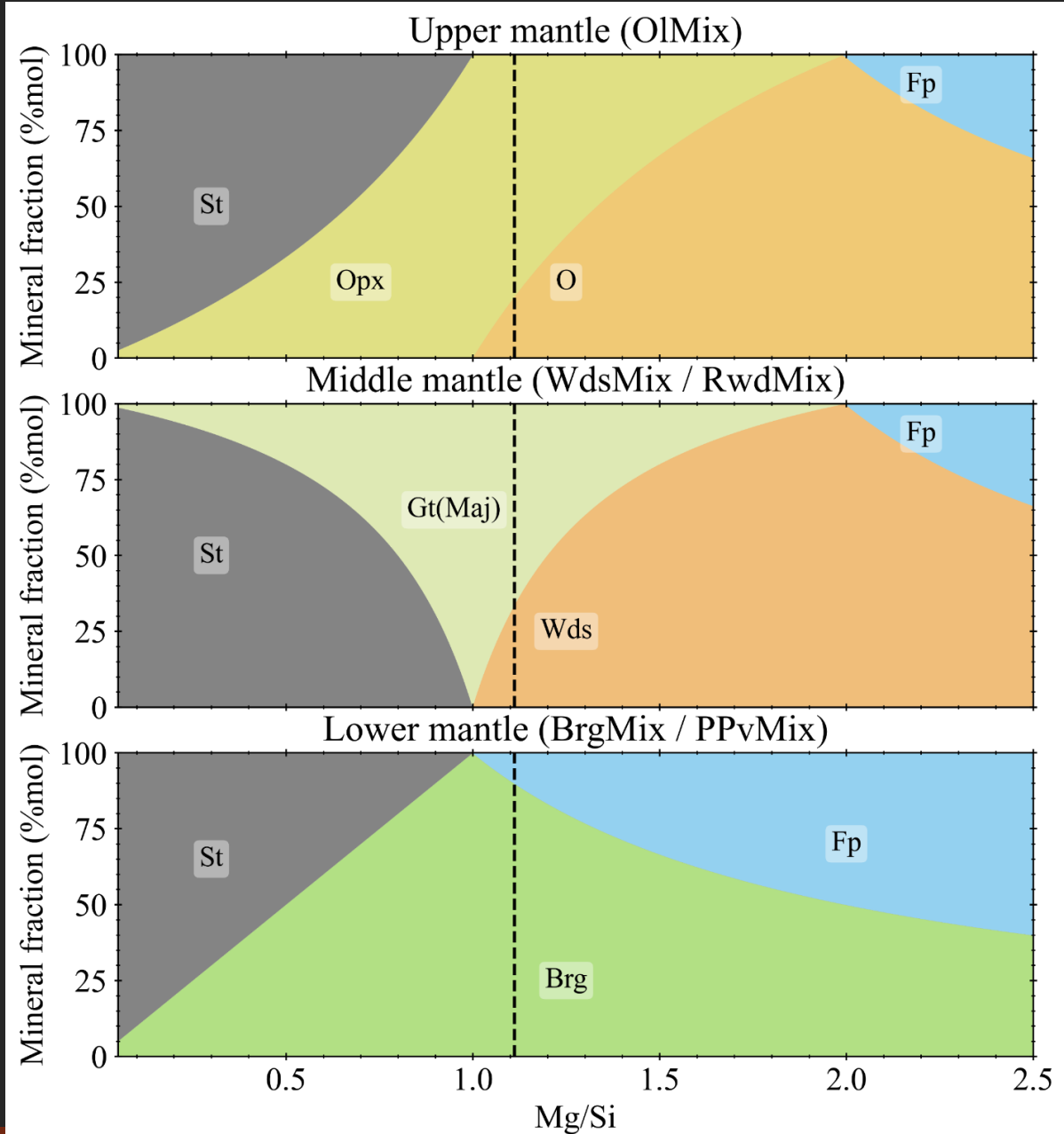
Middle:
Wds/Rng 96% 90-100%
Gt 4% Stx: C2/C or St 10-0%

Lower:
Pv 55% 70%
Wus 45% 30%

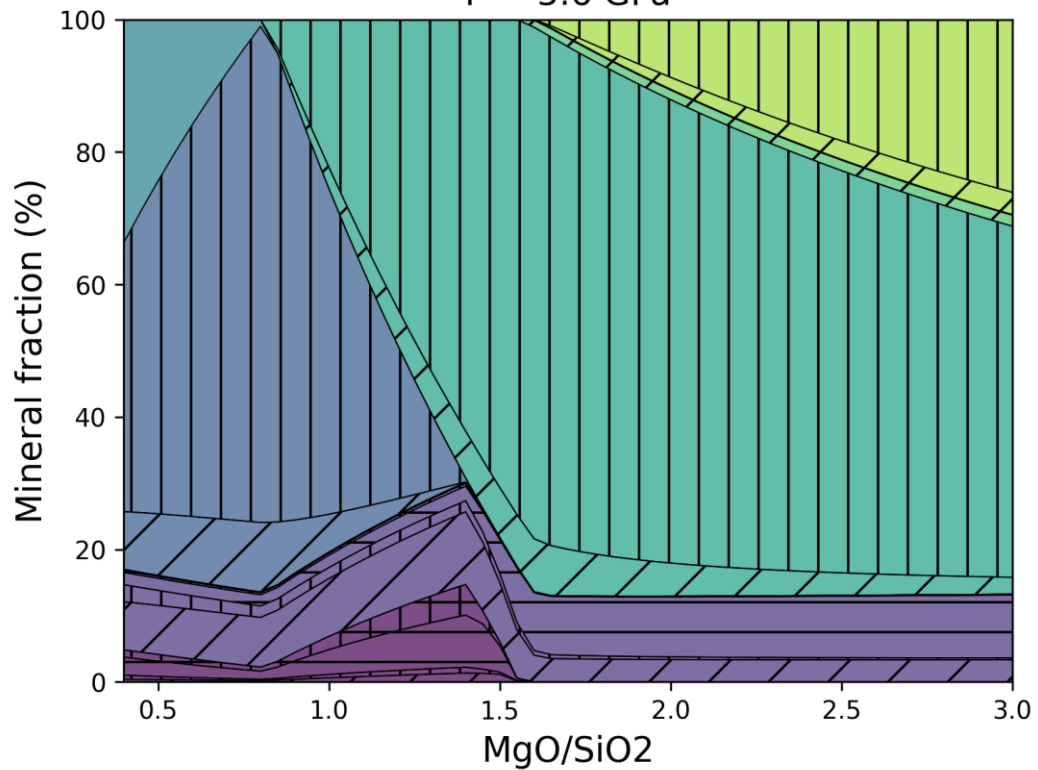
High Minor
 INPUTS USED:
 Ca/Mg=0.15,
 Al/Mg=0.15,
 Si/Mg=0.9,
 Fe/Mg=0,
 Mg# = 1



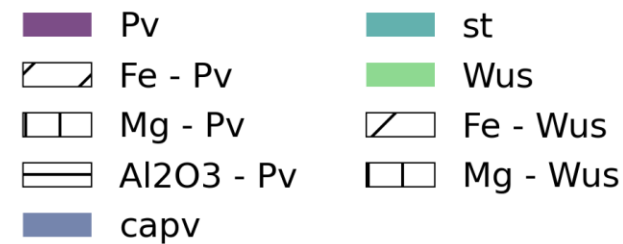
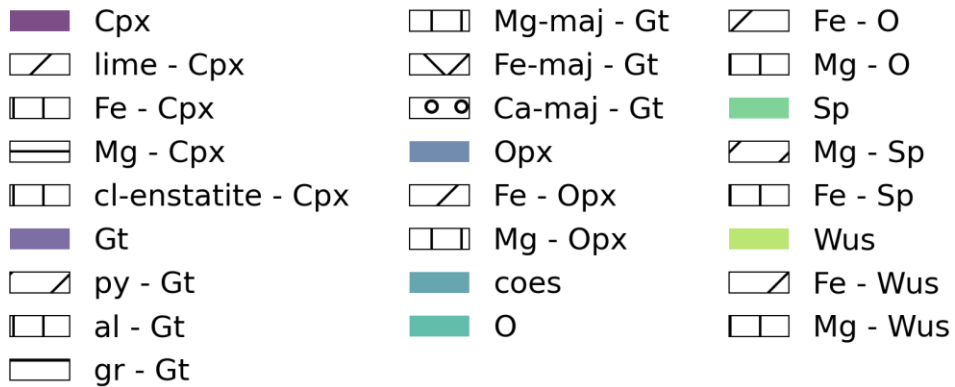
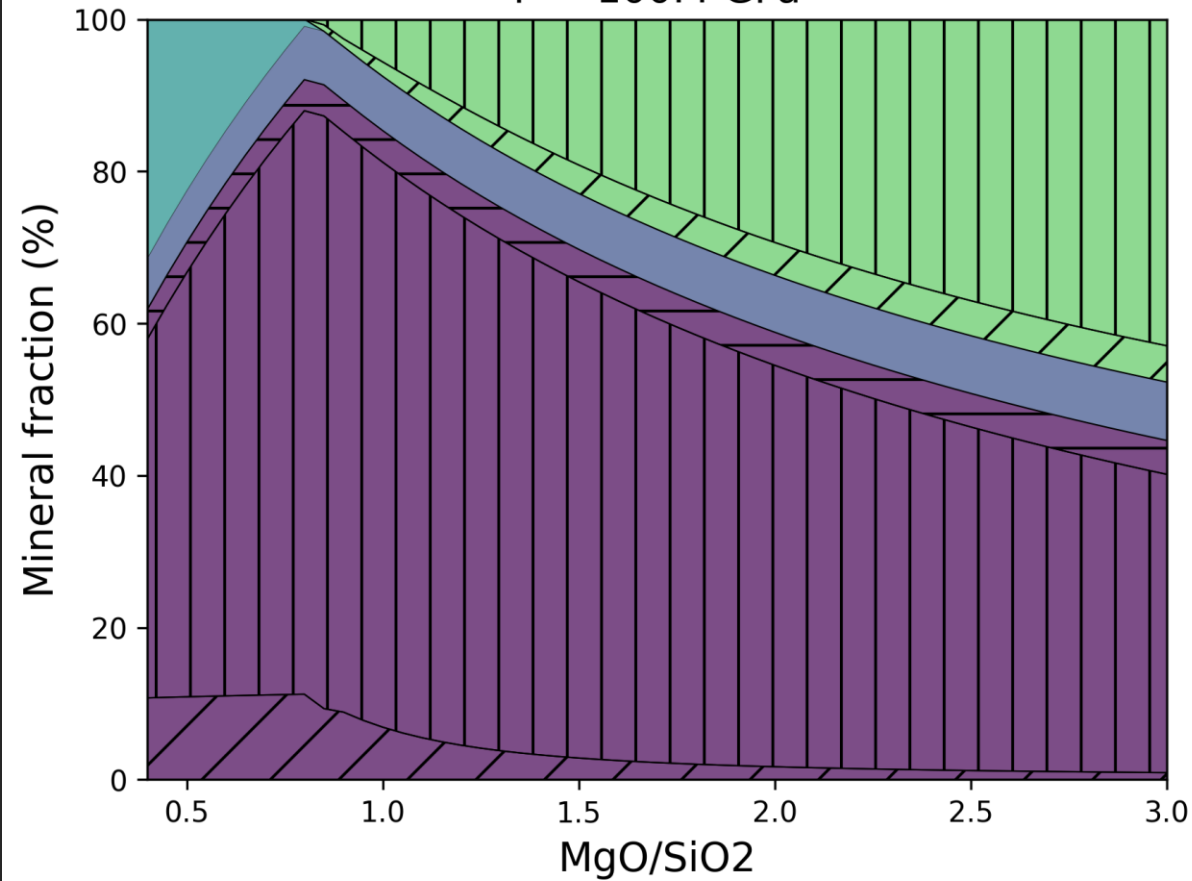


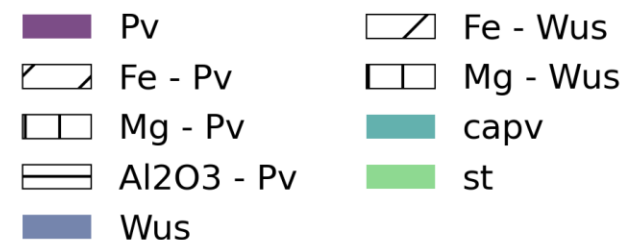
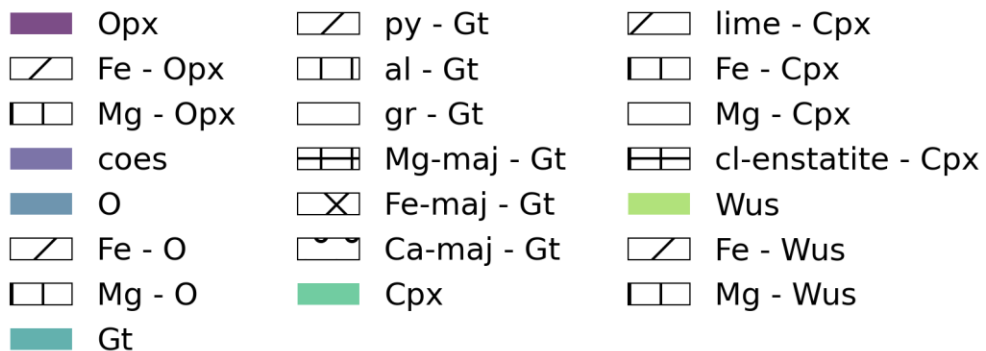
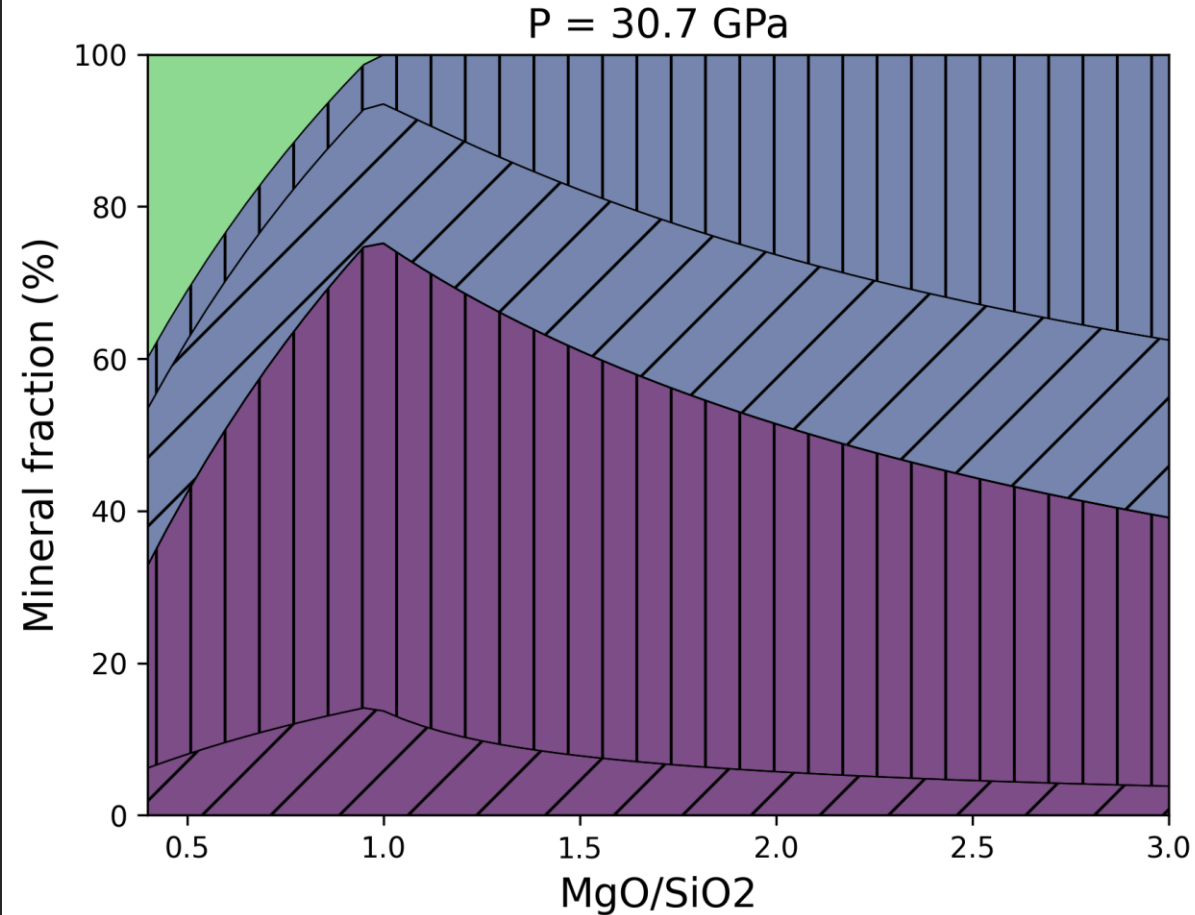
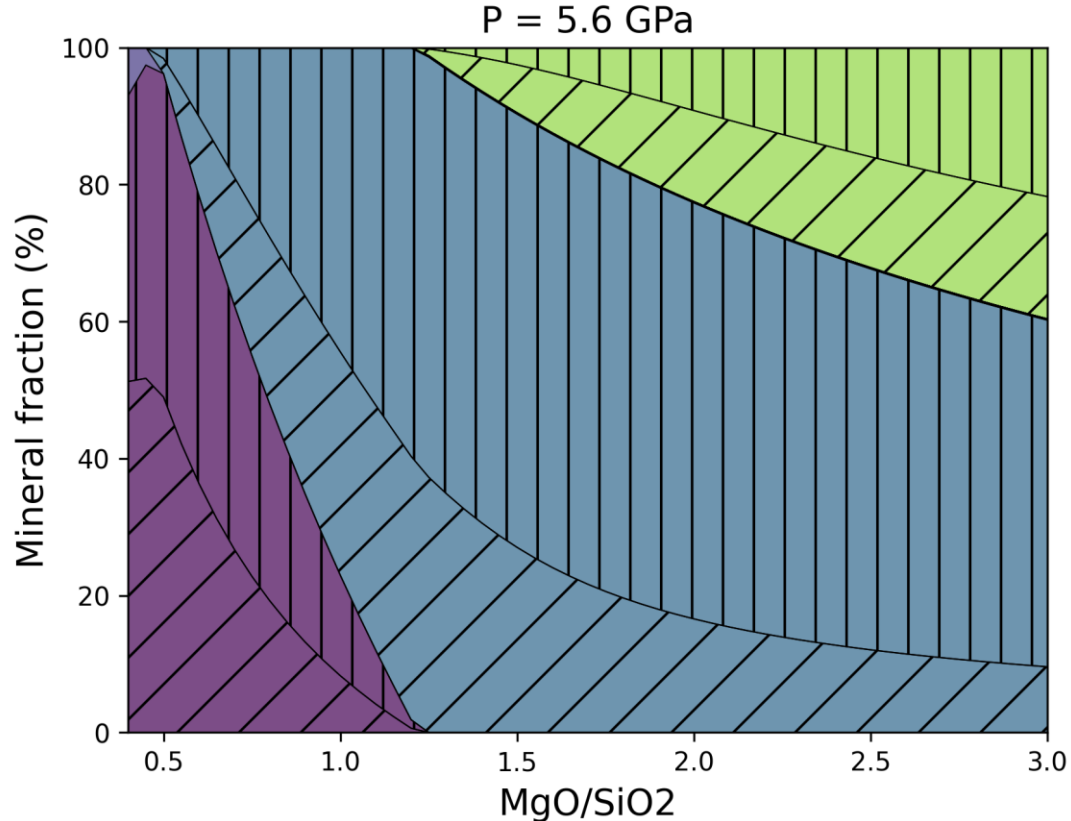


P = 5.6 GPa



P = 100.4 GPa



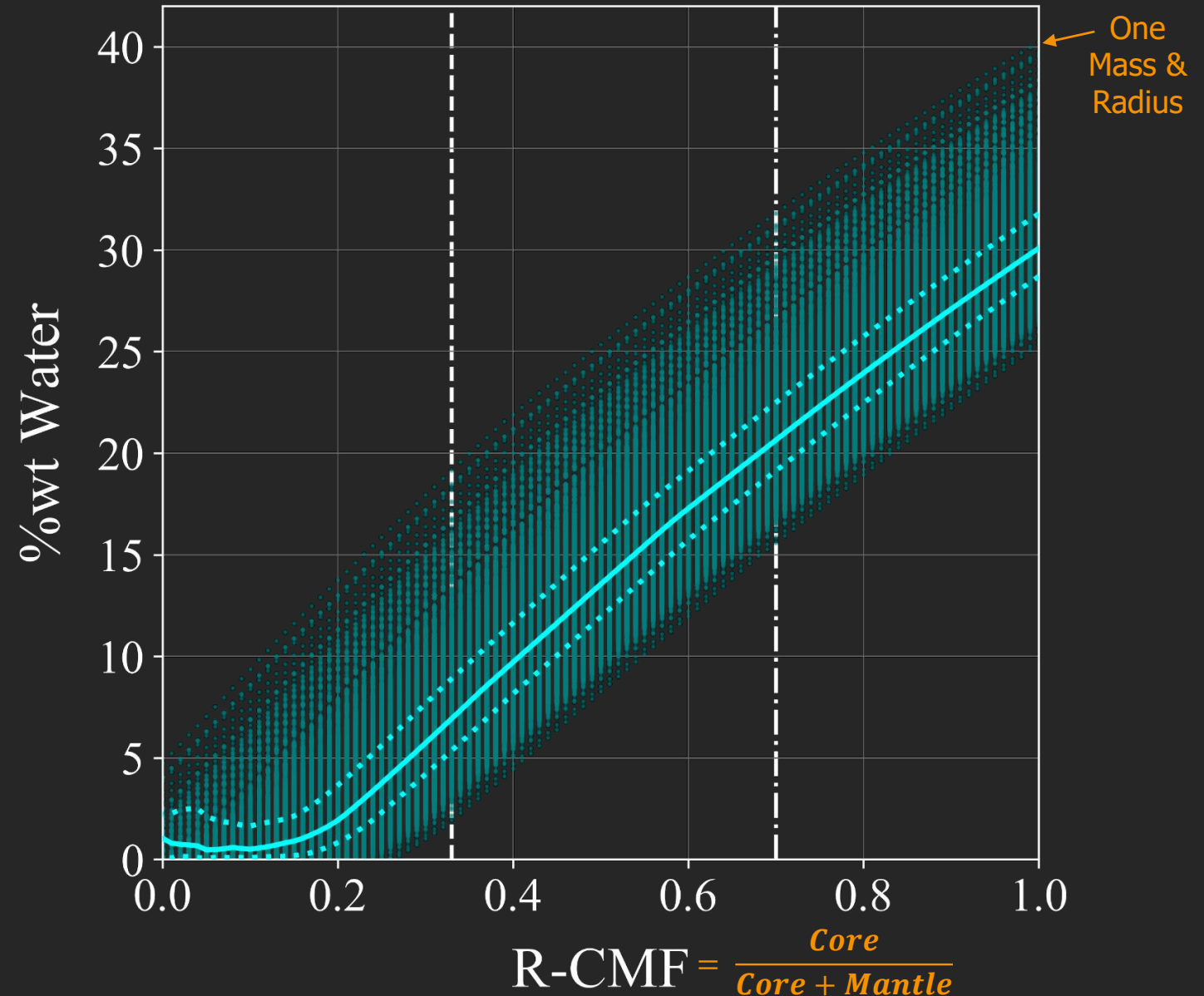


v2.0 Standardized Planet Solvers

3-Layer Secant Method Solver:

1. Given a Planet Mass
2. Hold 2 layers in mass ratio
3. Shoot for 3rd layer mass
4. Match Planet Radius

500,000 WMFs –
2.5 million runs of
Magrathea

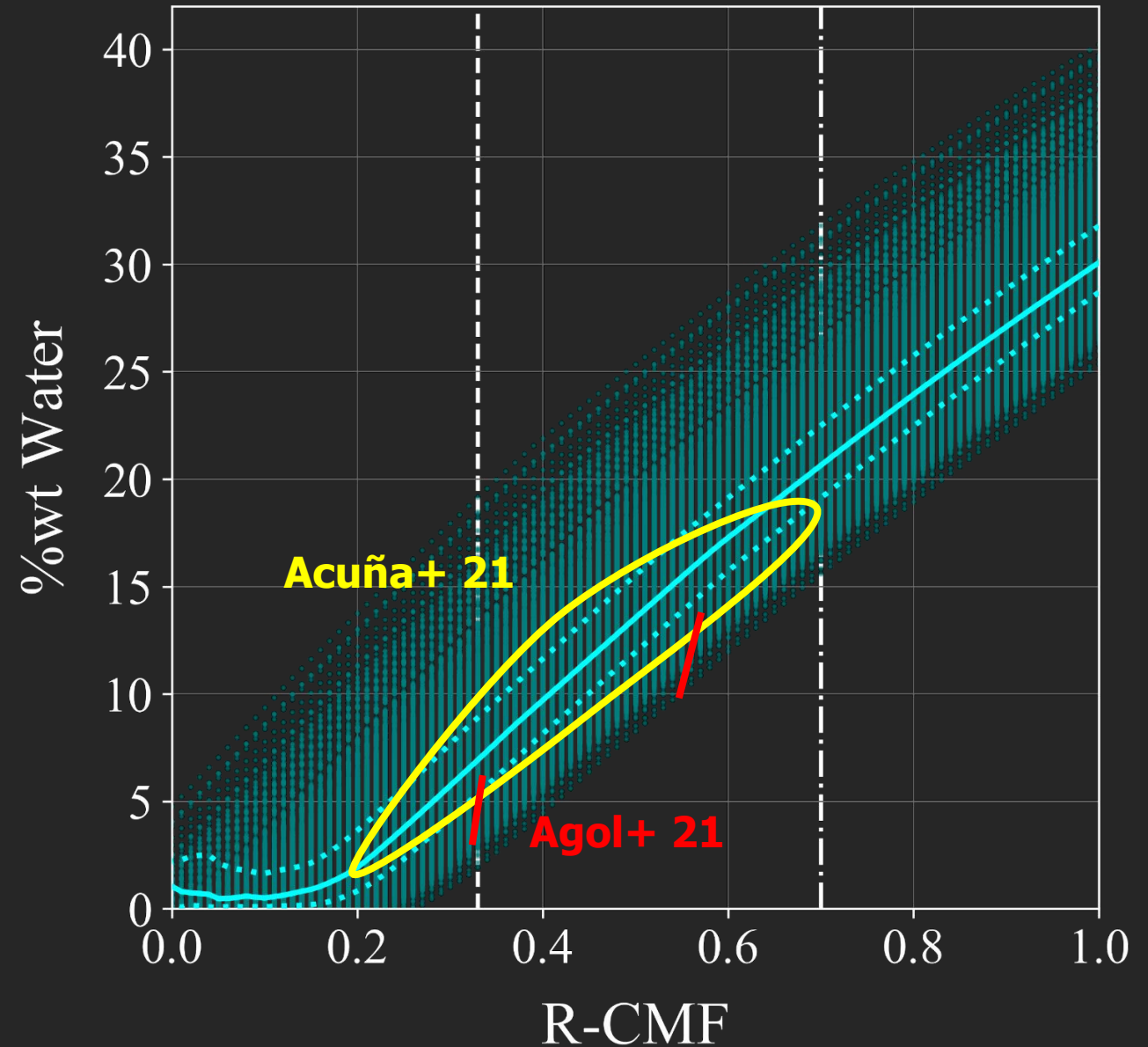


v2.0 Standardized Planet Solvers

Interior of **Trappist-1f**

Agol+ 21
 $1.045 \pm 0.013 R_{\oplus}$
 $1.039 \pm 0.031 M_{\oplus}$

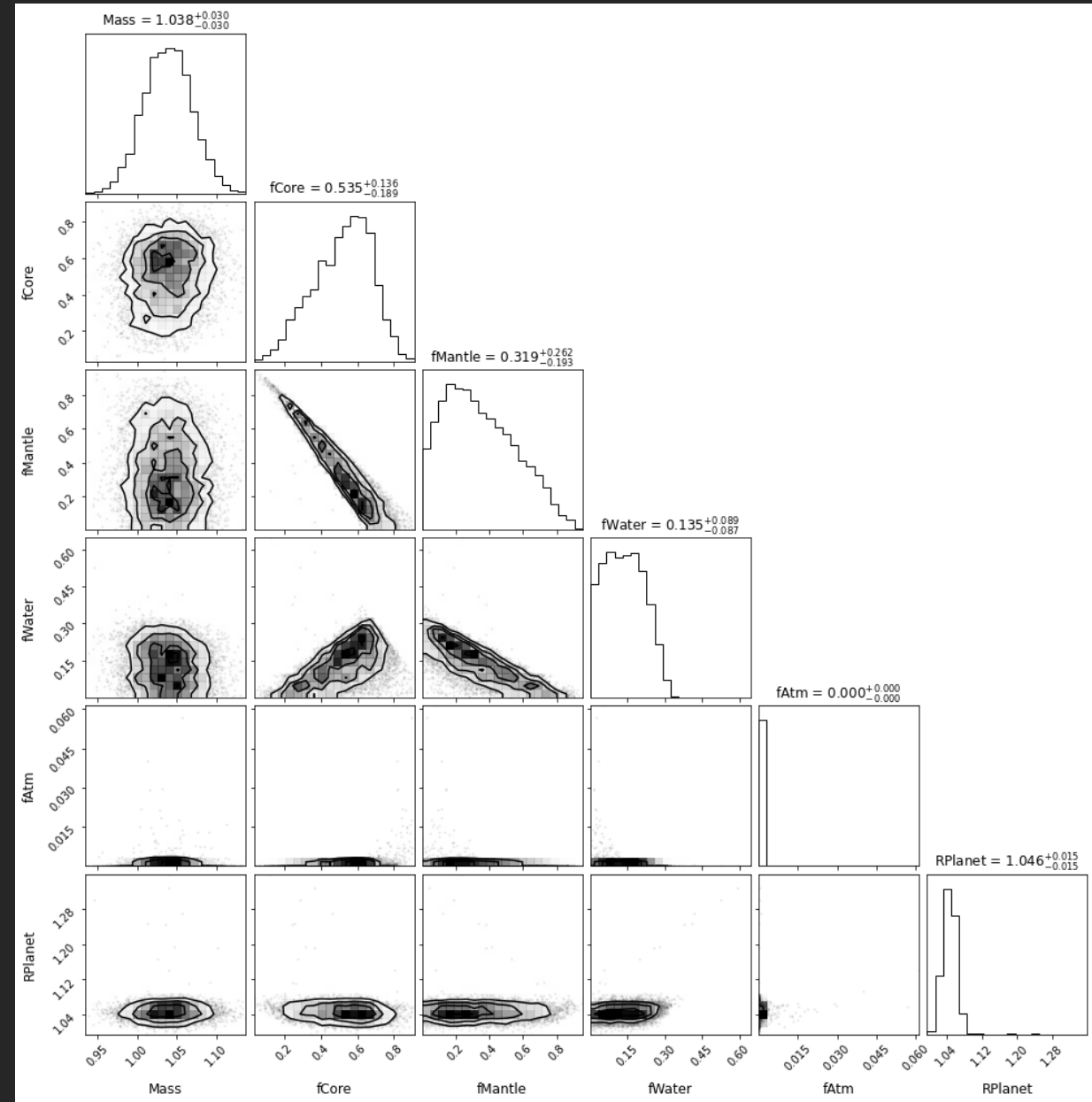
Rice+ 25 we explore
obs. and model
uncertainties to WMF

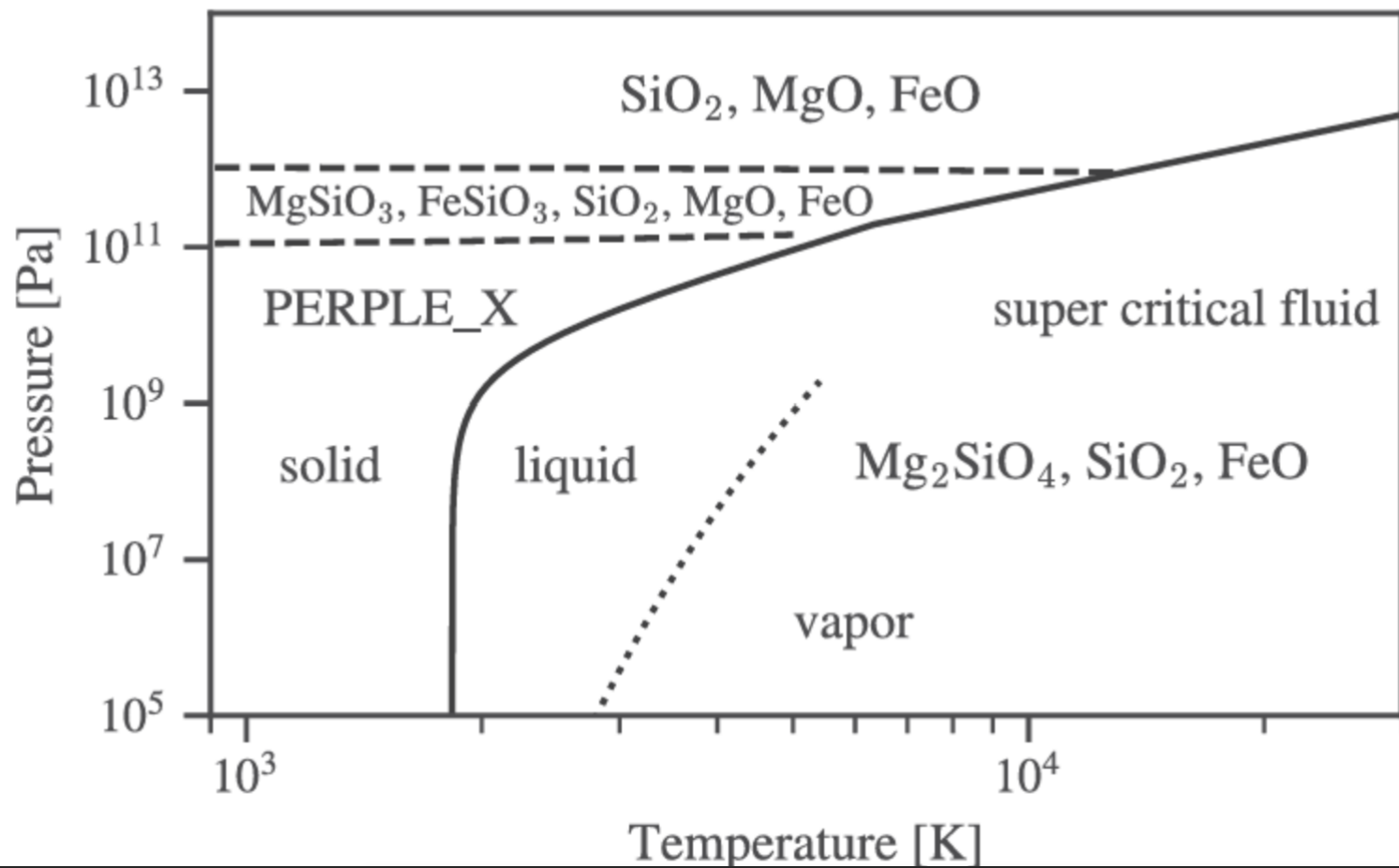


v2.0 Standardized Planet Solvers

MCMC composition
retrieval

Needs Testing





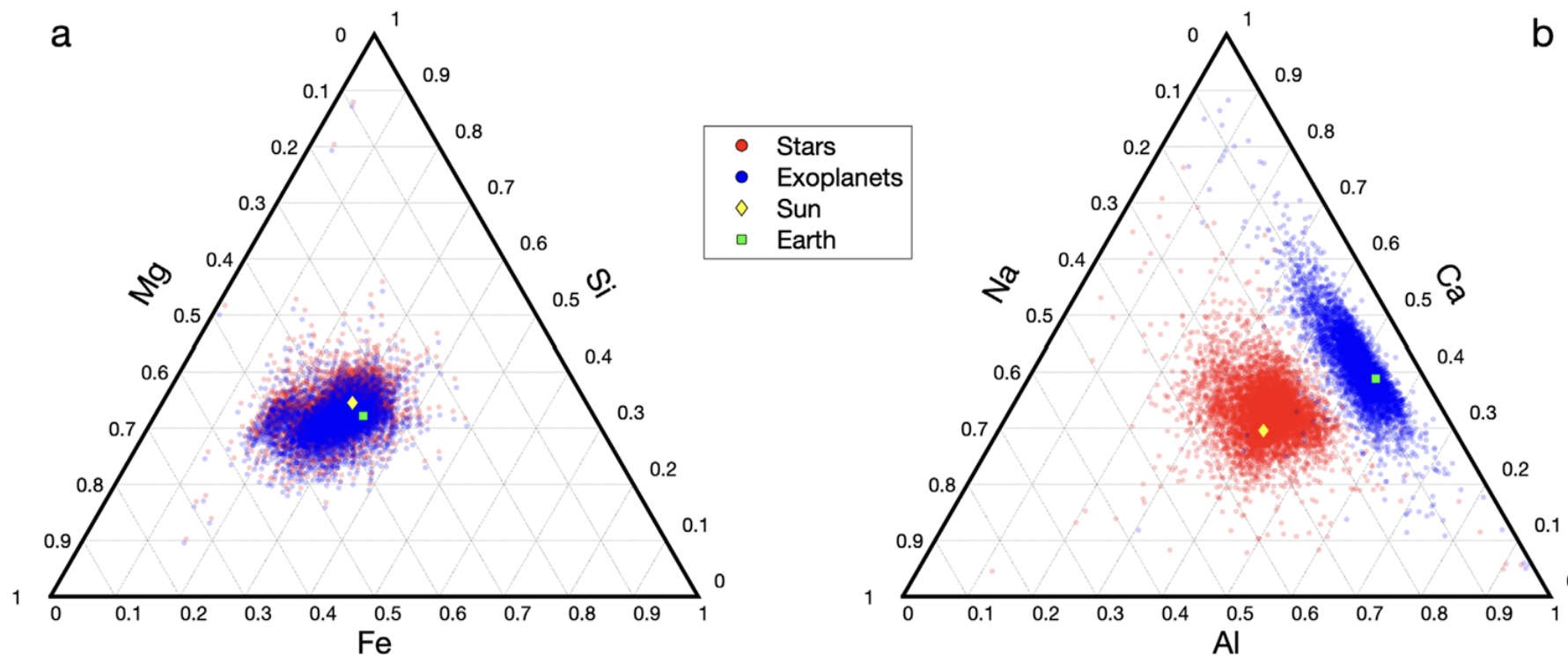


Figure 2. Bulk compositions of stars in the solar neighborhood (red; Hinkel et al. 2014; Buder et al. 2018), planet compositions calculated in this work (blue), solar composition (yellow diamond; Lodders et al. 2009), and Earth composition (green square; McDonough 2003) molar compositions, in the Fe–Mg–Si (left) and Ca–Al–Na (right) systems.

Magrathea's Composition Finder

