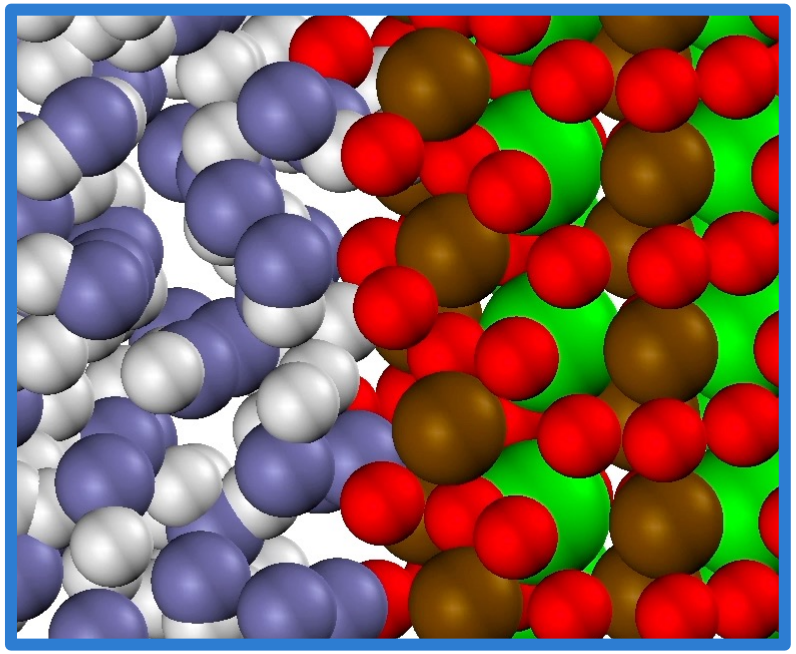
# Heat Until it Mixes

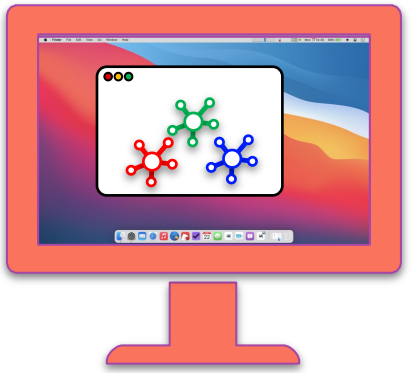
# A first principles exploration of the miscibility of ($MgO/MgSiO_3$)-$H_2O$ at HED conditions

Tanja Kovačević Ph.D. Candidate

# Hello there!

Tanja Kovačević
4th year Ph.D. Candidate
U.C. Berkeley - EPS
Burkhard Militzer





DFT(MD) = density functional theory molecular dynamics

# AGENDA

**BEGINNING**

#

- Motivation

**MIDDLE**

#

- Method
- Results

**END**

#

- Implications
- Summary

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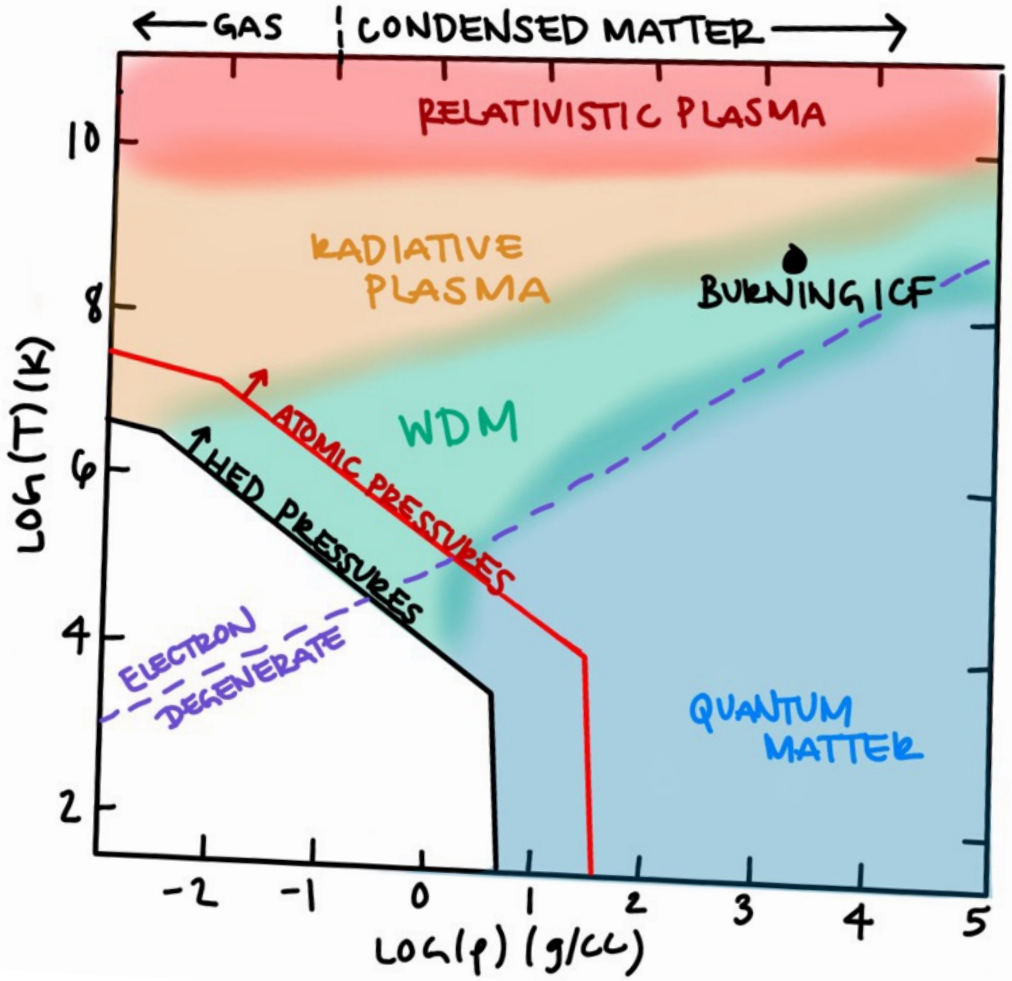
# The importance of HED science

From the perspective of a graduate student

...and the National Academies Consensus Study Report on Fundamental HEDS Research




R. Collins (2023) NAS Consensus Report

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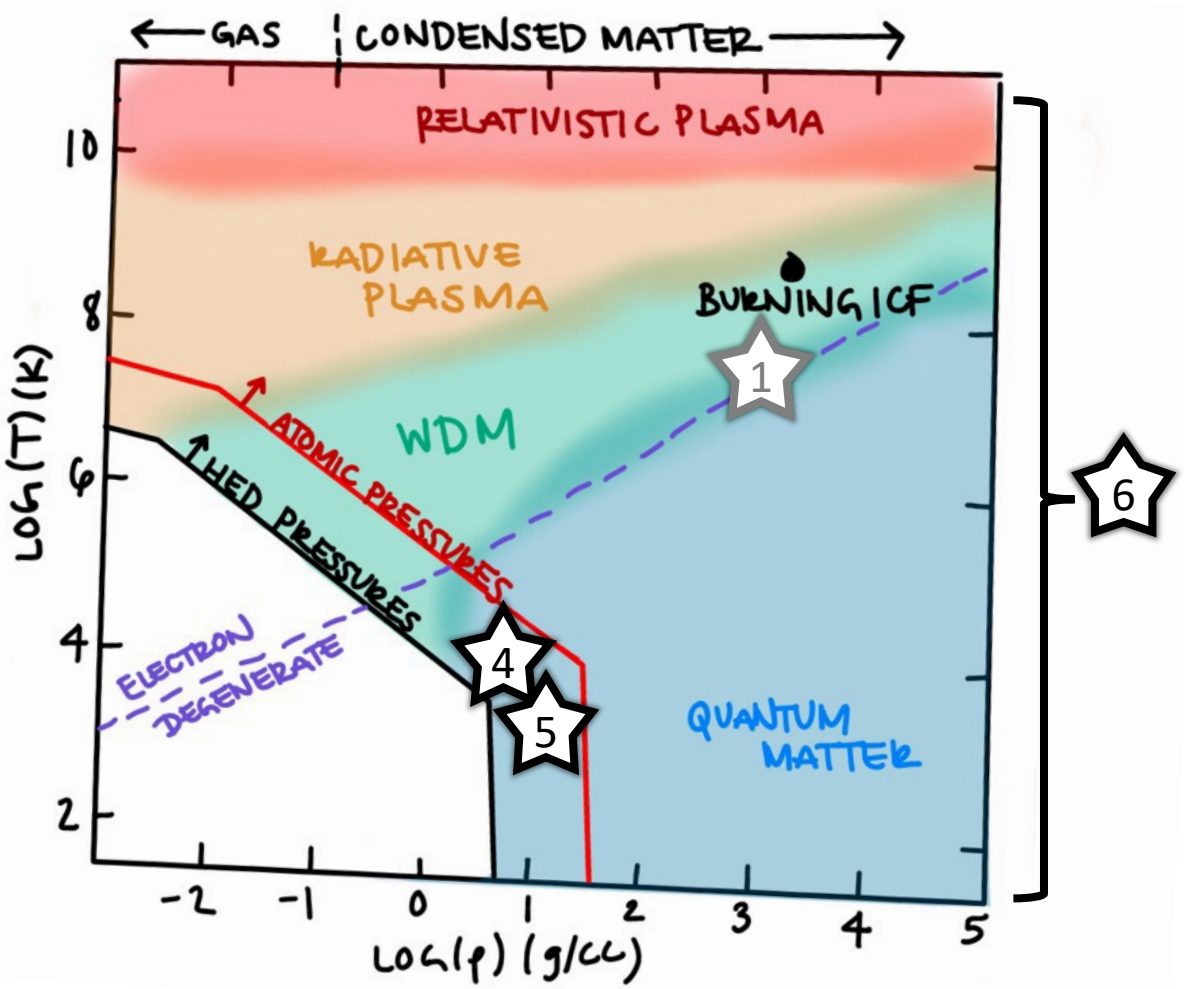


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From the perspective of a graduate student

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1 Laboratory based nuclear fusion

4 New chemistry

5 Evolution of planets / conditions for life

6 Cross cutting science
(Multi-scale nature of HED science)

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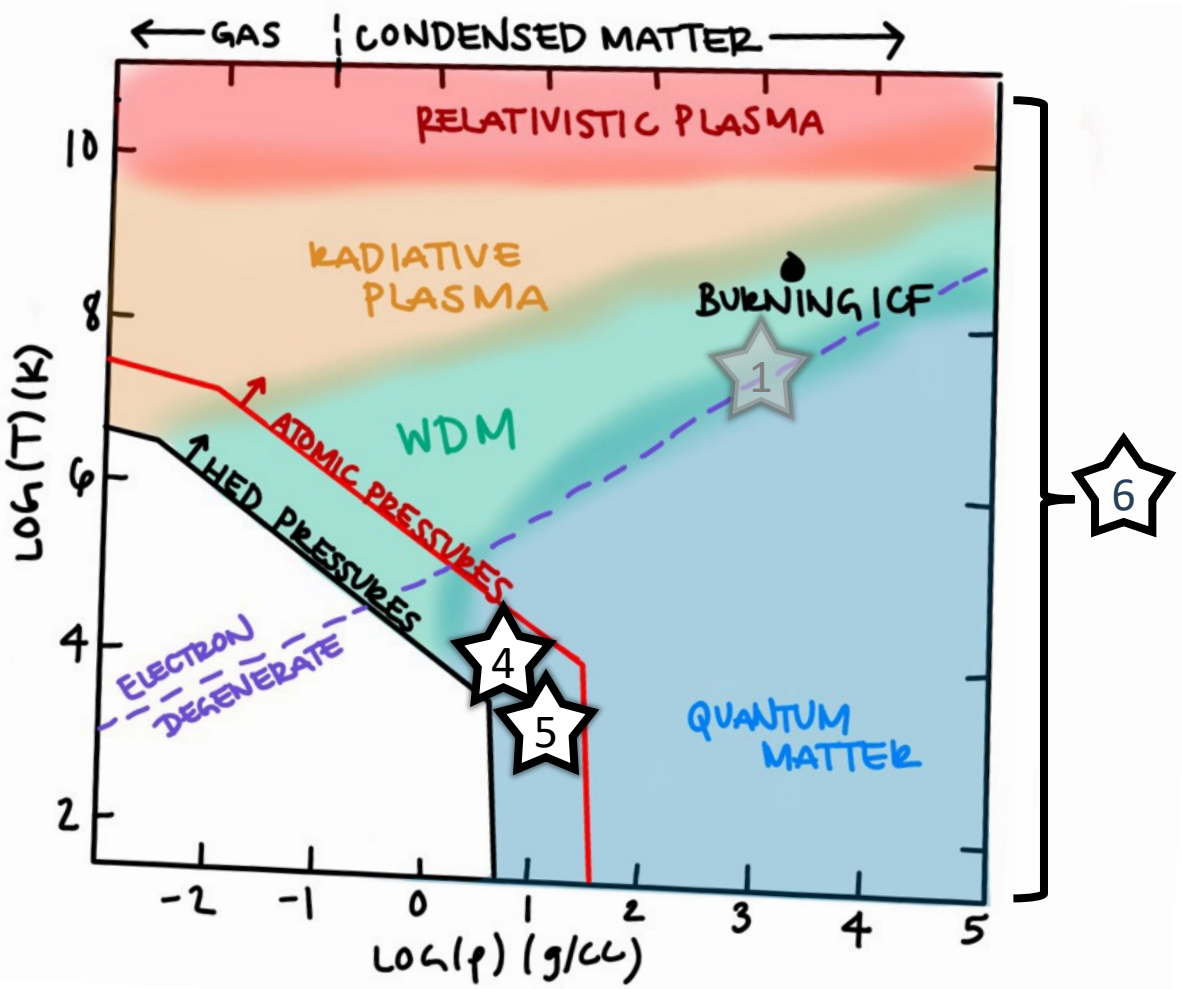


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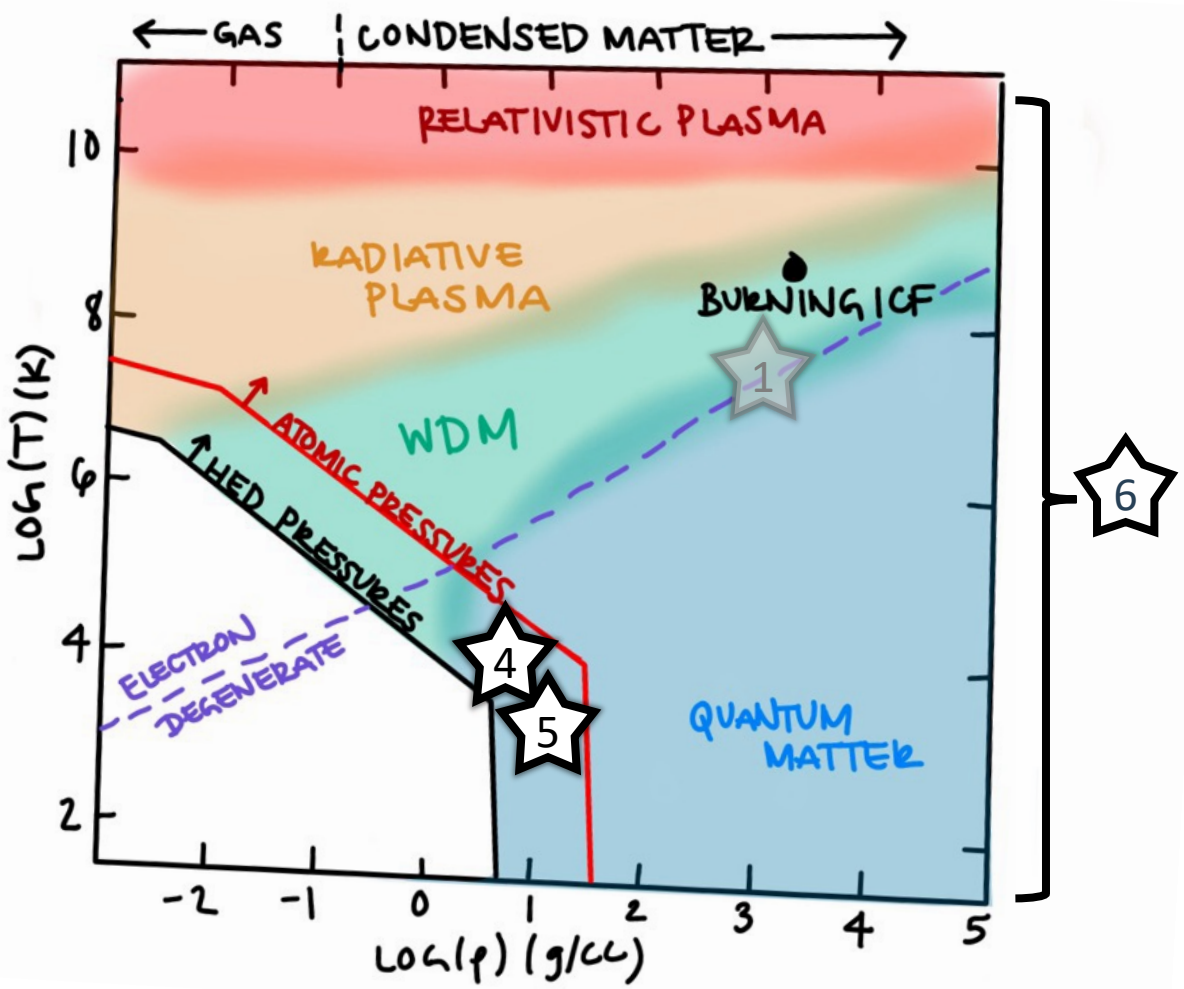


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- rheology, formation, evolution of planets/exoplanets

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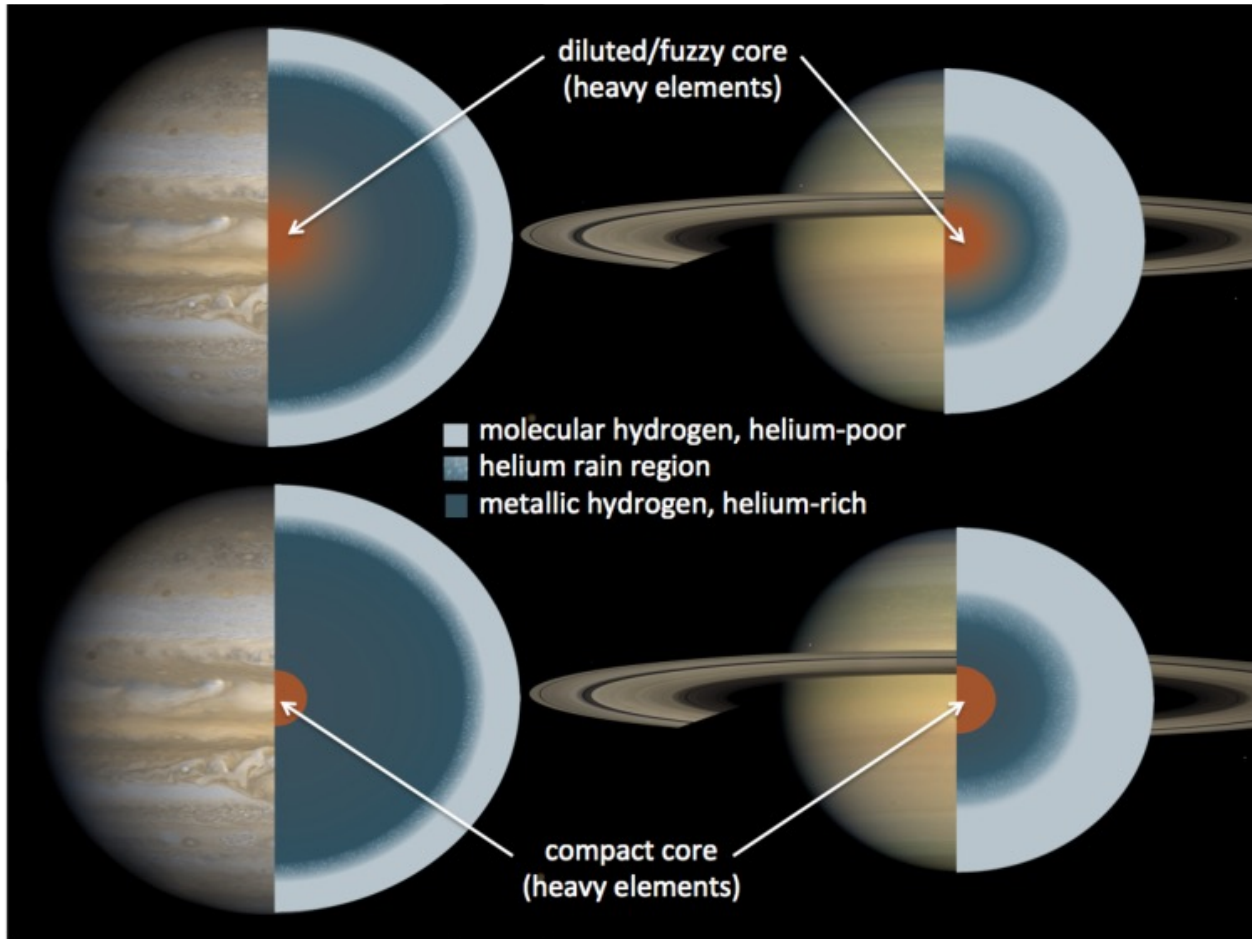
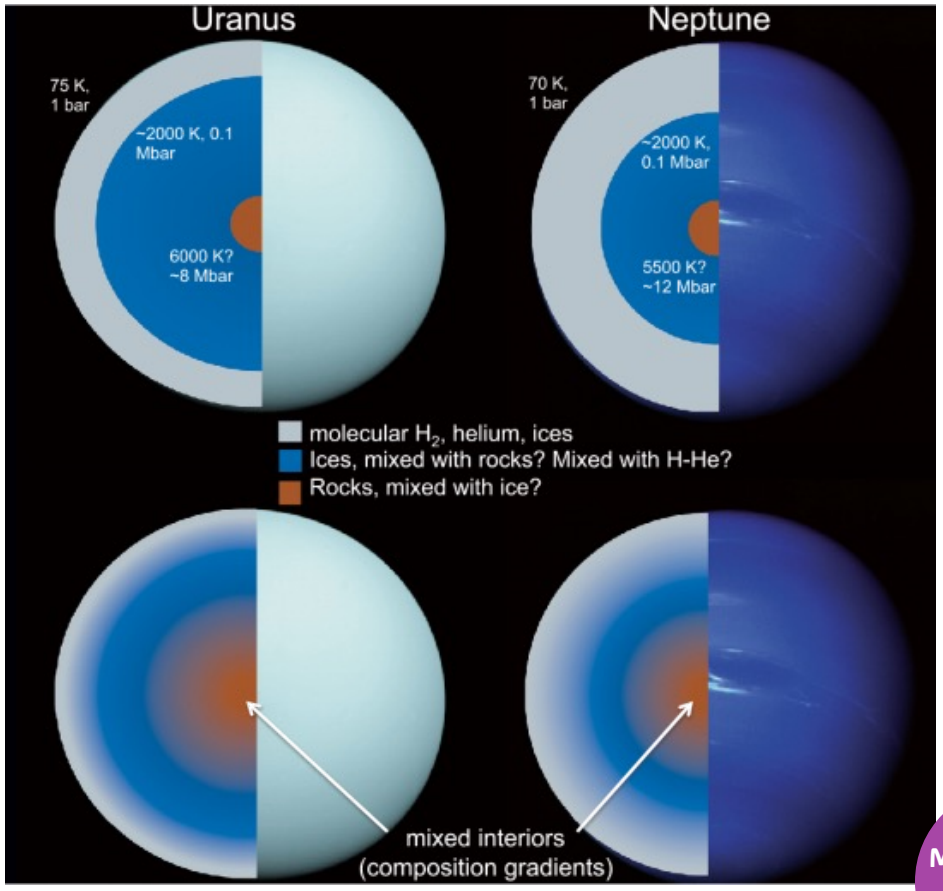
(Multi-scale nature of HED science)

# An aside… grand challenge 5 Planets!




R. Helled+ *OREs* (2019)

R. Helled+ *Space Sci Rev* **216**, 38 (2020)



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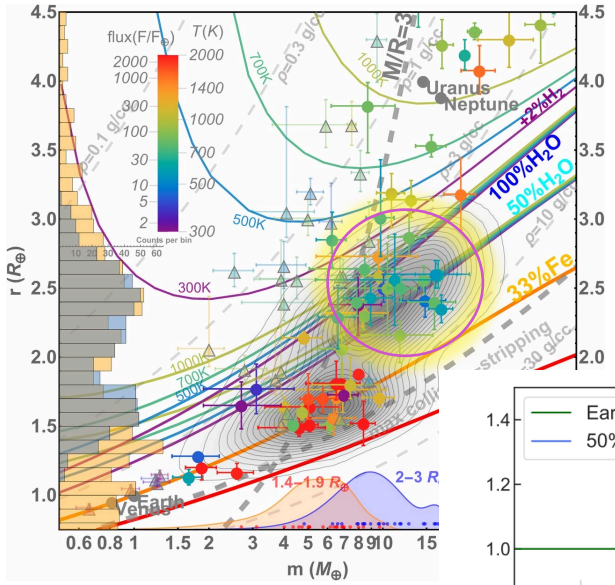
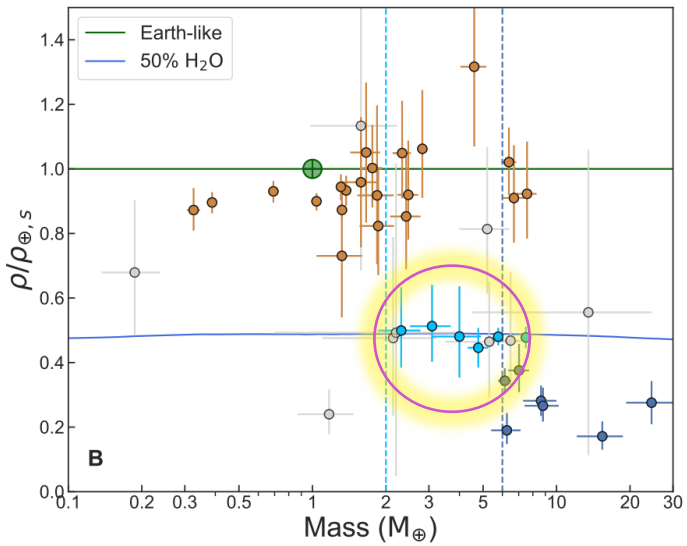
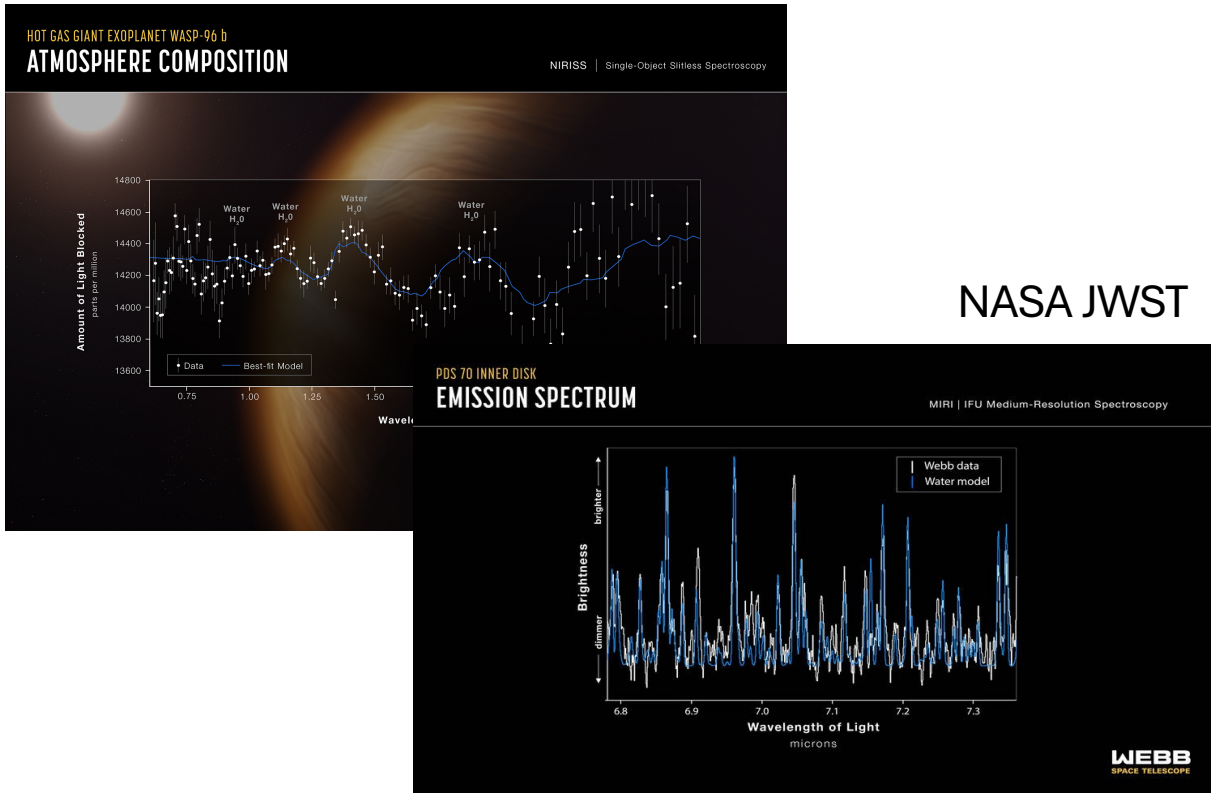



Zeng+ PNAS (2022)

Luque+ Science (2022)



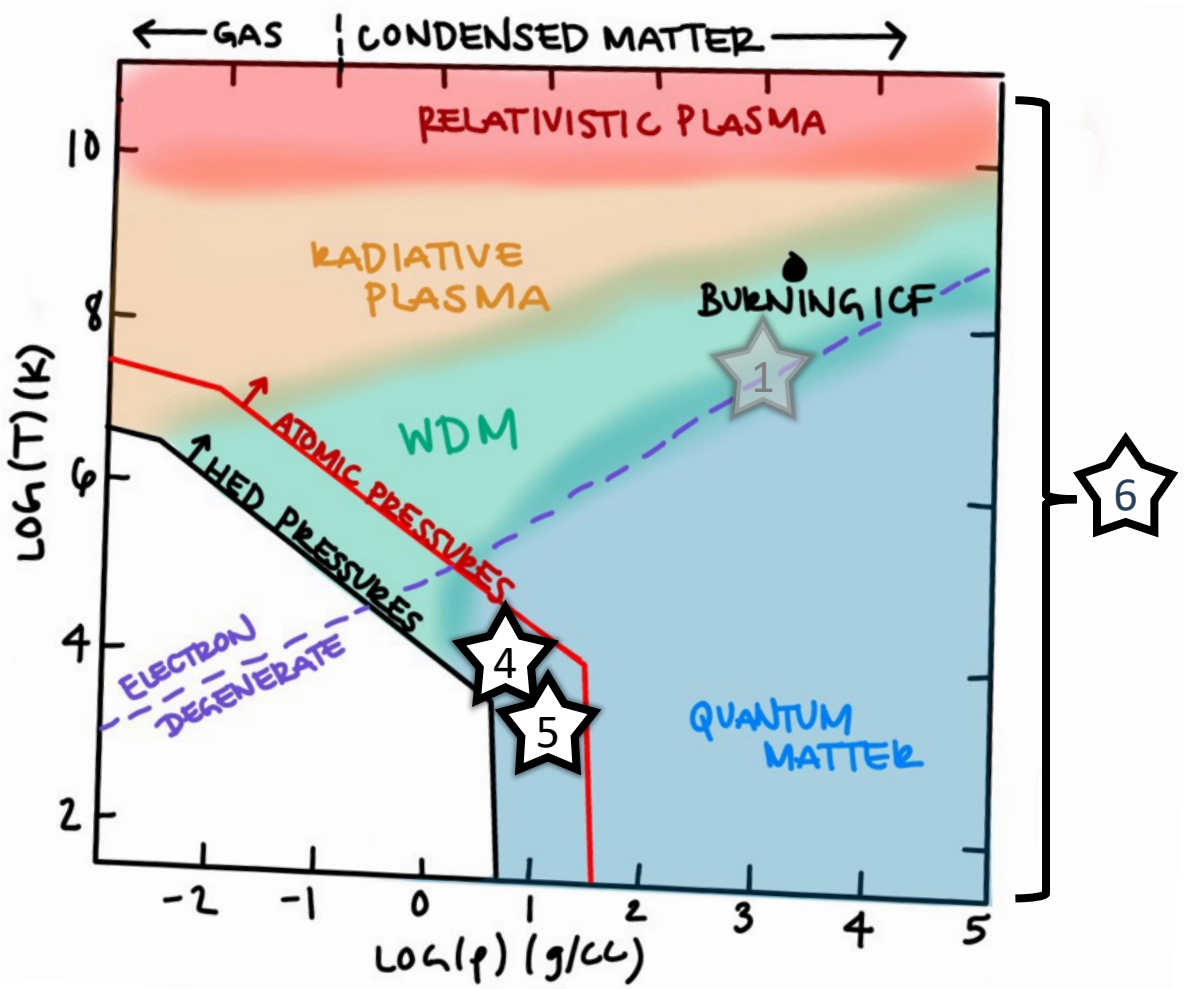

theoretical




NASA JWST

observational

# The importance of HED science

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1 Laboratory based nuclear fusion

- high pressure phase chemistry
- rheology, formation, evolution of planets/exoplanets
- cuts across many fields of science, bridging - energy, distance, and time scales

# My work!

## PUBLISHED RESULTS

ORIGINAL ARTICLE

**The homogeneous mixing of MgO and $H_2O$ at extreme conditions**

Tanja Kovačević ✉, Felipe González-Cataldo, Burkhard Militzer

First published: 03 May 2023 | https://doi.org/10.1002/ctpp.202300017

Article | Open Access | Published: 29 July 2022

**Miscibility of rock and ice in the interiors of water worlds**

Tanja Kovačević ✉, Felipe González-Cataldo, Sarah T. Stewart & Burkhard Militzer

*Scientific Reports* **12**, Article number: 13055 (2022) | Cite this article

miscibility – homogeneous (or uniform) mixing
(examples: coffee, rainwater, mouthwash)

**$MgO + H_2O$**
pressures – 120–200 GPa
temperatures – 500-8,000 K

**$MgSiO_3 + H_2O$**
pressures – 60–200 GPa
temperatures – 500–8,000 K

# AGENDA

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**MIDDLE**

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- Results

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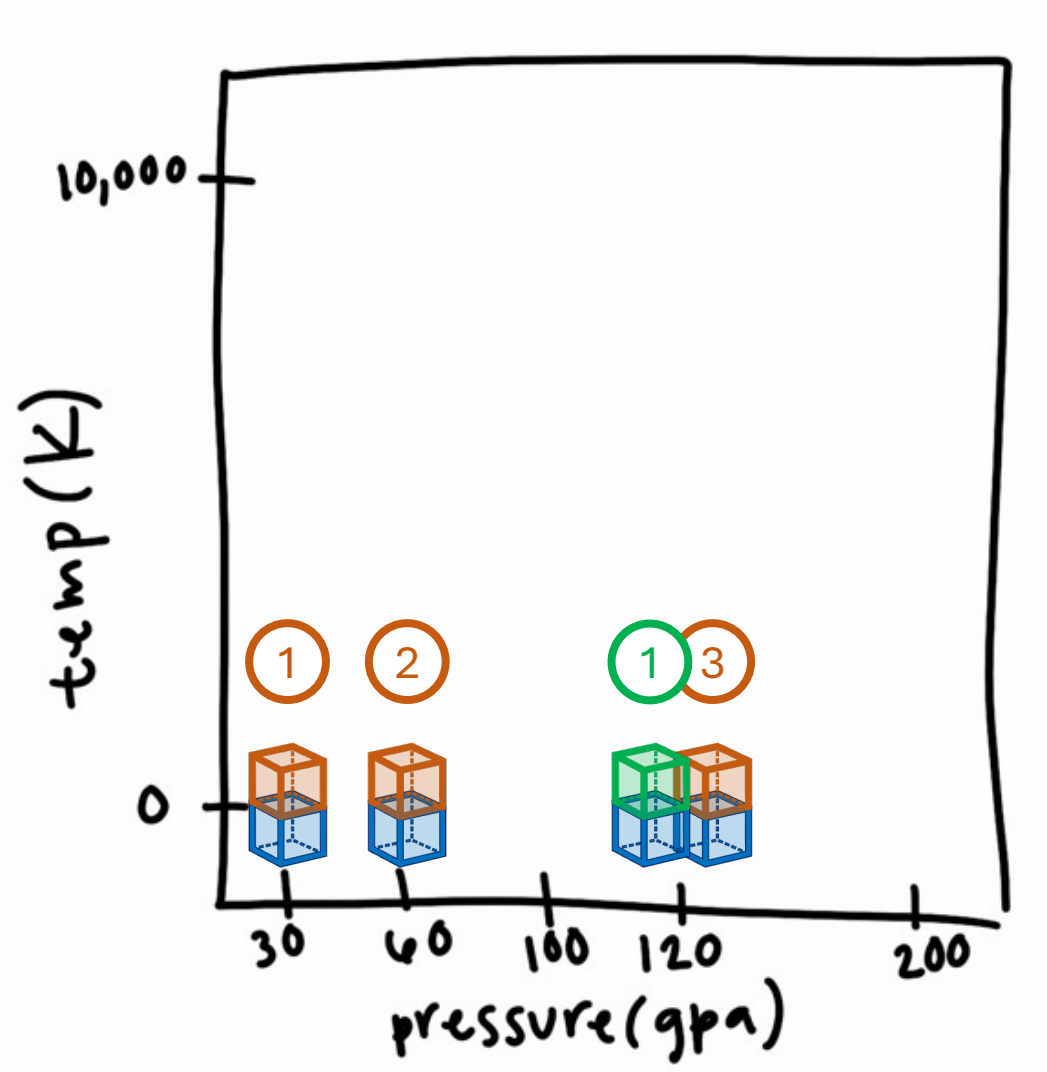
- Implications
- Summary

# Heat Until it Mixes (HUMix)




1 $MgSiO_3$ – perovskite
$H_2O$ – ice VIII

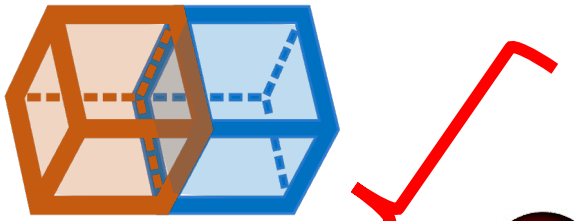
2 $MgSiO_3$ – perovskite
$H_2O$ – ice X

3 $MgSiO_3$ – post-perovskite
$H_2O$ – ice X

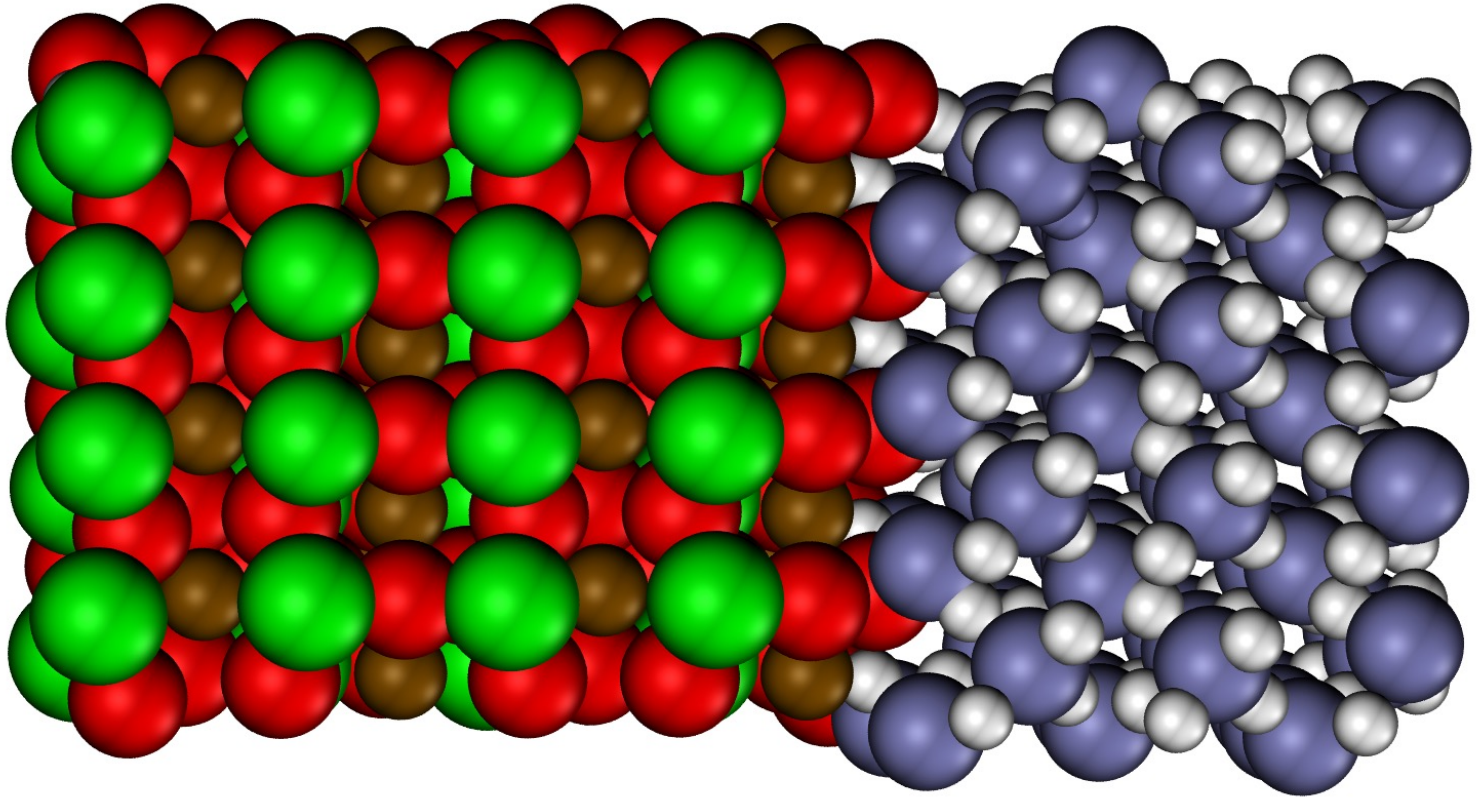
1 MgO – B1
$H_2O$ – ice X

METHOD 19

# Visualizing the system



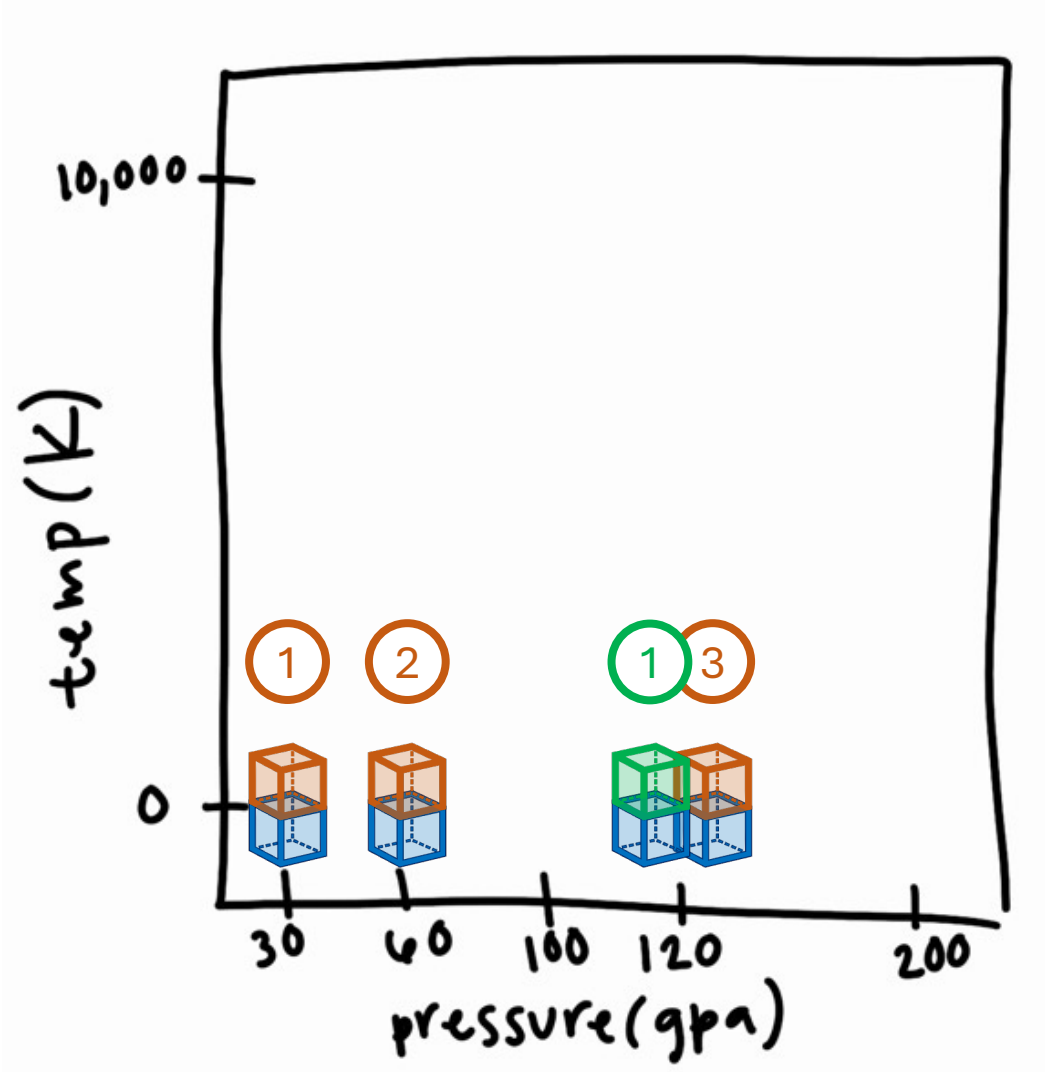
$MgSiO_3 + H_2O$






METHOD 20

# Heat Until it Mixes (HUMix)

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METHOD 21

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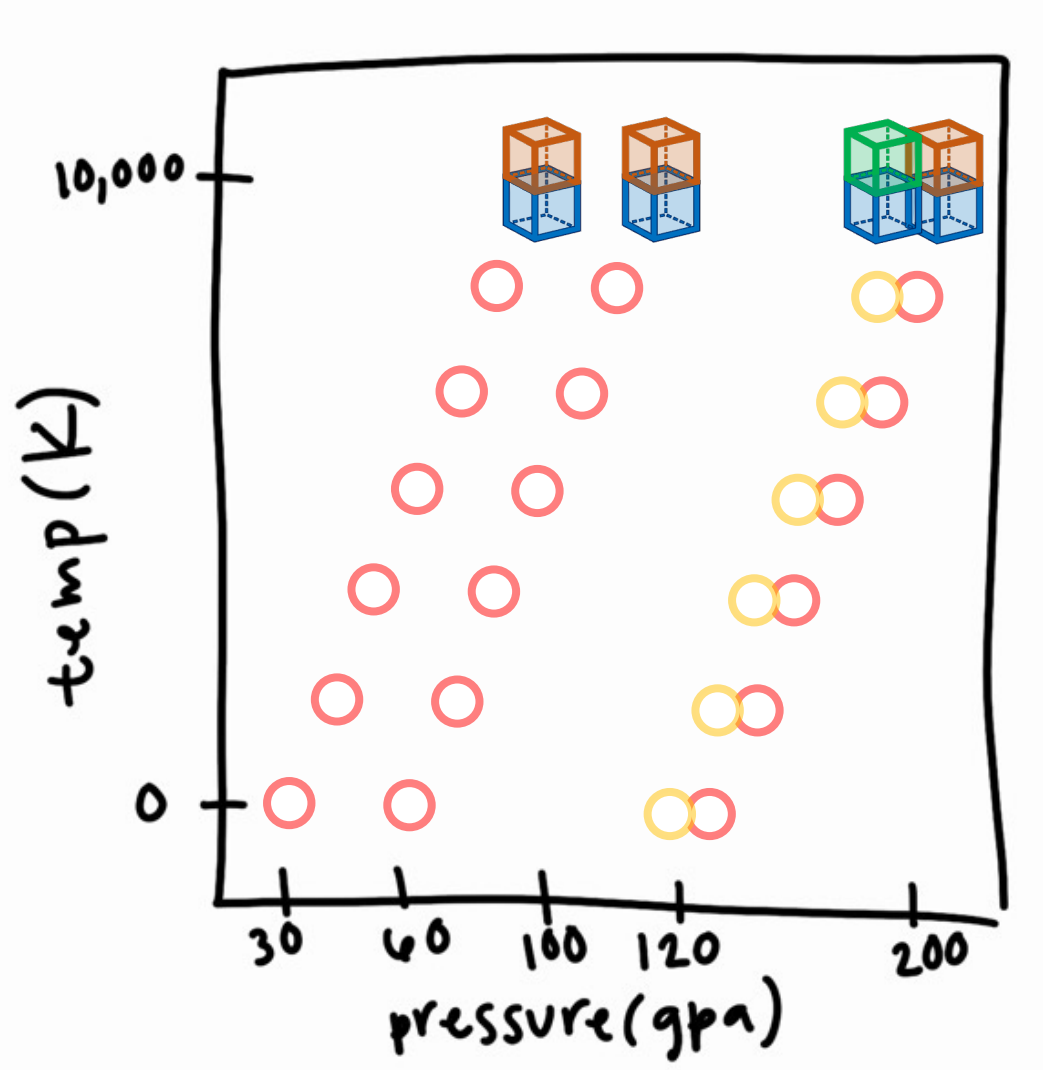


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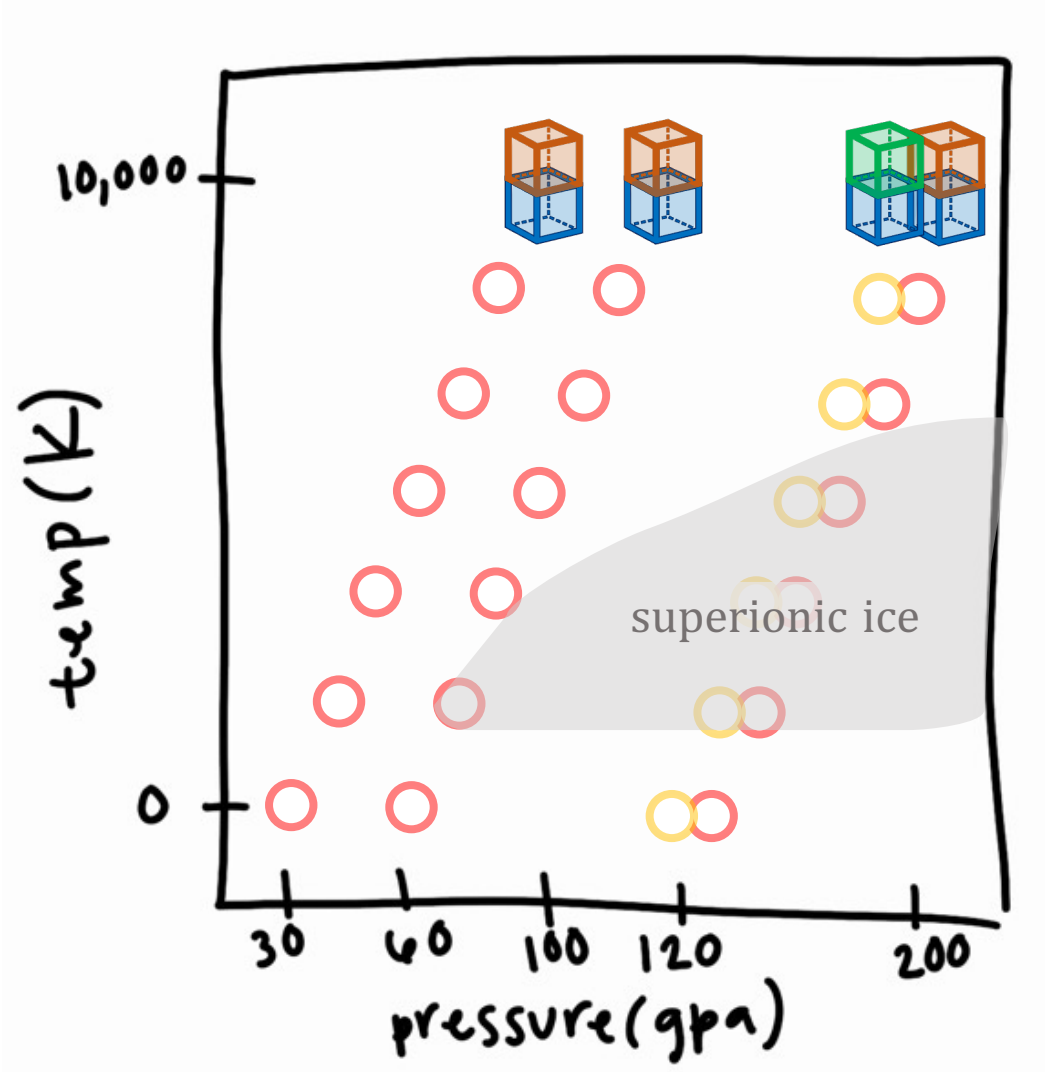
METHOD 22

# Heat Until it Mixes (HUMix)

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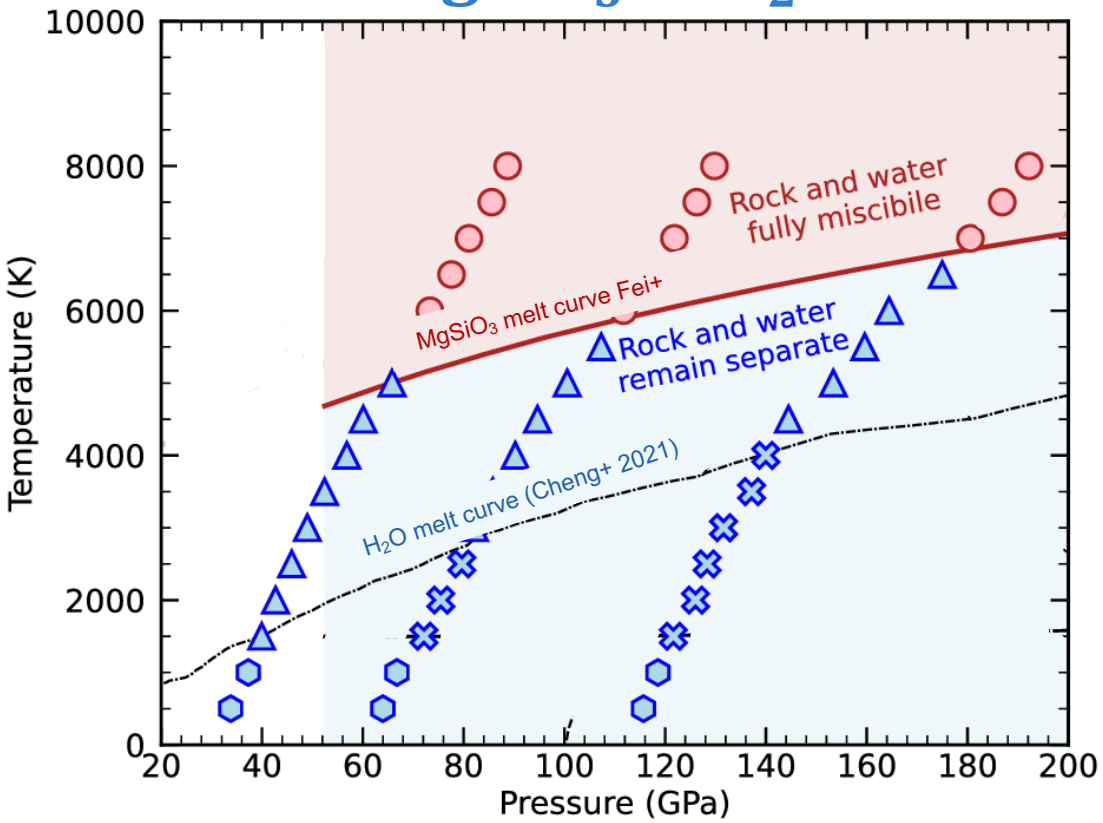
1 — MgO – B1
$H_2O$ – ice X

METHOD 23

# HUMix Isochores

## $MgSiO_3 + H_2O$

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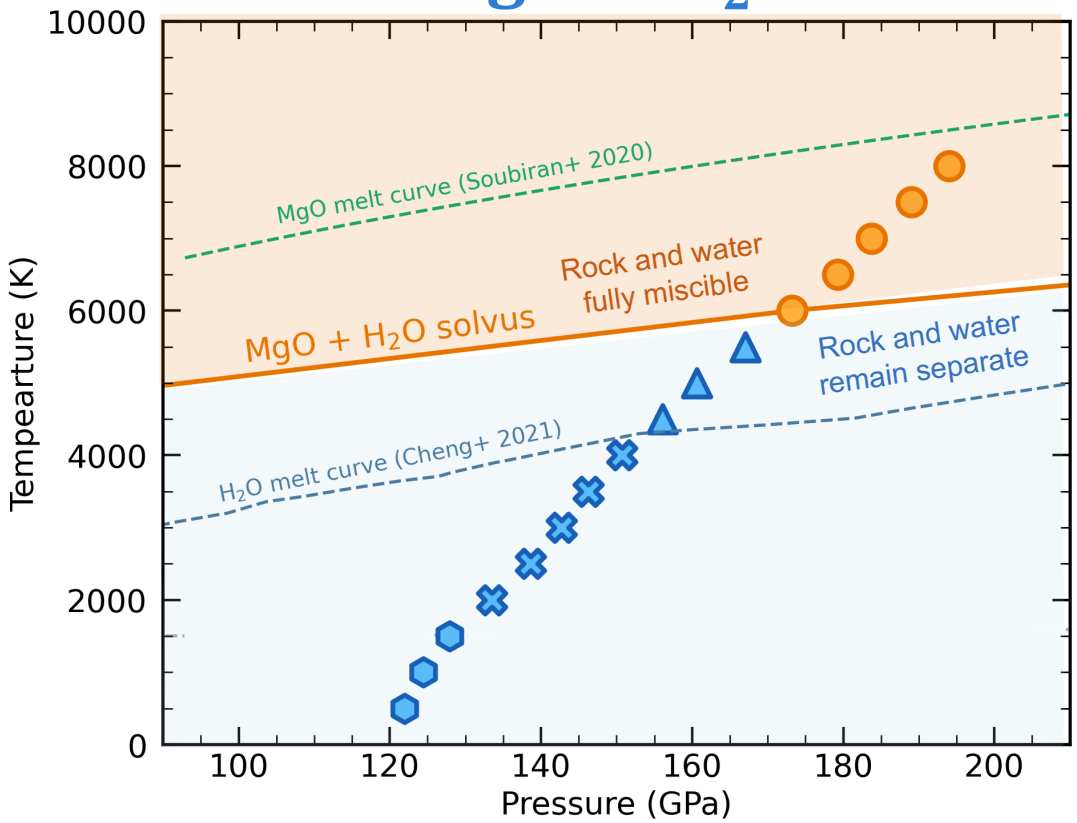
## $MgO + H_2O$

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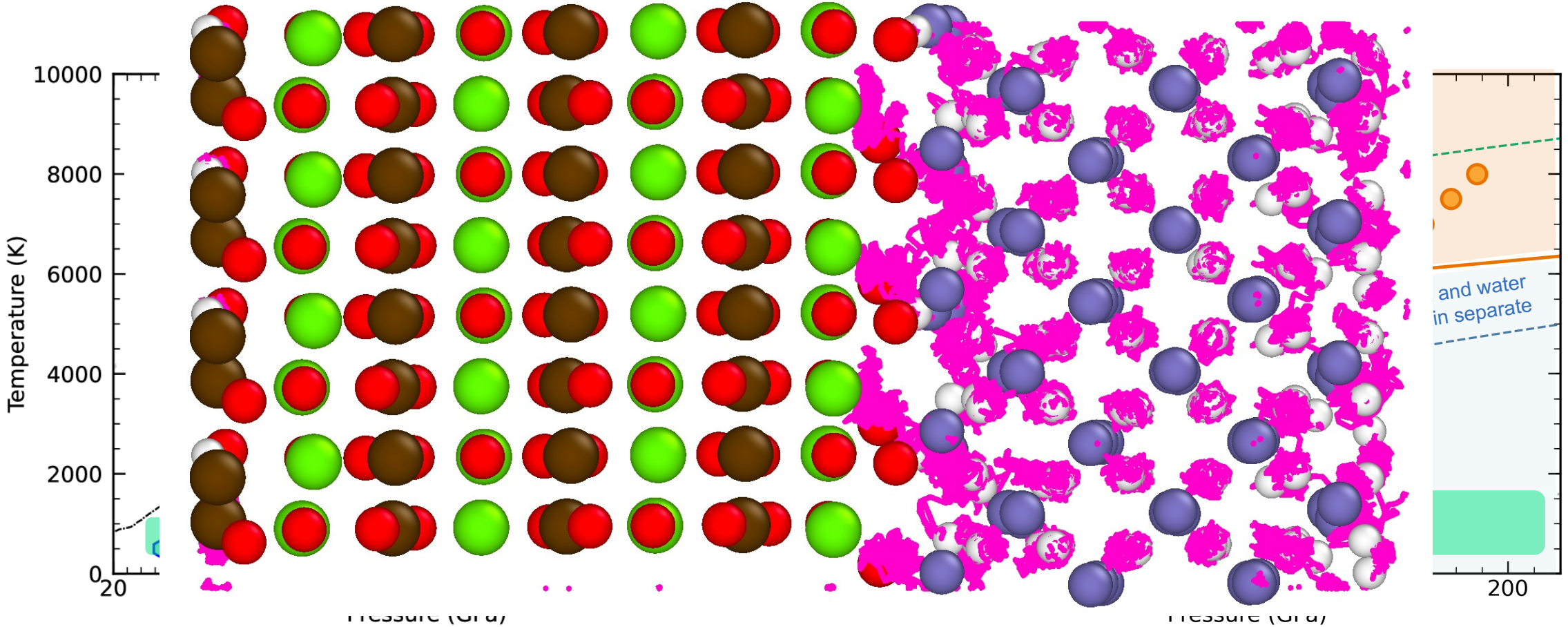
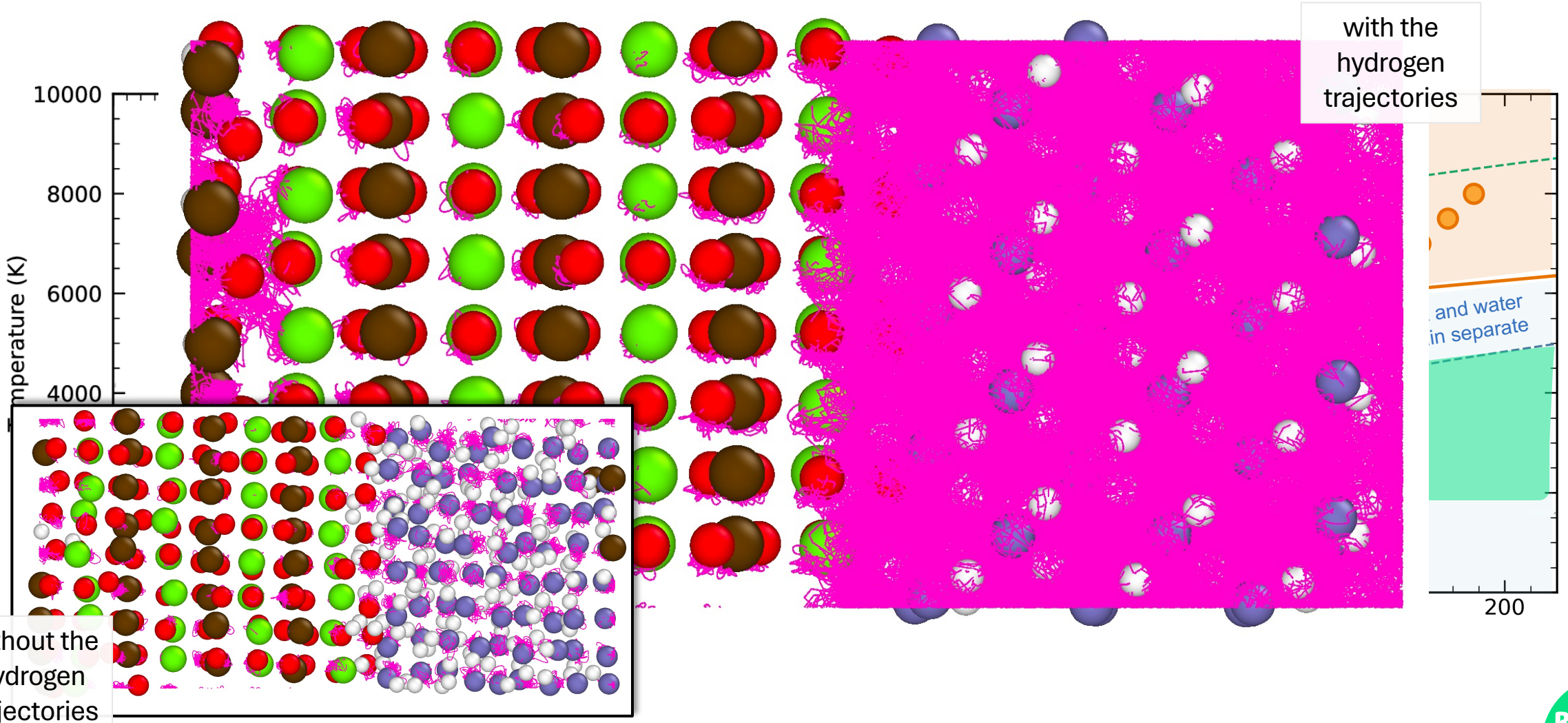
RESULTS 24

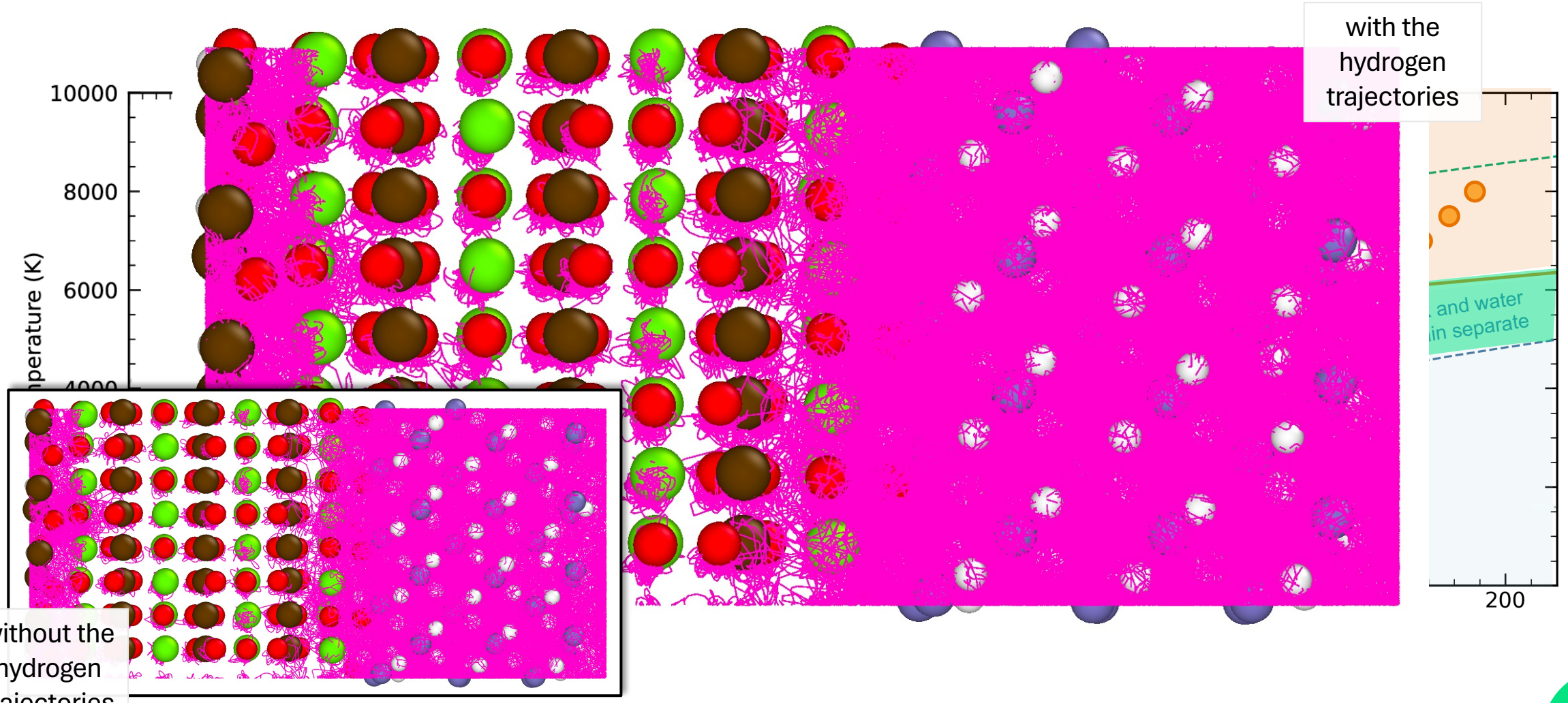
# Trajectories: rock(solid) water(solid)



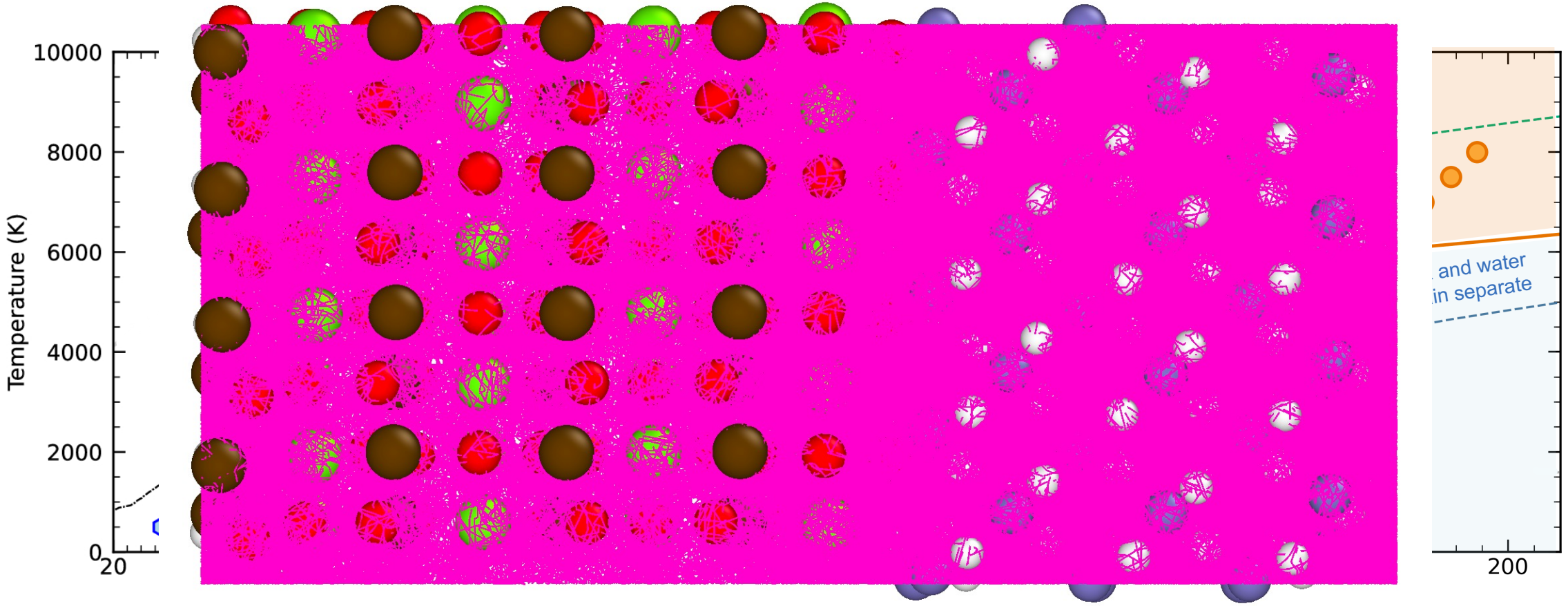
# Trajectories: rock(solid) water(superionic)



# Trajectories: rock(solid) water(ionic liquid)



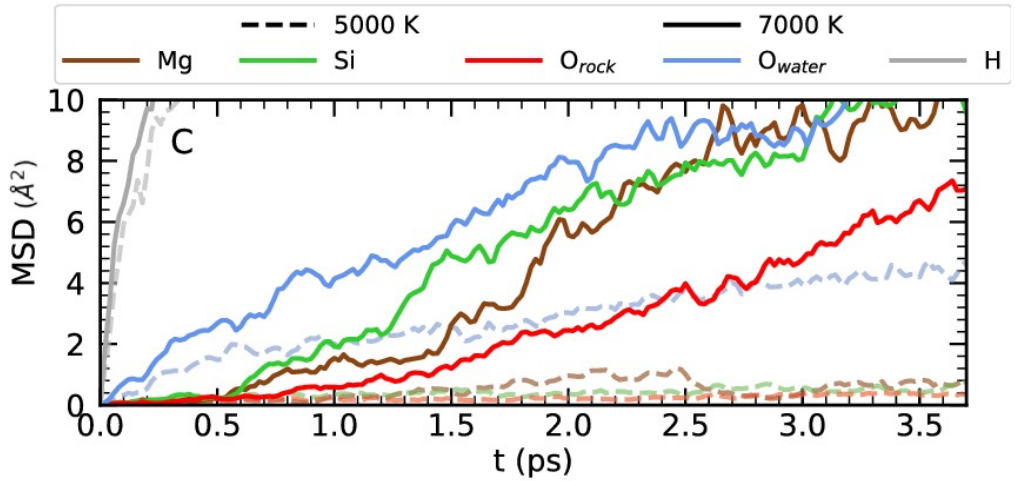
# Trajectories: rock-water(mixed)




RESULTS
28

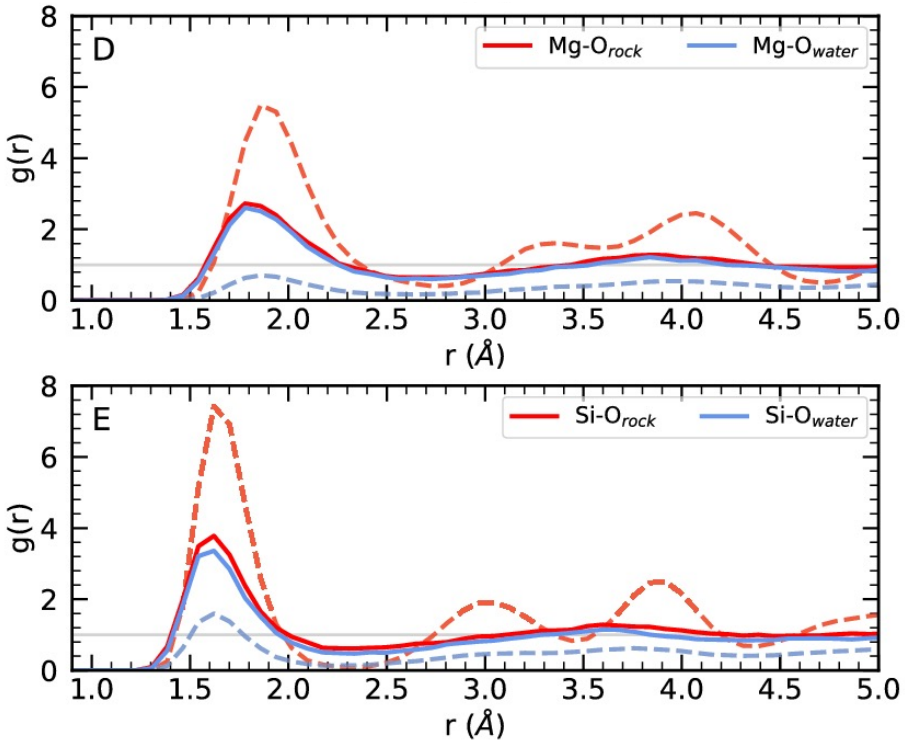
# Quantitative evidence for mixing

## Mean Squared Displacement




Kovacevic+ *Sci Rep* **12**, 13055 (2022)

## Radial Distribution Function

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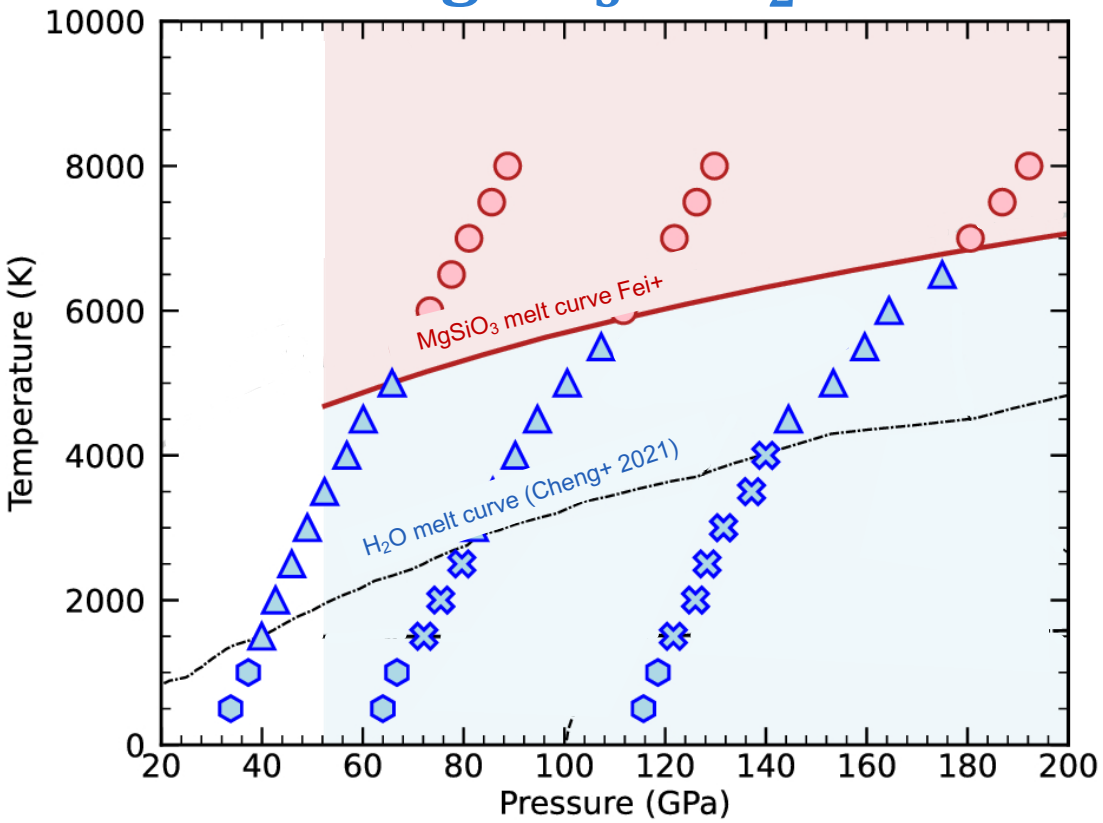
# HUMix Isochores

## $MgSiO_3 + H_2O$

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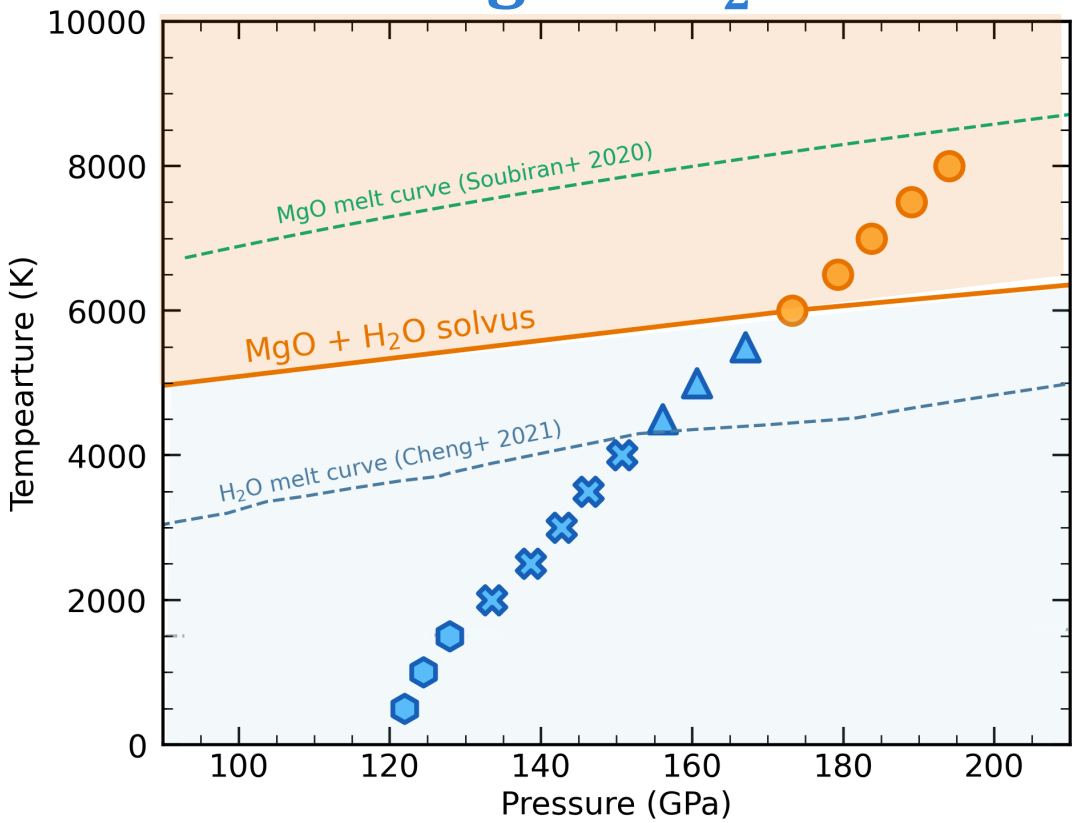


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RESULTS 31

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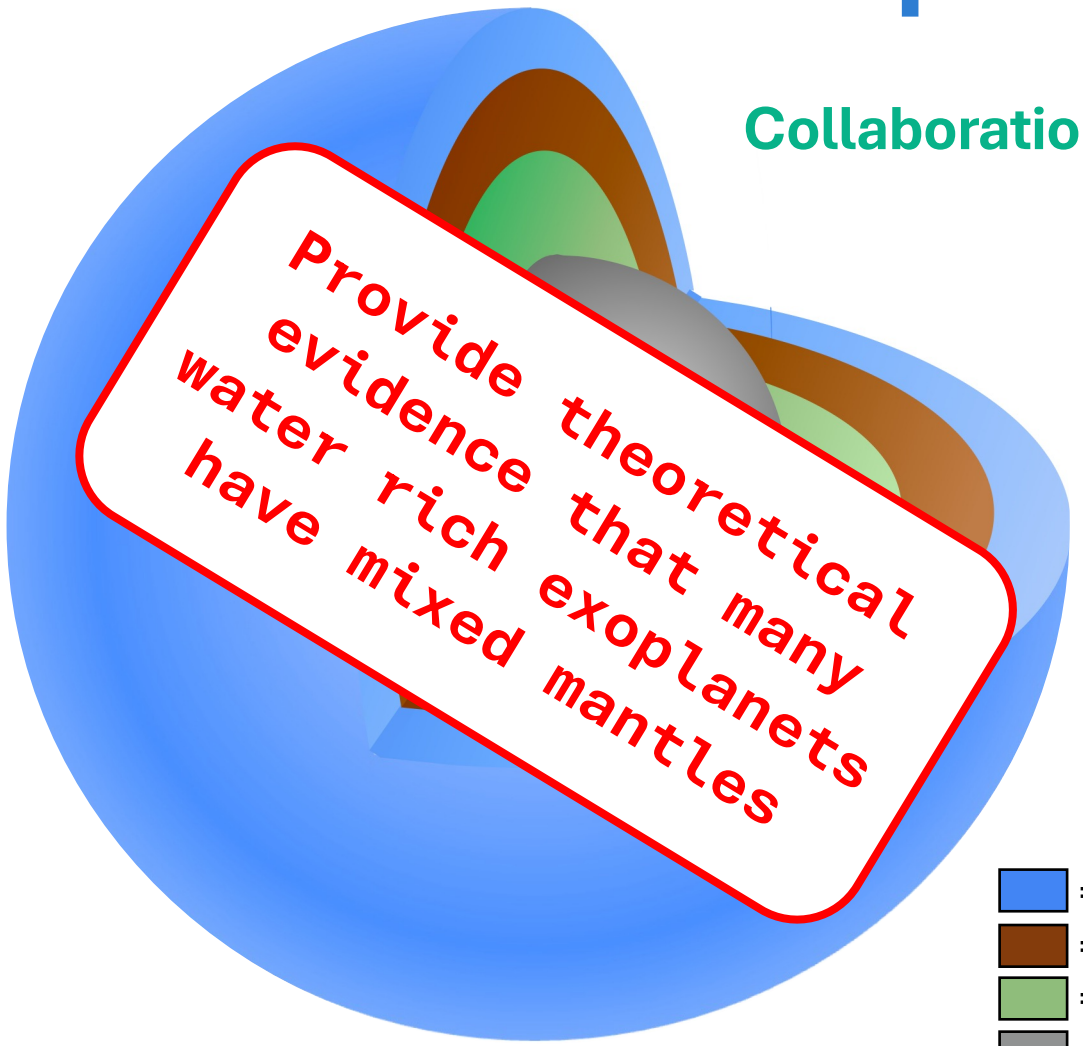
# Implications

## Collaboration with Sarah T. Stewart at U.C. Davis




**INITIAL CONDITIONS**

$M_{planet}$ (0.7 – 4.68 $M_{\oplus}$)

wt% $H_2O$ (15 – 44%)

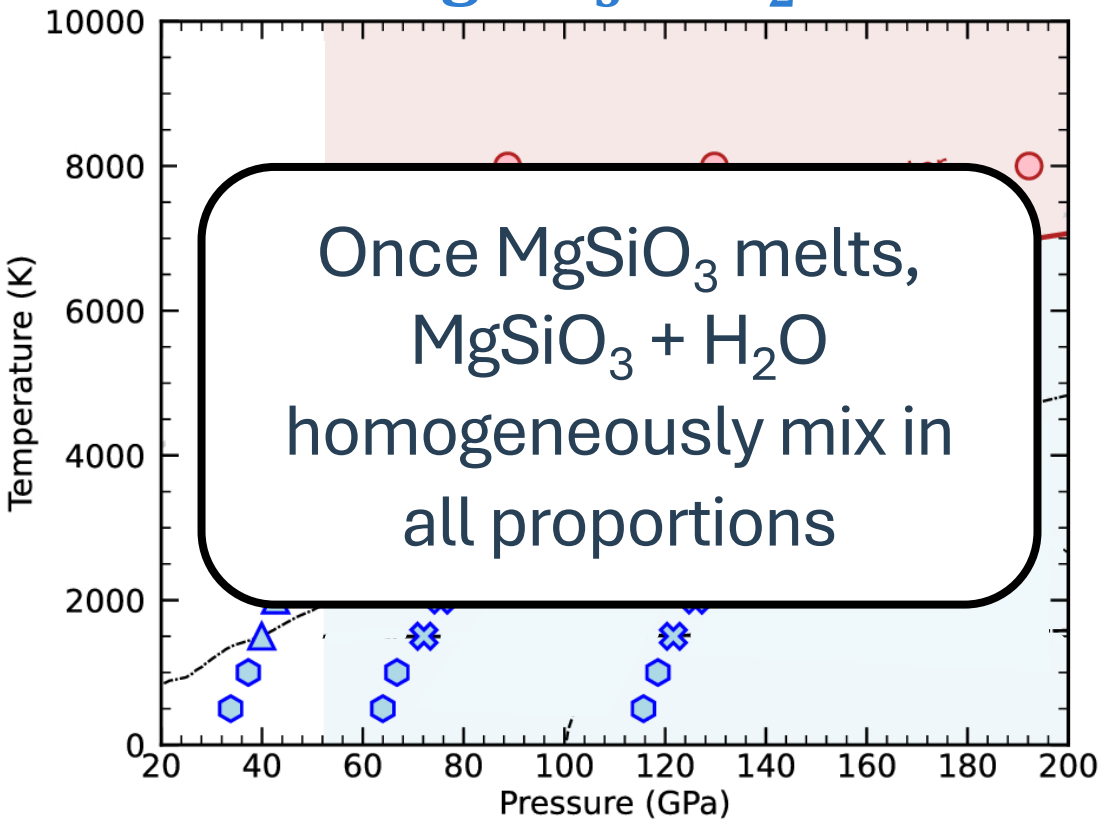
$R_{planet}$ (1 – 1.86 $R_{\oplus}$)

**6 – 22 % 'rock' mechanically mixed up into the $H_2O$ layer**

= water
= mixture
= rock
= iron

# Summarized DFT Results

## $MgSiO_3 + H_2O$

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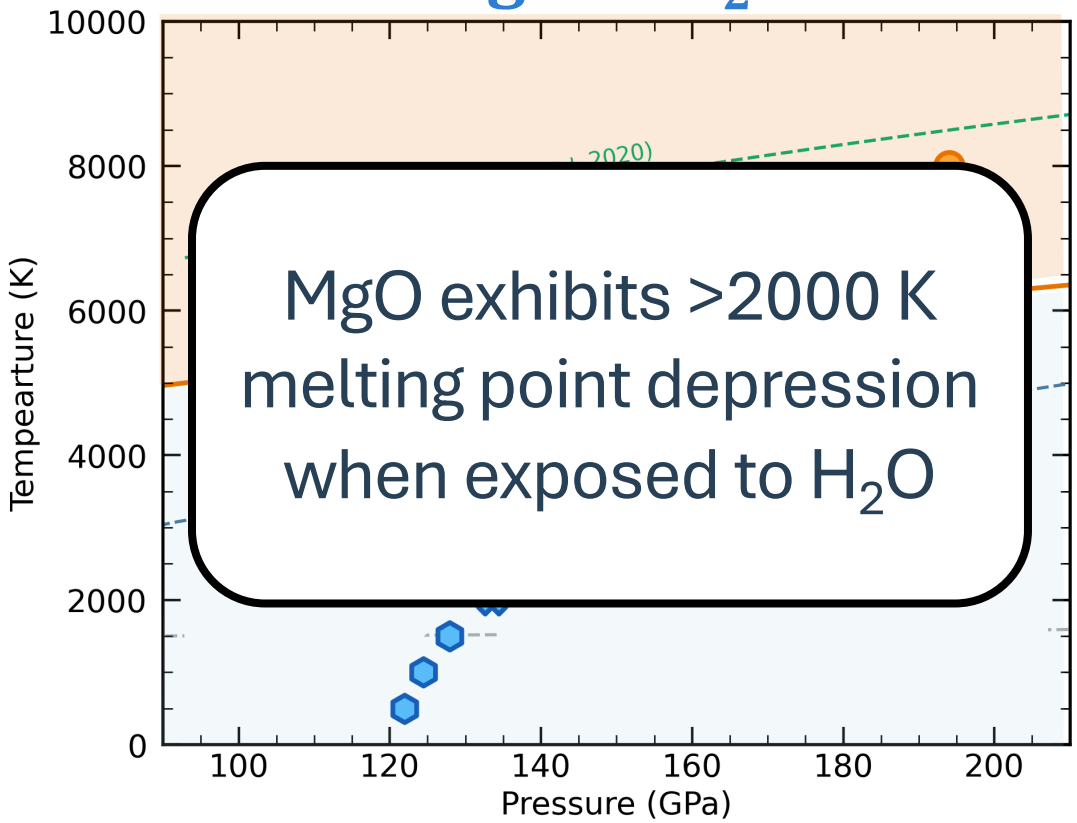

# THANK YOU!

**Militzer Group**

Salma Ahmed
Felipe Cataldo-Gonzalez
Kyla De Villa
Burkhard Militzer
Victor Naden Robinson
Jizhou Wu

Sarah T. Stewart

Lawrence Livermore National Laboratory

NSF

CMEC

HEARTS TO H2H HUMANITY ETERNAL


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looking for post-doc opportunities!

THANKS!