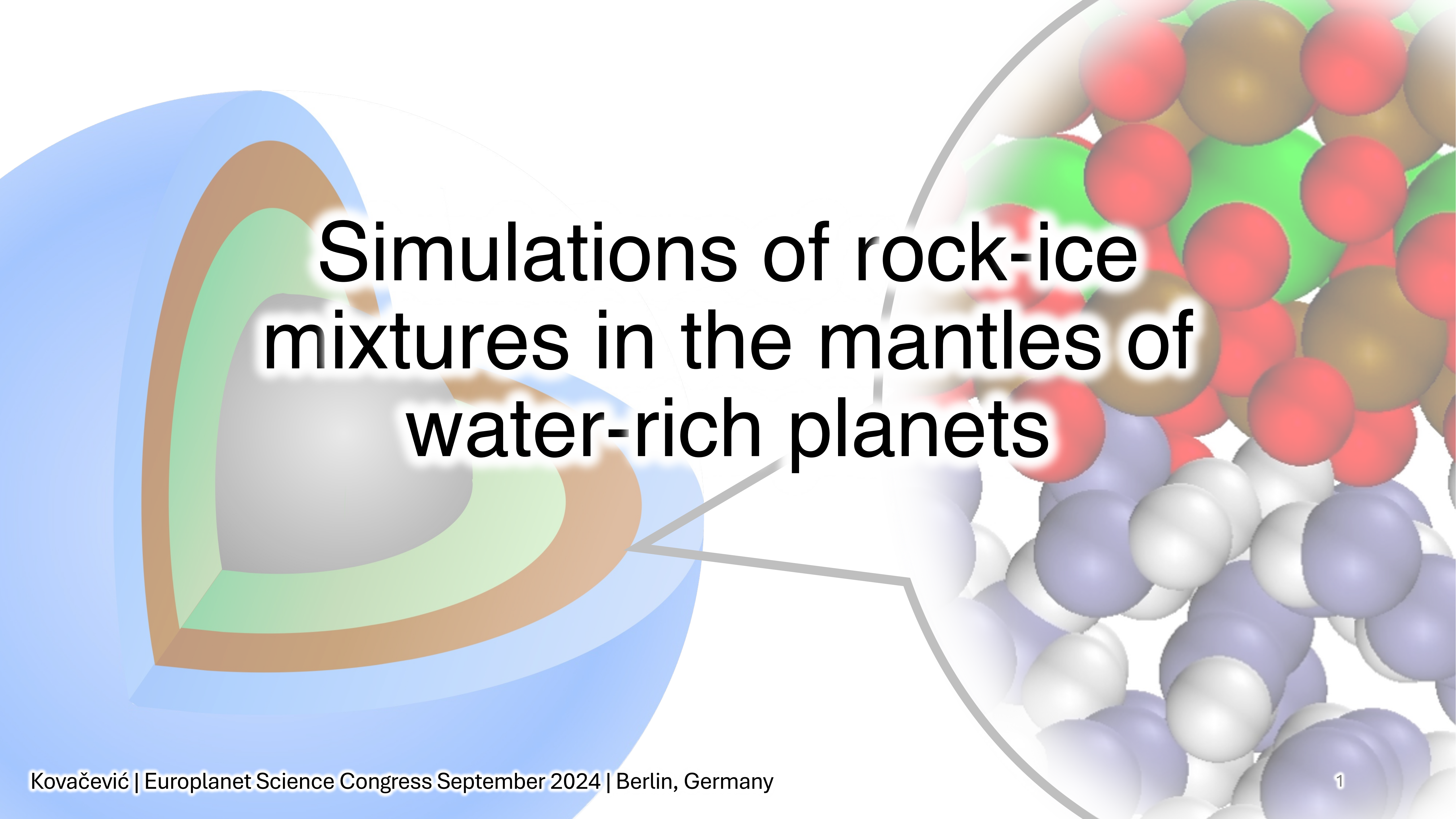


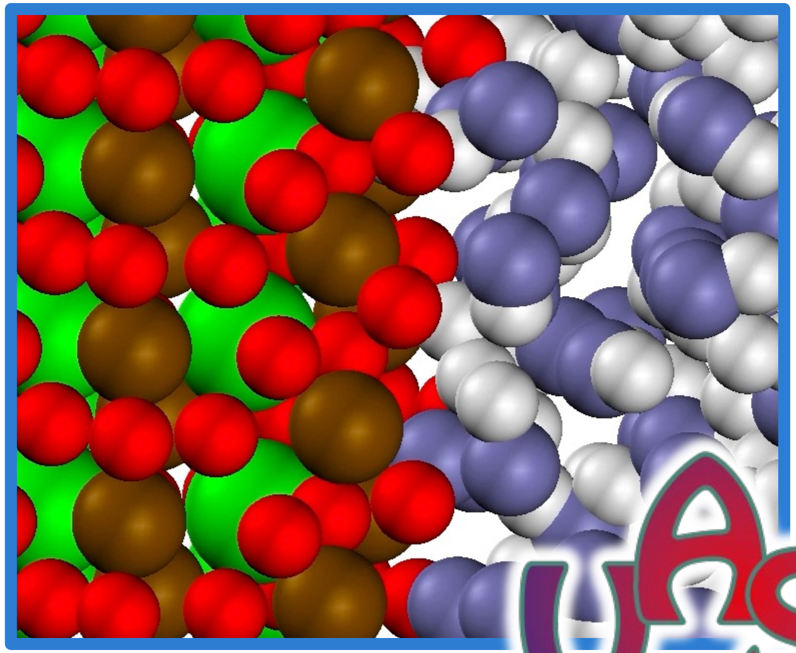
Simulations of rock-ice mixtures in the mantles of water-rich planets

Tanja

5^{th} year Ph.D. Candidate
U.C. Berkeley – Earth & Planetary Science
Burkhard Militzer

- Density Functional Theory Molecular Dynamics (DFT-MD)
- HED binary mixtures
  - Magnesium silicates + H_2O

High **E**nergy **D**ensity



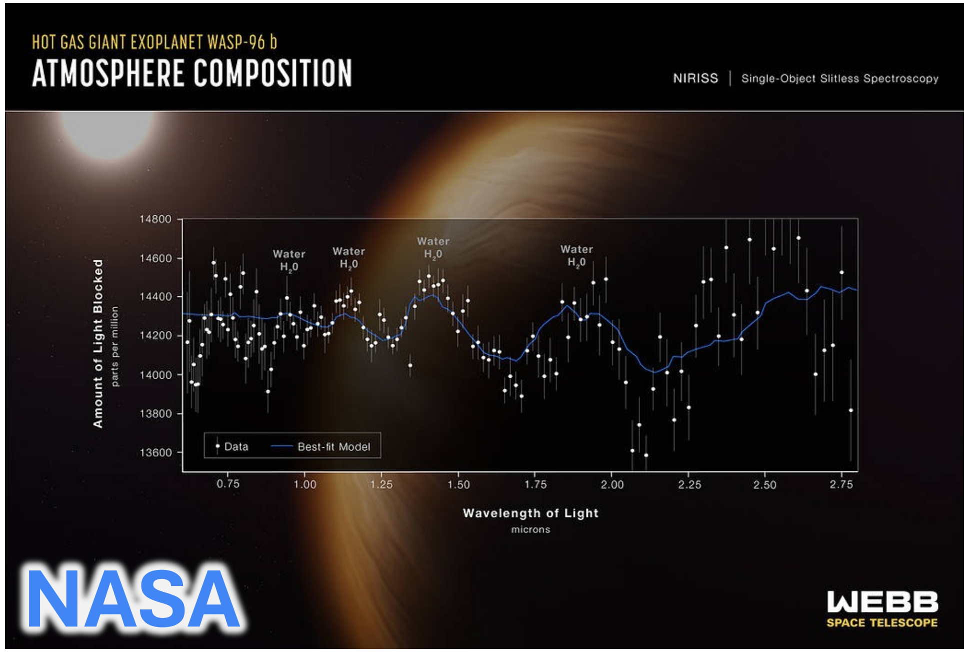
Are there water rich exoplanets?

Mousis+ 2020 ApJ - Irradiated Ocean Planets Bridge Super-Earth and Sub-Neptune Populations

Zeng+ 2019 PNAS – "exoplanets (2–4$R_\oplus$) upwards of 50% by mass H_2O-dominated ices"

Luque+ 2022 Science- Density, not radius, separates rocky and water-rich small planets orbiting M dwarf stars

Parc+ 2024 A&A. From super-Earths to sub-Neptunes: Observational constraints and connections to theoretical models



Growing evidence for rock-ice mixing

Luo+ 2023 – The interior as the dominant water reservoirs in super-Earths and sub-Neptunes

Kim+ 2021 Nat. Astron - Atomic-scale mixing between MgO and H_2O in the deep interiors of water-rich planets

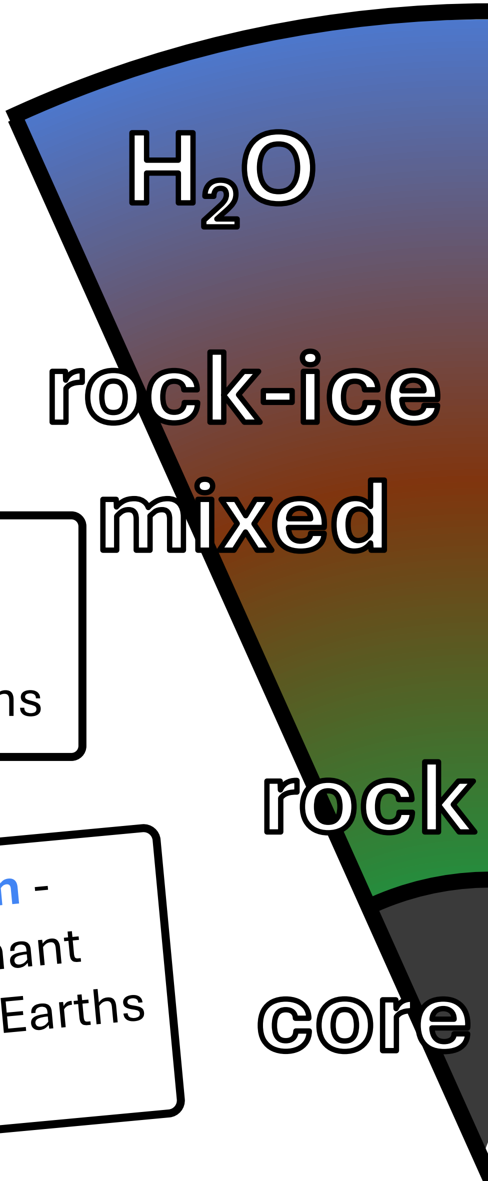
Kovacevic+ 2023 CPP - The homogeneous mixing of MgO and H2O at extreme conditions

Kovacevic+ 2022 Sci. Rep. - Miscibility of rock and ice in the interiors of water worlds

Dorn+ 2021 ApJL - Hidden water in magma ocean exoplanets

Vazan+ 2022 ApJ - Ice–Rock Mixture Instead of Ice on Top of Rock

Luque+ 2024 Nat. Astron - The interior as the dominant water reservoir in super-Earths and sub-Neptunes



AGENDA

- Approaches to determine the phase diagram for these mixtures
- DFT to calculate the EOS for these mixtures
    - Method
    - Results
- Giant impact simulations – a collaboration with Sarah Stewart
    - Results
- Conclusion

Calculating the EOS of binary mixtures

classical thermodynamics

(indirect) fitting the EOS for the mixture as a linear combination of end-member EOSs

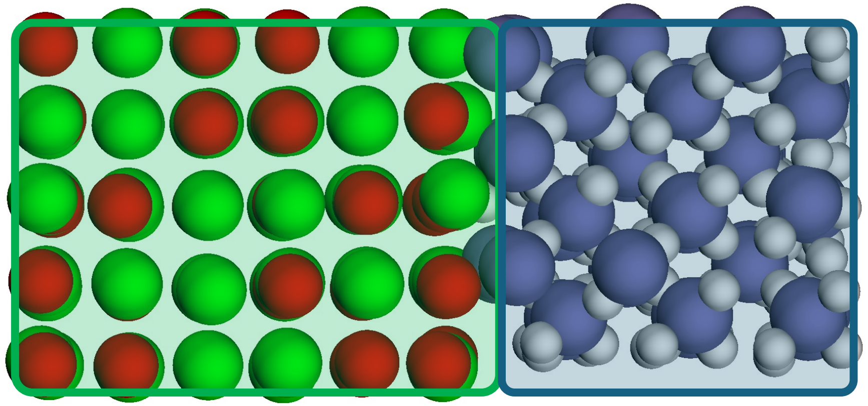
MgO EOS

H_2O EOS

Mix EOS = $\sum_{\chi=H_2O\ conc.}(1-\chi_i)(\text{MgO EOS}) + (\chi_i)(\text{H}_2\text{O EOS})$

dft

(direct) simulate EOS of the mixture with DFT



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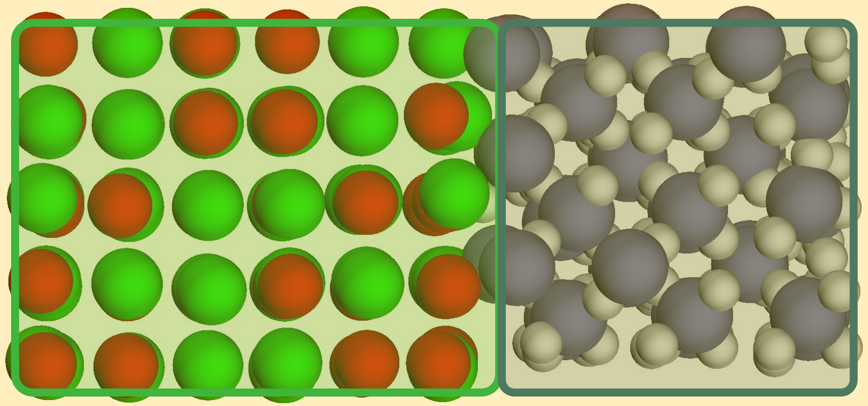
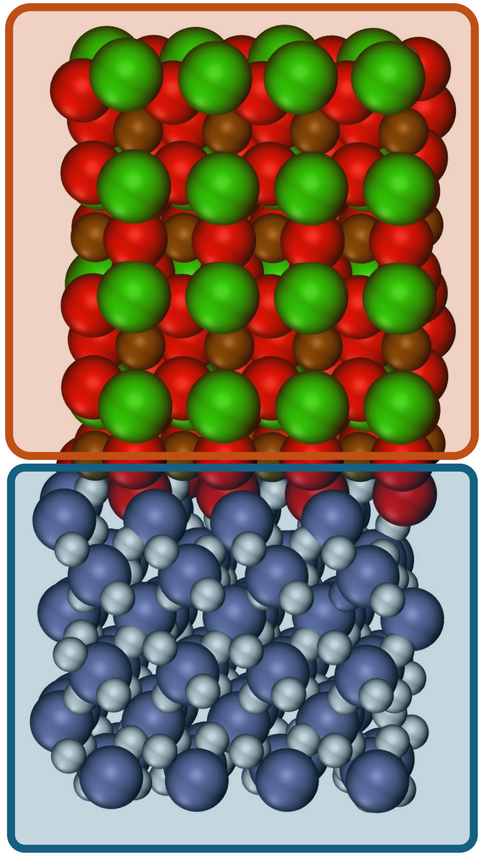


MgO : H_2O

$MgSiO_3$: H_2O

Method: building the rock-ice systems

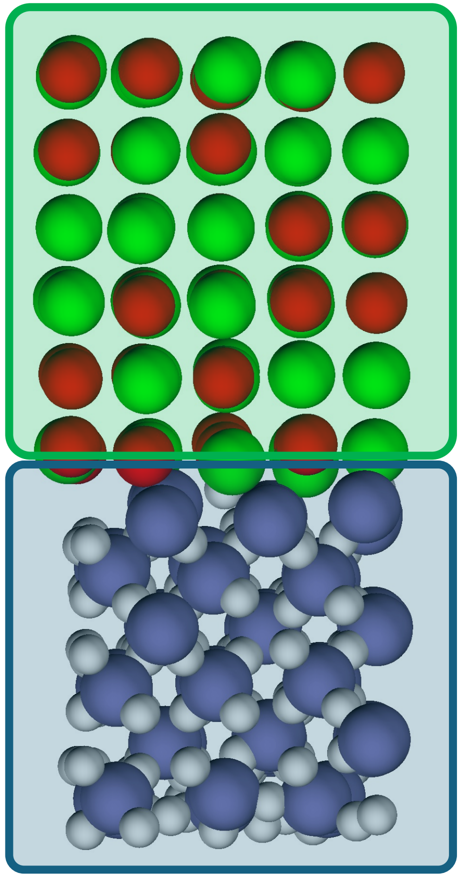


$MgSiO_3$ – pv, ppv
H_2O – ice VIII, ice X

32 formula unit's $MgSiO_3$
72 formula unit's H_2O

concentration (wt. %)

29 wt. % H_2O



MgO – B1
H_2O – ice X

48 formula unit's MgO
54 formula unit's H_2O

concentration (wt. %)

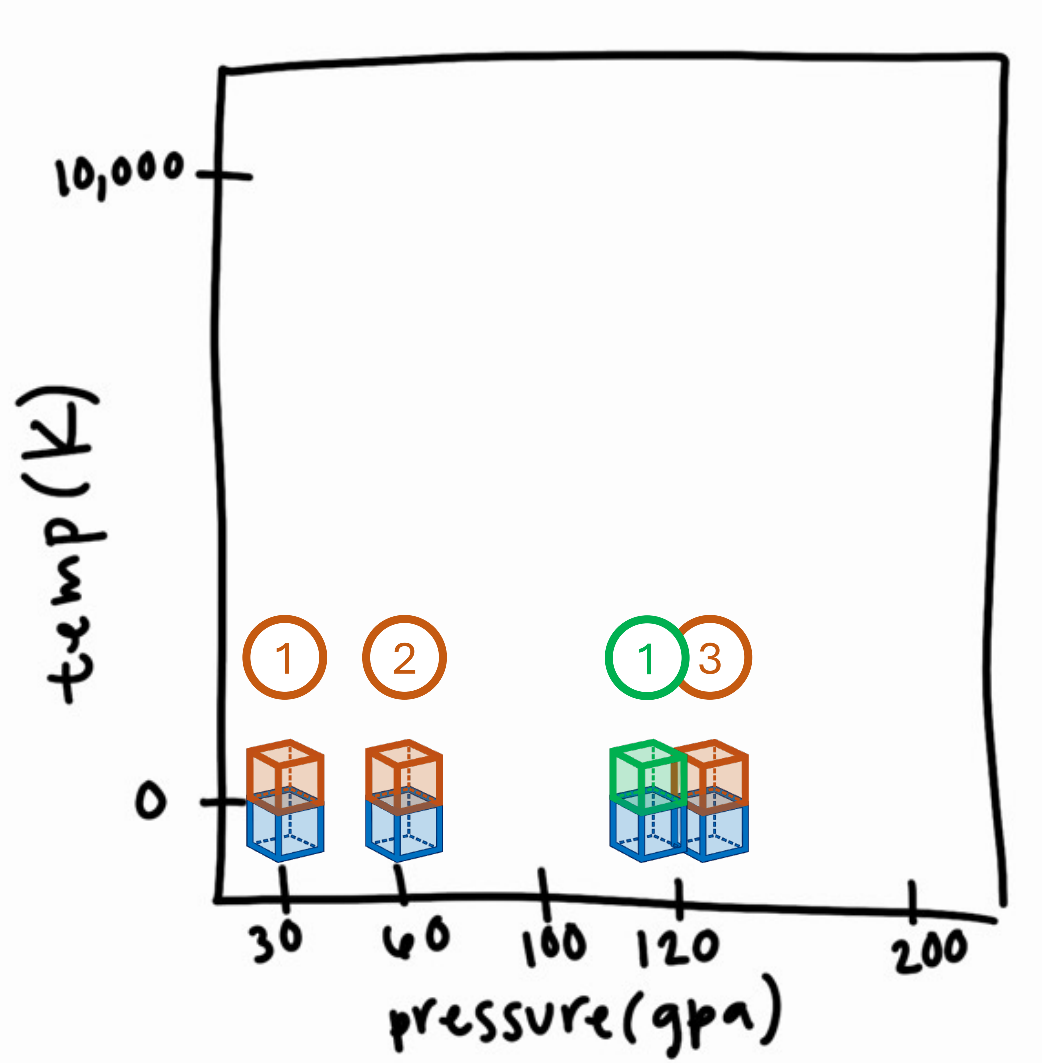
33 wt. % H_2O

Method: calculating isochores

composition (wt. %)

$MgSiO_3$: H_2O 29 wt. % H_2O

MgO : H_2O 33 wt. % H_2O



material – solid phase

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

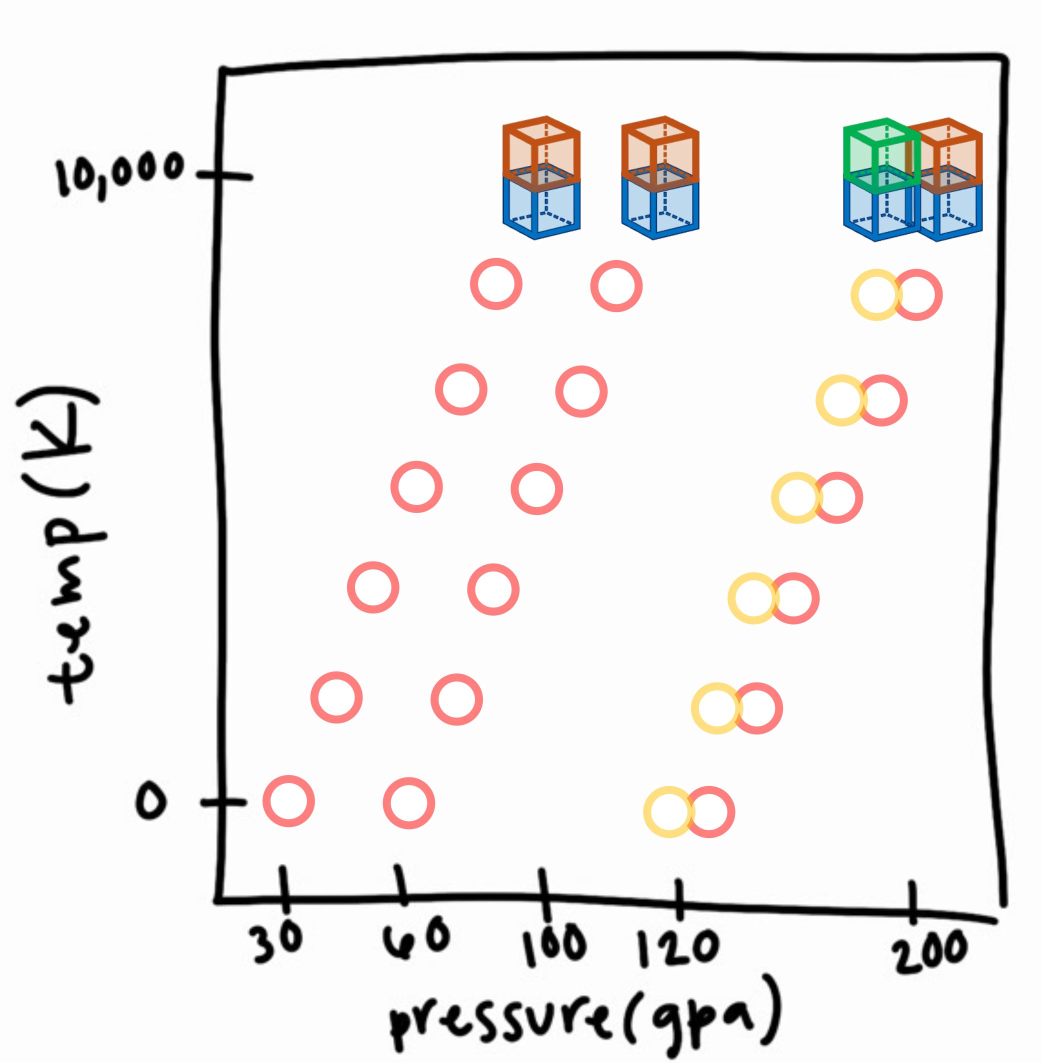
1 (MgO). **MgO** – B1; **H_2O** – ice X

composition (wt. %)

$MgSiO_3 : H_2O$ — 29 wt. % H_2O

$MgO : H_2O$ — 33 wt. % H_2O

Method: calculating isochores



material – solid phase

1. $MgSiO_3$ – perovskite; H_2O – ice VIII
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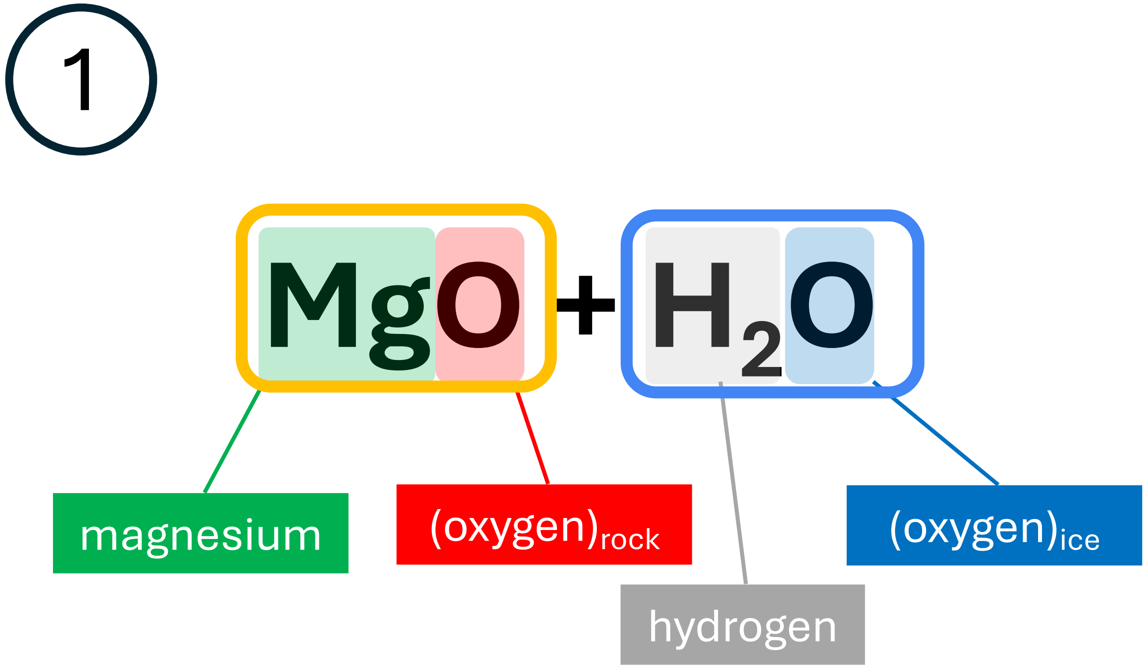
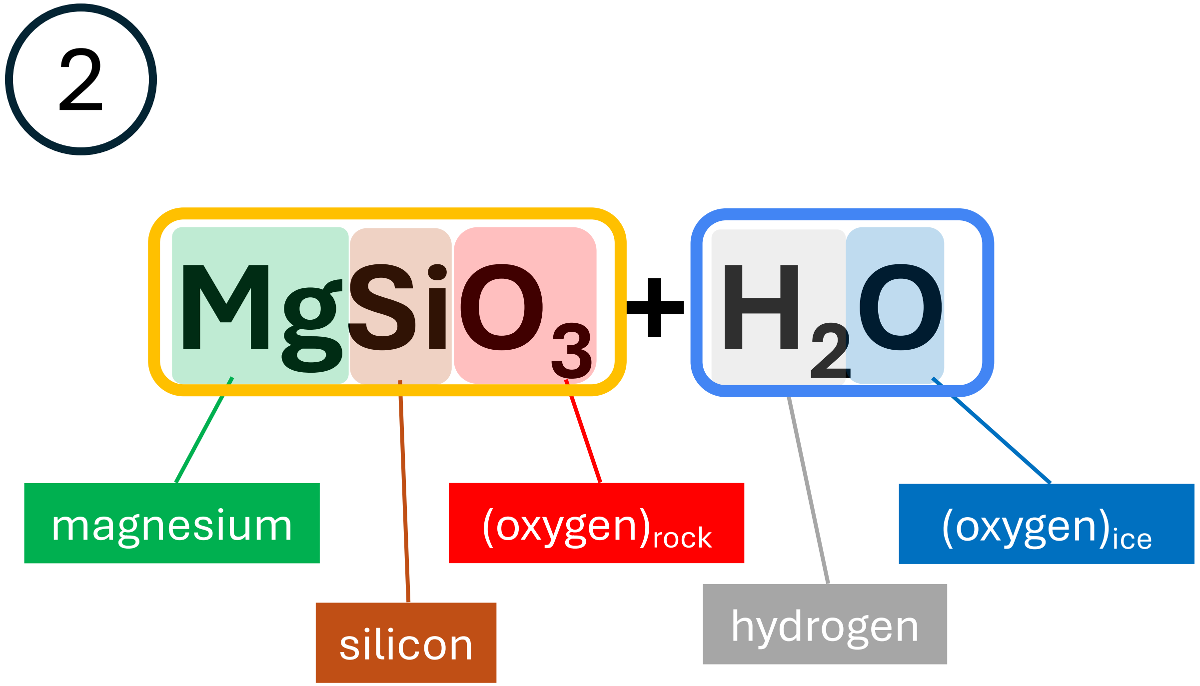
3. $MgSiO_3$ – post-perovskite; H_2O – ice X

1. MgO – B1; H_2O – ice X

Method: analyzing simulations

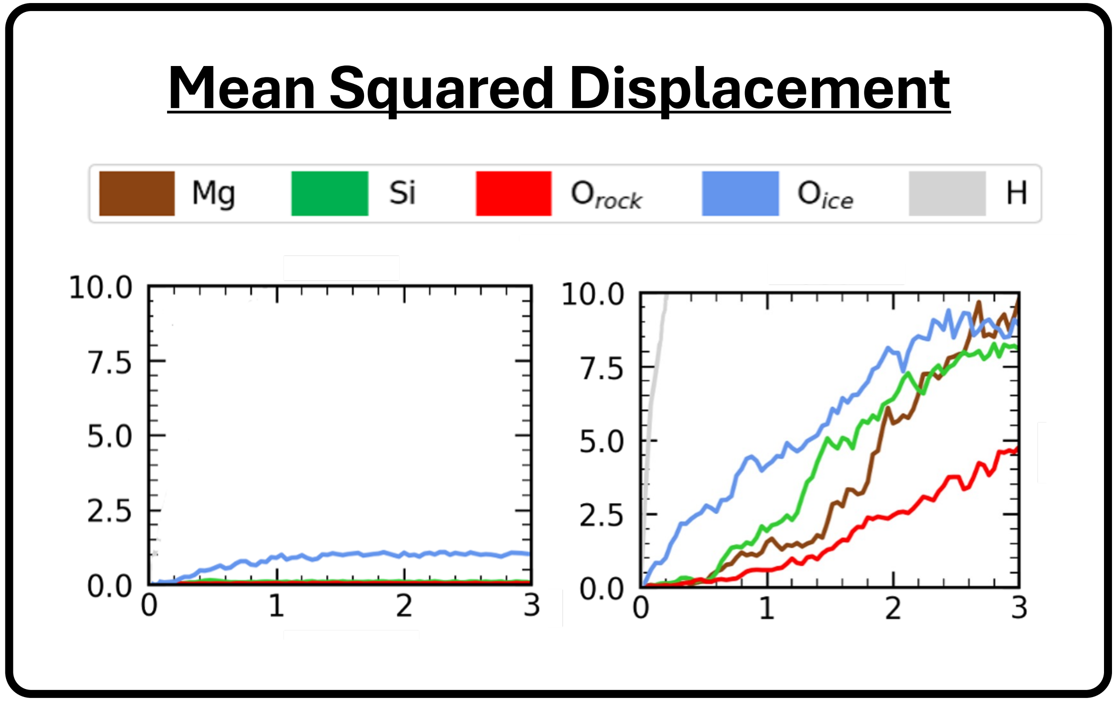
These binary mixtures contain several elemental species



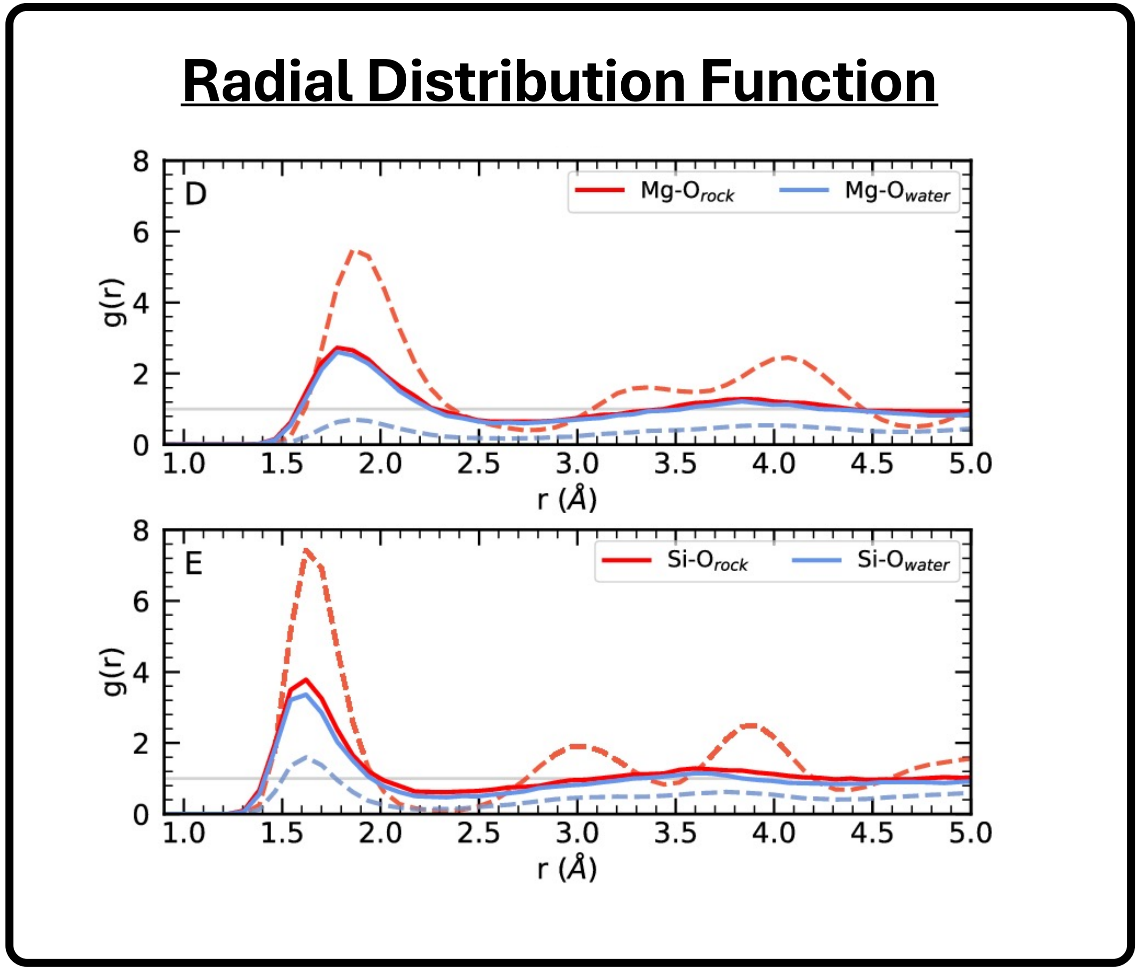


For analysis purposes, it was beneficial to consider the **rock** & **ice** oxygens separately

Method: quantitative evidence for mixing



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



Results: isochore plots

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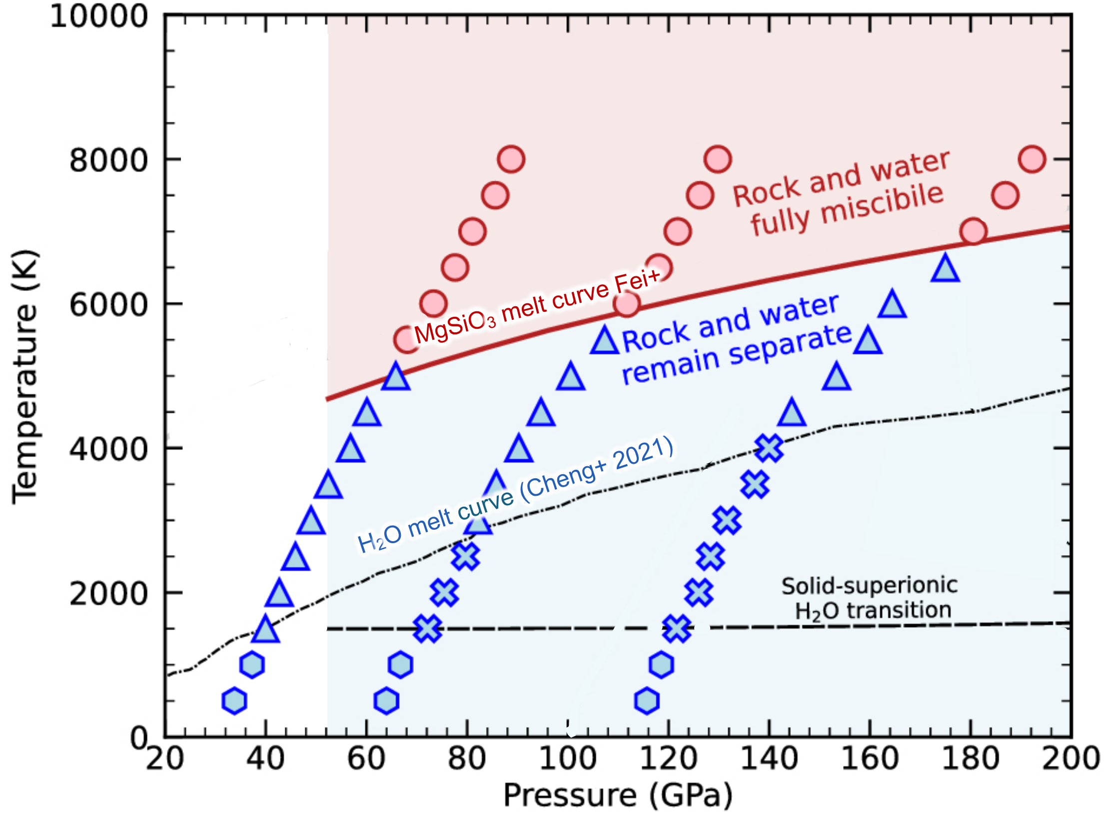
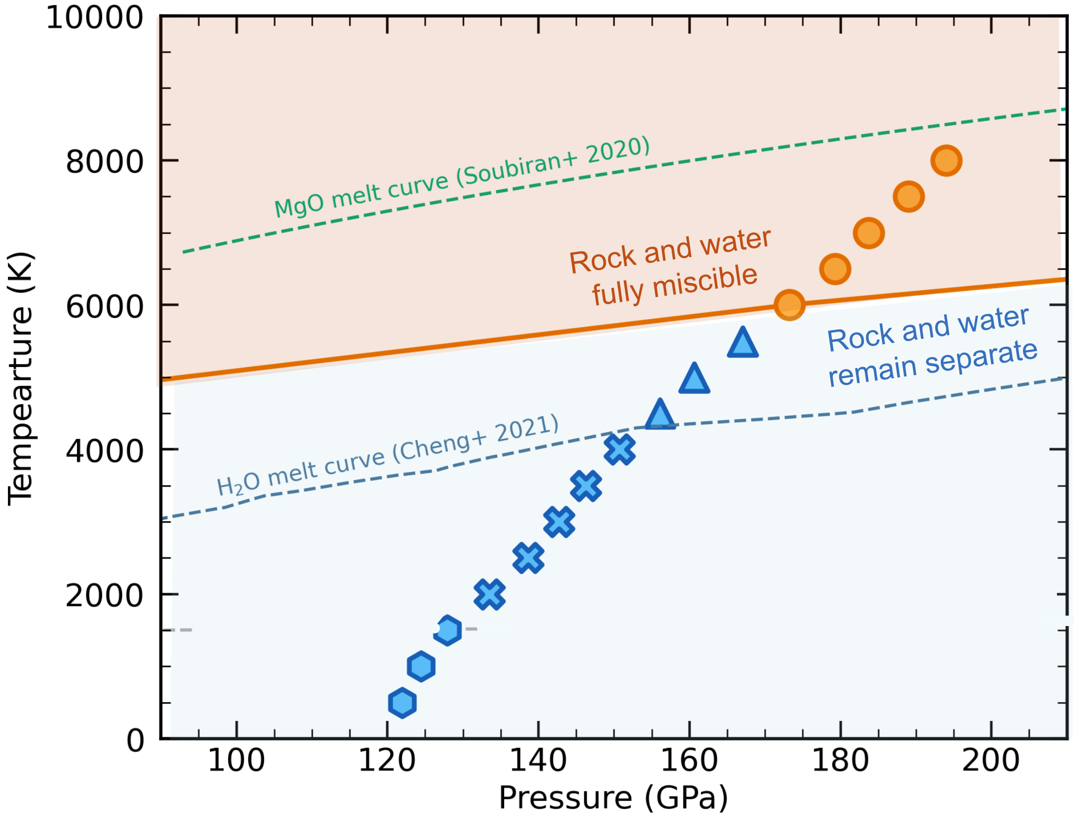
$MgSiO_3$: H_2O - 29 wt. % H_2O



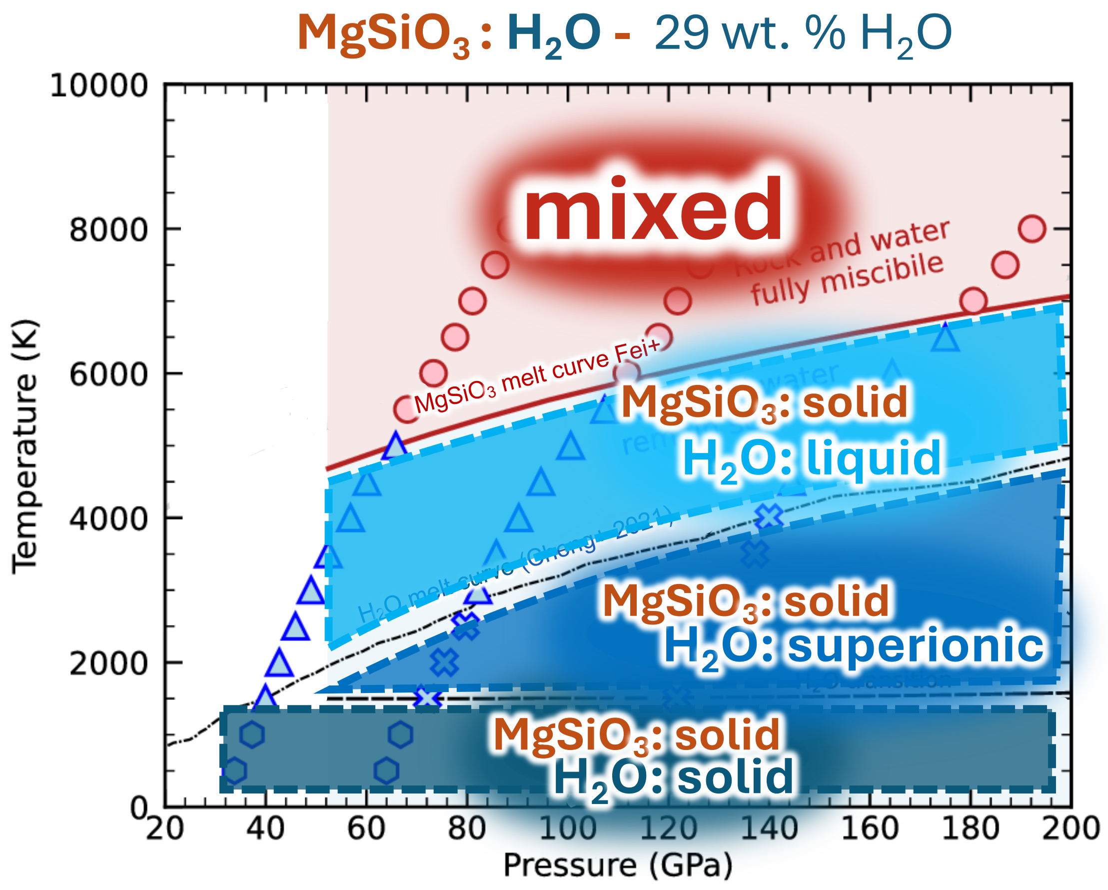
Kovačević+ ***Sci. Rep.*** (2022)

MgO : H_2O - 33 wt. % H_2O

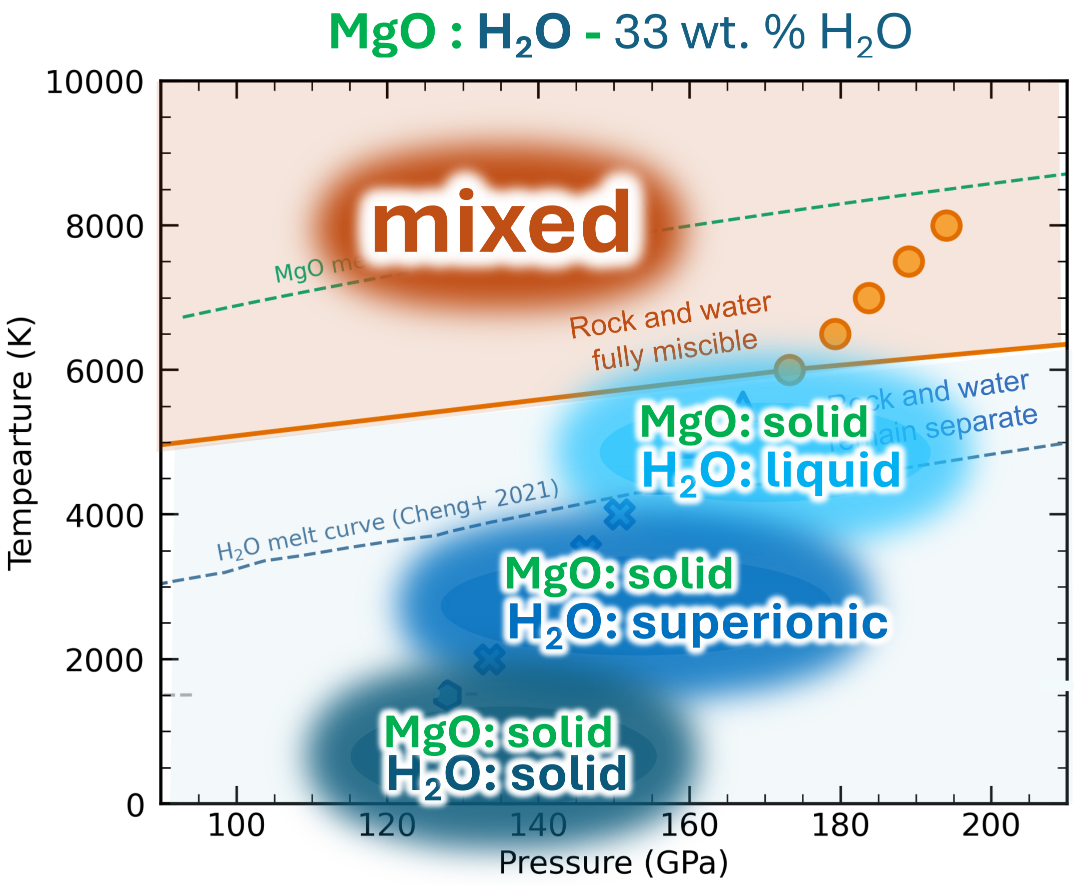


Kovačević+ ***CPP*** (2023)

Results: isochore plots



Kovačević+ ***Sci. Rep.*** (2022)



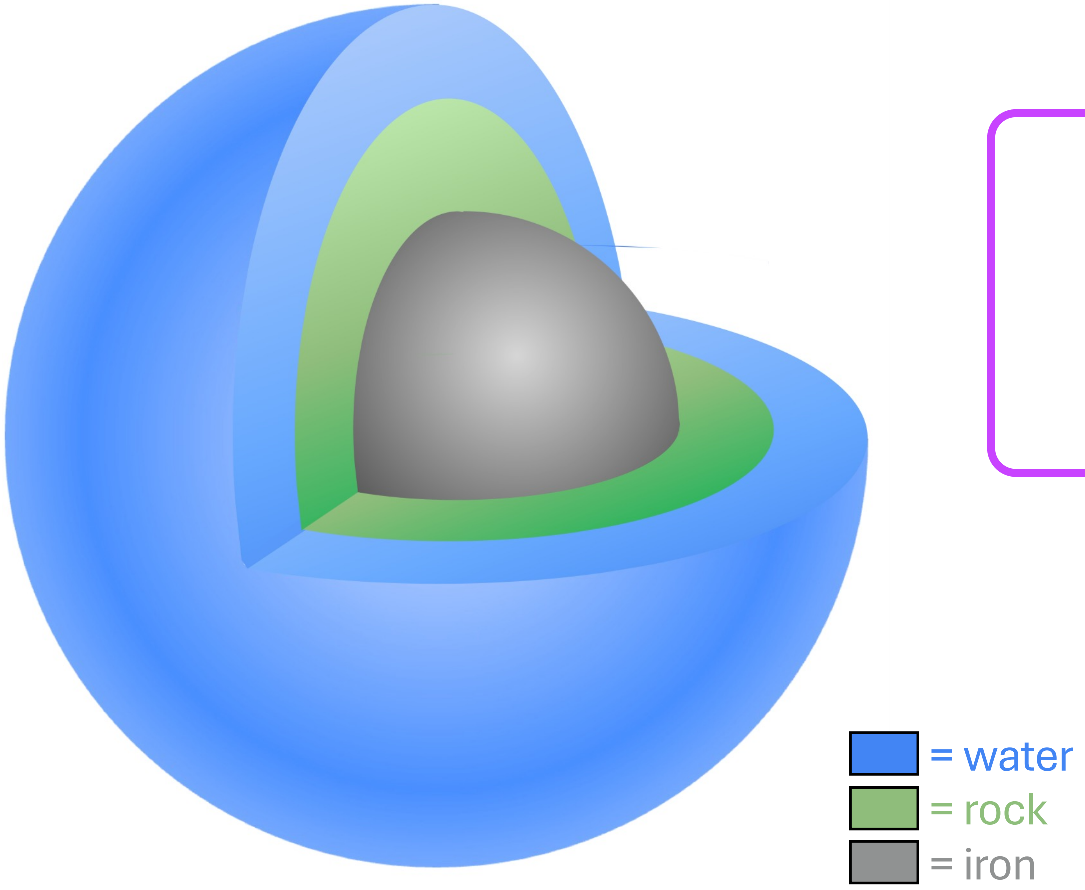
Kovačević+ ***CPP*** (2023)

composition (wt. %)

$MgSiO_3 : H_2O$	$MgO : H_2O$
29 wt. % H_2O	33 wt. % H_2O

Collab: giant impact simulations

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

composition (wt. %)

$MgSiO_3 : H_2O$	$MgO : H_2O$
29 wt. % H_2O	33 wt. % H_2O

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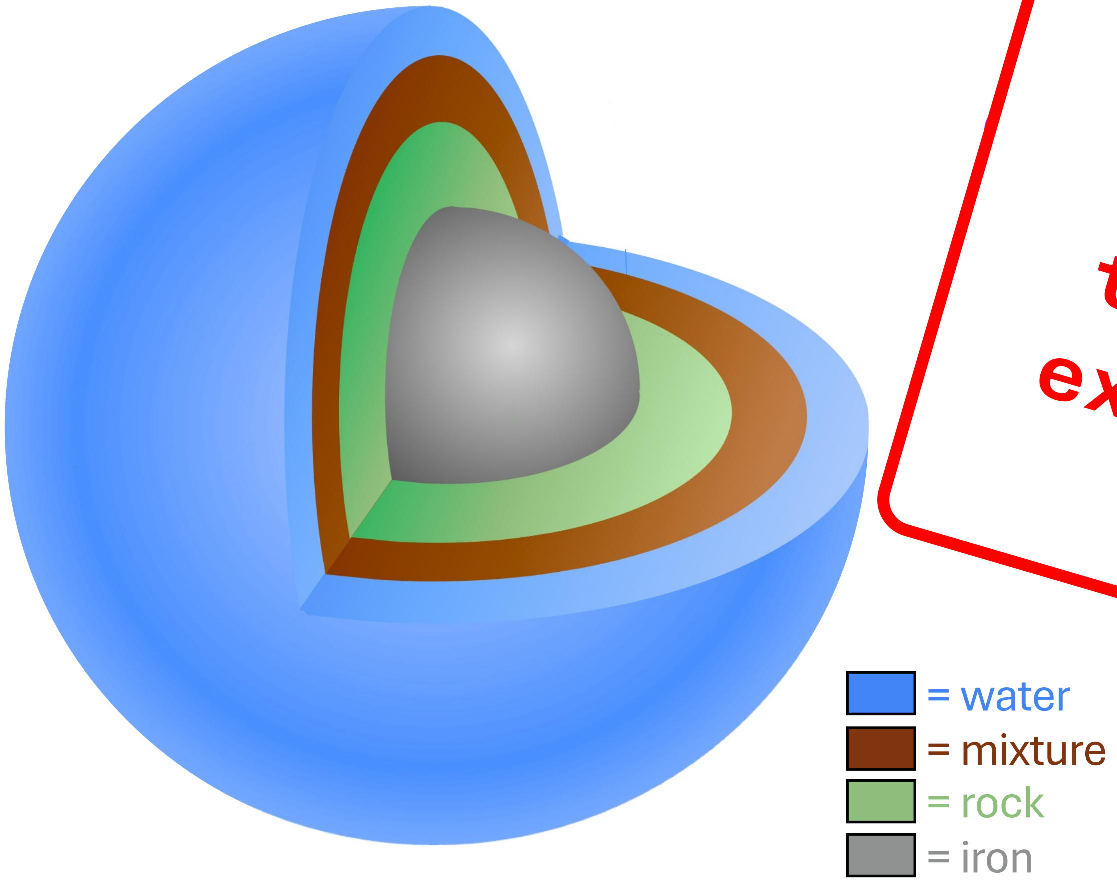

Our work provides theoretical evidence that many water rich exoplanets have mixed mantles

THANK YOU!

Militzer Group

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CMEC

HEARTS TO H2H HUMANITY ETERNAL

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