Unlocking the Rocky Exoplanet Interior-Atmosphere Connection via Laboratory Experiments

Maggie Thompson[1,2]

Paolo Sossi[2], Dan Bower[2], Anat Shahar[3], Sylvain Petitgirard[2], Meng Tian[4]

[1]NASA Sagan Fellow, Earth and Planets Laboratory, Carnegie Institution for Science

[2]Experimental Planetology Group, Institute of Geochemistry and Petrology, ETH-Zürich

[3]Earth and Planets Laboratory, Carnegie Institution for Science

[4]University Observatory Munich, Ludwig-Maximilians-University

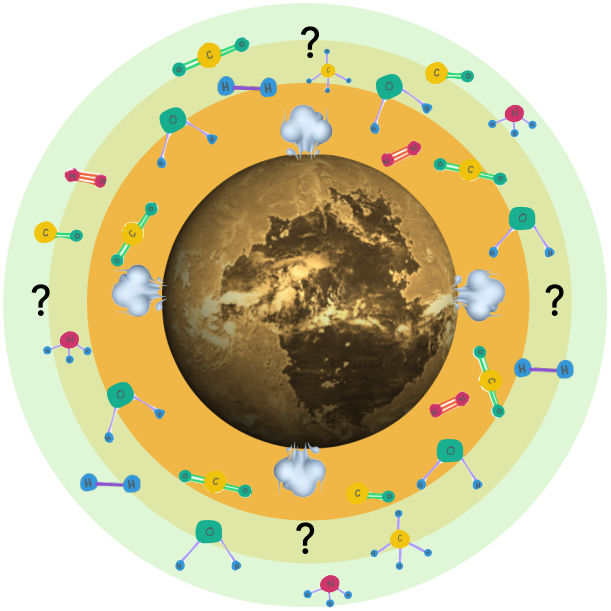
NASA Hubble Fellowship Program

NHFP Symposium
Caltech, Pasadena, CA
September 16, 2024

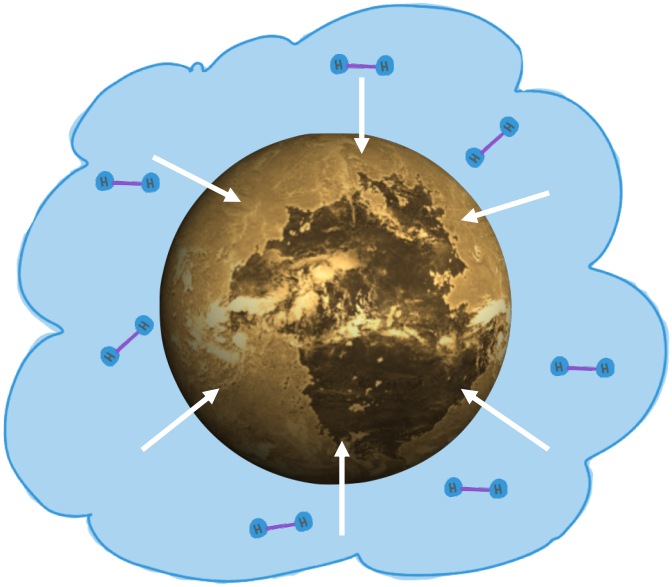
PLANETOLOGY GROUP

ETH zürich

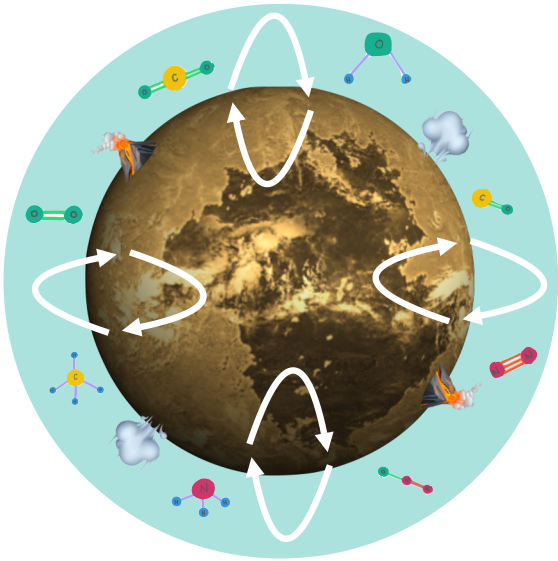
What Controls the Mass and Composition of Rocky Planet Atmospheres?



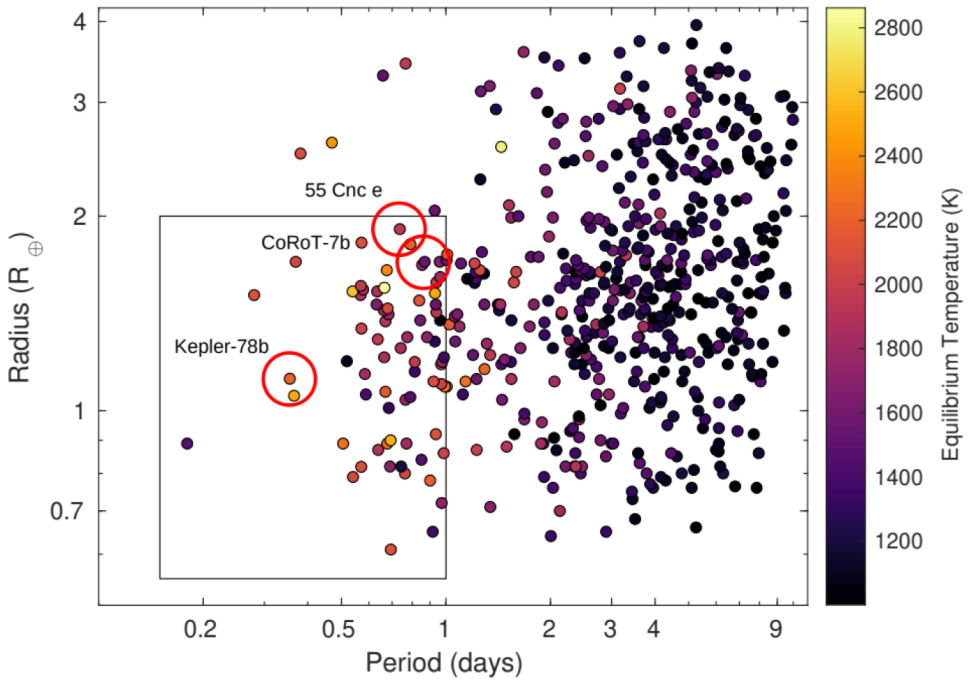
Experimental Constraints: Volatile Solubility and Outgassing Experiments

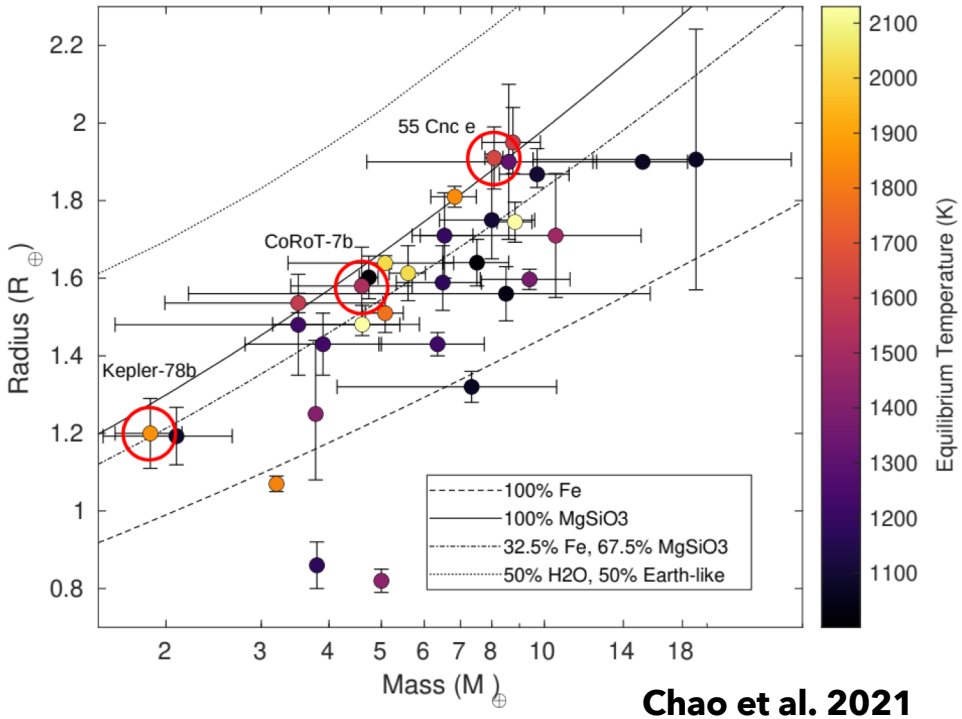


Numerical Constraints: Connecting Planetary Interiors and Atmospheres with *Atmodeller*



Magma Worlds: Near-Term Windows into Rocky Exoplanet Diversity

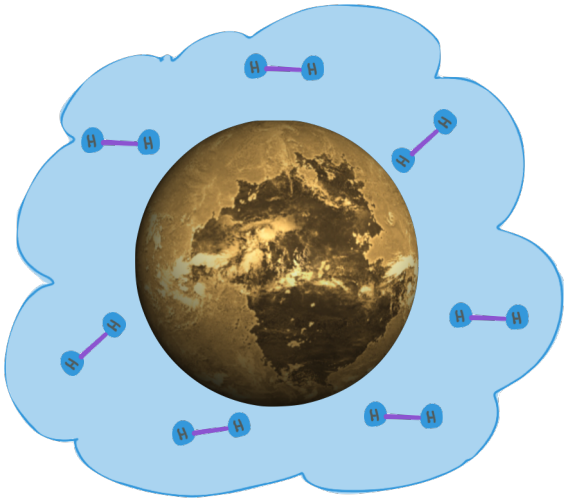




Chao et al. 2021

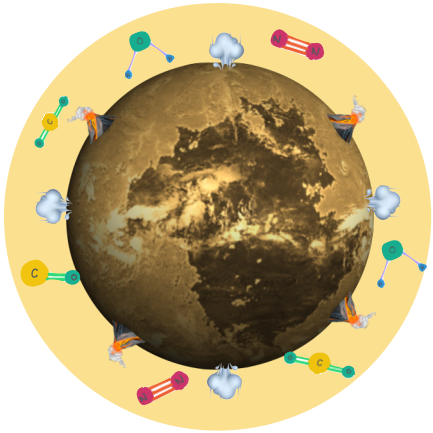
- Magma planets: extensive lava or magma oceans at their surfaces
- **Observational advantage**: short orbital periods and bright day-side fluxes in infrared light

Formation of Rocky Planet Atmospheres



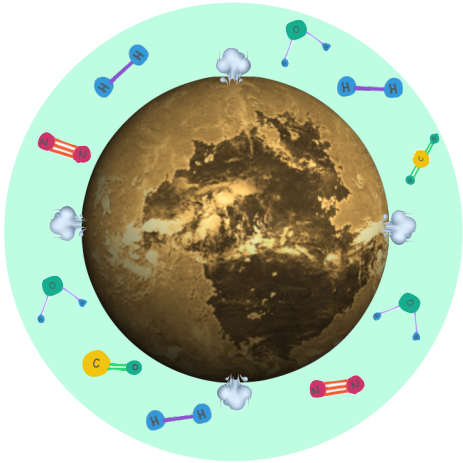
Primary Atmospheres

Form via capturing H_2-rich nebular gas



Secondary Atmospheres

Form via outgassing during planetary accretion and later through subsequent tectonic processes



Hybrid Atmospheres

Combination of residual primary atmosphere and outgassing

Tian & Heng 2023

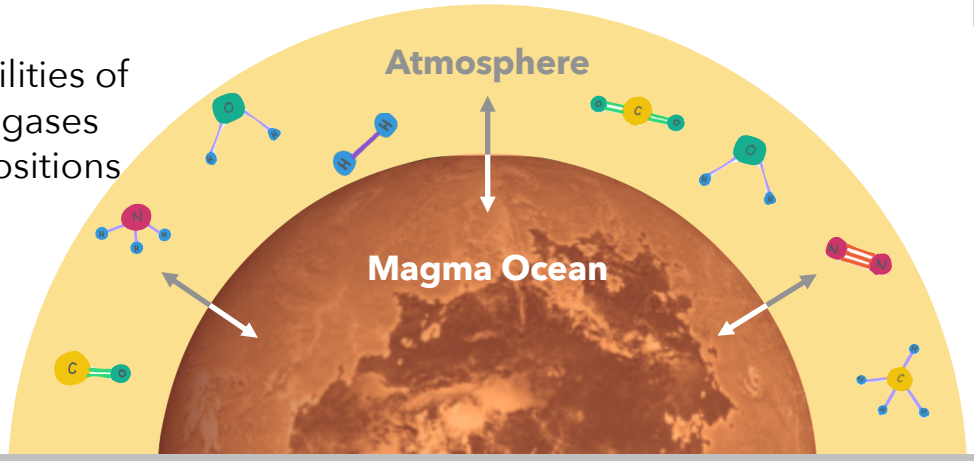
What Controls the Mass and Composition of Hot, Rocky Planet Atmospheres?

Magma planet atmospheres depend on:

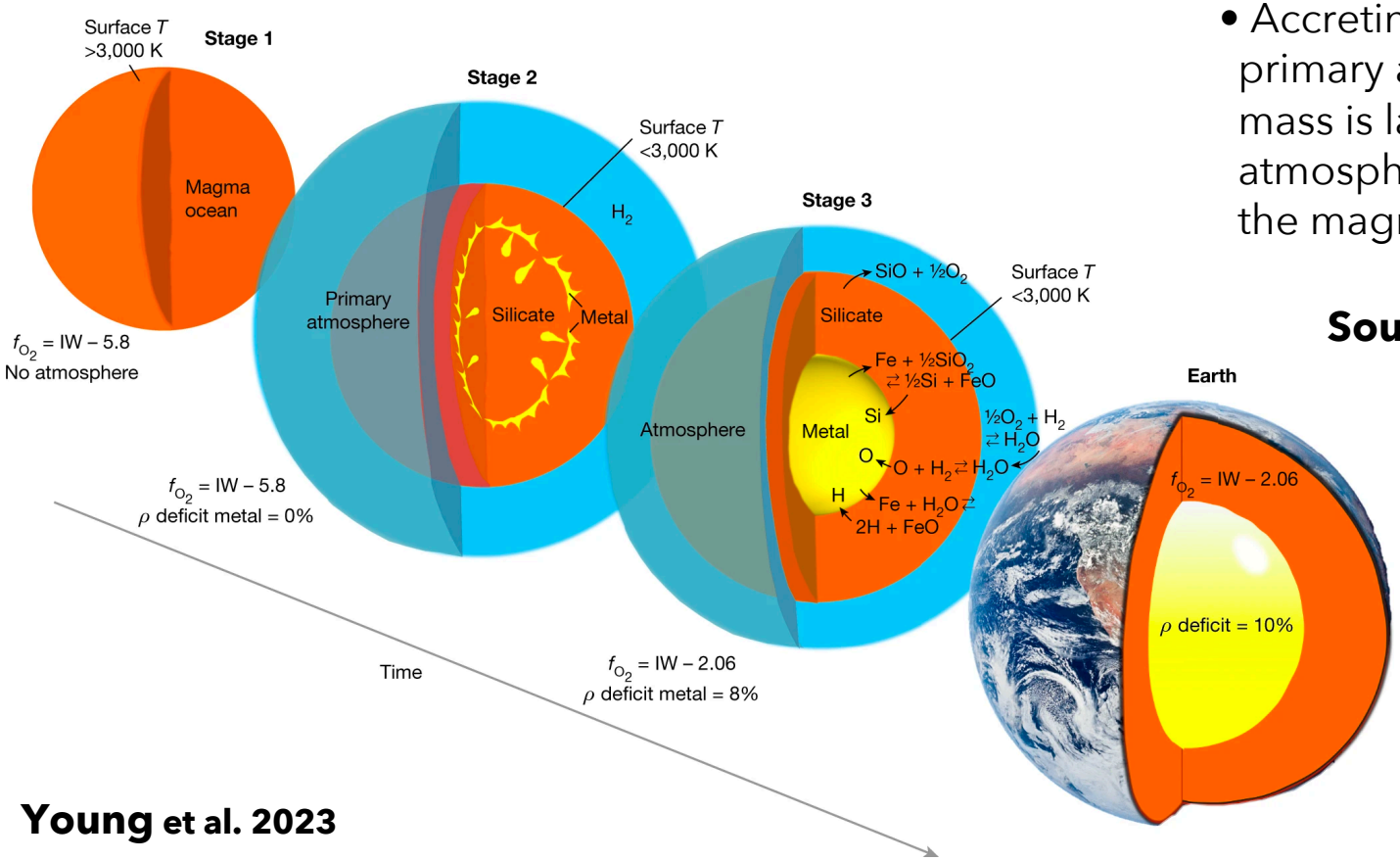
- Rocky precursor material
- Solubilities of major gas species in the magma ⟶ $\chi_i = \alpha P_i^{\beta}$

χ_i = Mole fraction of species i dissolved in melt
α = Solubility constant
P_i = Partial pressure of i in atmosphere
β = Stoichiometric coefficient

*There is currently limited experimental data on solubilities of major atmosphere-forming gases in a range of magma compositions relevant for exoplanets



H_2 Solubility and the Influence of Primary Atmospheres for Magma Planets



Young et al. 2023

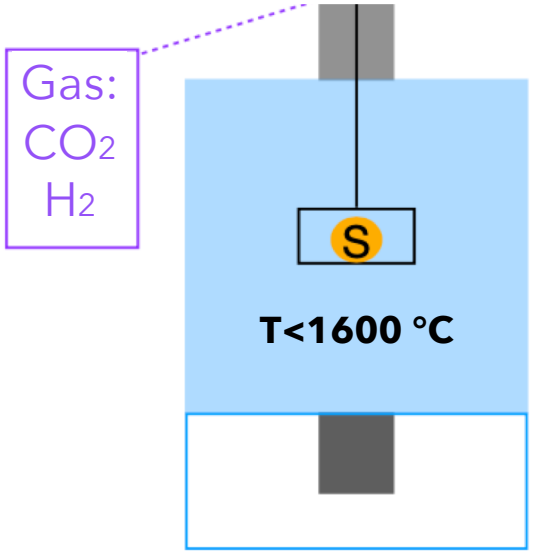
- Accreting planets can form primary atmospheres if the planet mass is large enough and the atmospheric H_2 can dissolve into the magma ocean

Source of Earth's Water?

- Earth's water may have originated from reactions between oxygen in the magma ocean and hydrogen in the nebular atmosphere

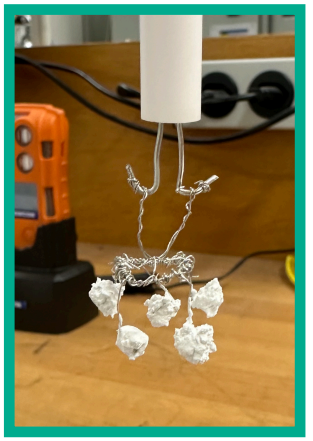
H_2 Solubility Experiments: Instrument and Set-Up

1-bar Gas-Mixing Furnace

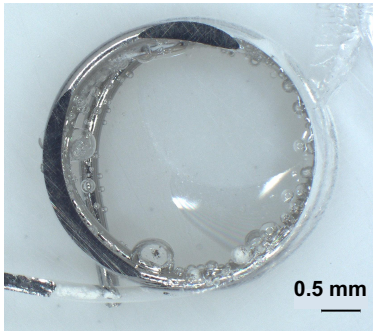


S : Samples

Samples Pre-Experiment



A Quenched Glass Sample Post-Experiment



H_2 Solubility Experiments: Spectral Analysis

Melt Compositions in the Ca-Mg-Al-Si-Fe System

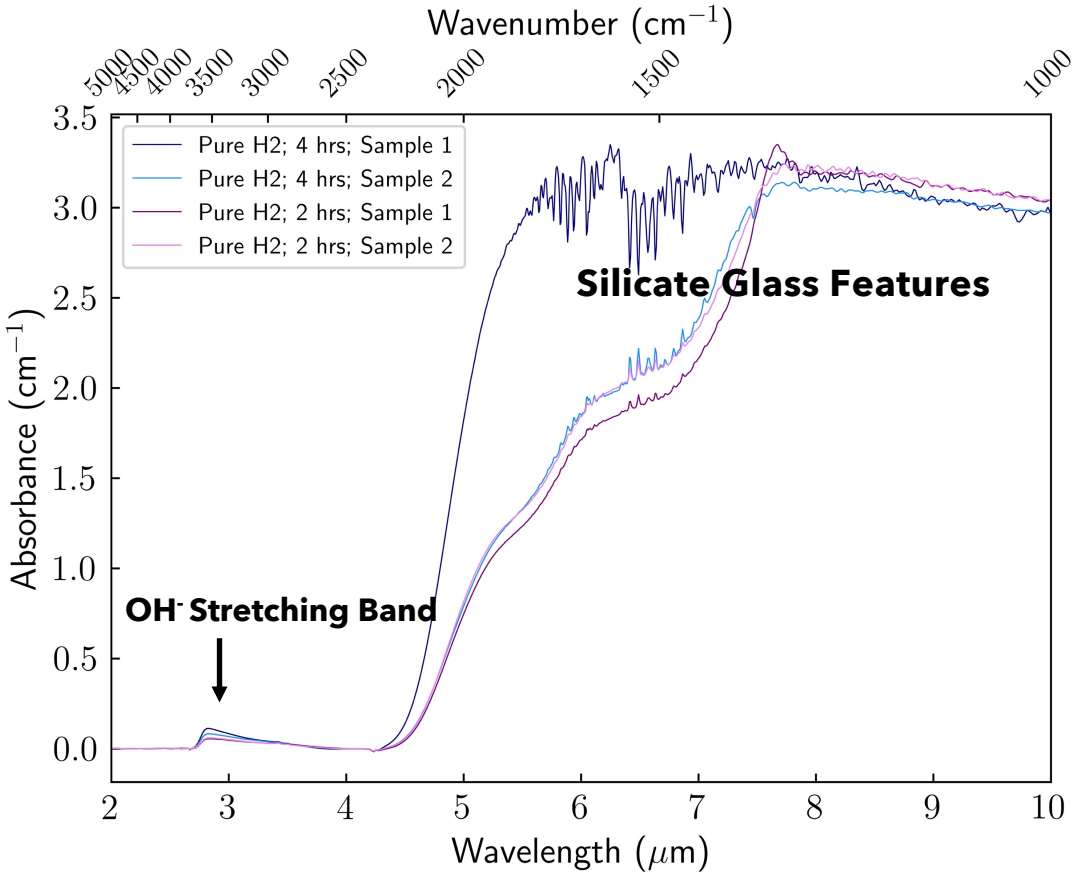
Melt	CaO	MgO	Al_2O_3	SiO_2	FeO
AD eutectic	24.1	10.6	15.2	50.1	–
AD+Fo (15%)	20.5	16.9	12.9	49.6	–
AD+En (60%)	15.2	20.6	9.3	54.8	–
AD+Wo (140%)	38.0	4.6	6.6	50.6	–
AD+Qz (50%)	16.2	6.9	10.0	66.8	–
AD eutectic + 10 wt.% FeO	21.7	9.5	13.7	45.1	10.0
AD eutectic + 20 wt.% FeO	19.3	8.5	12.2	40.1	20.0
AD eutectic + 30 wt.% FeO	16.9	7.4	10.6	35.1	30.0

Anorthite-Diopside Eutectic:
42% Anorthite ($CaAl_2Si_2O_8$) 58% Diopside ($CaMgSi_2O_6$)

Gas Mix: H_2/CO_2 = 5, 10, Pure CO_2, Pure H_2

Temperatures: 1400, 1475, 1550 °C

Fourier-Transform Infrared (FTIR) Spectrometer



Thompson et al. 2024 (in prep.)

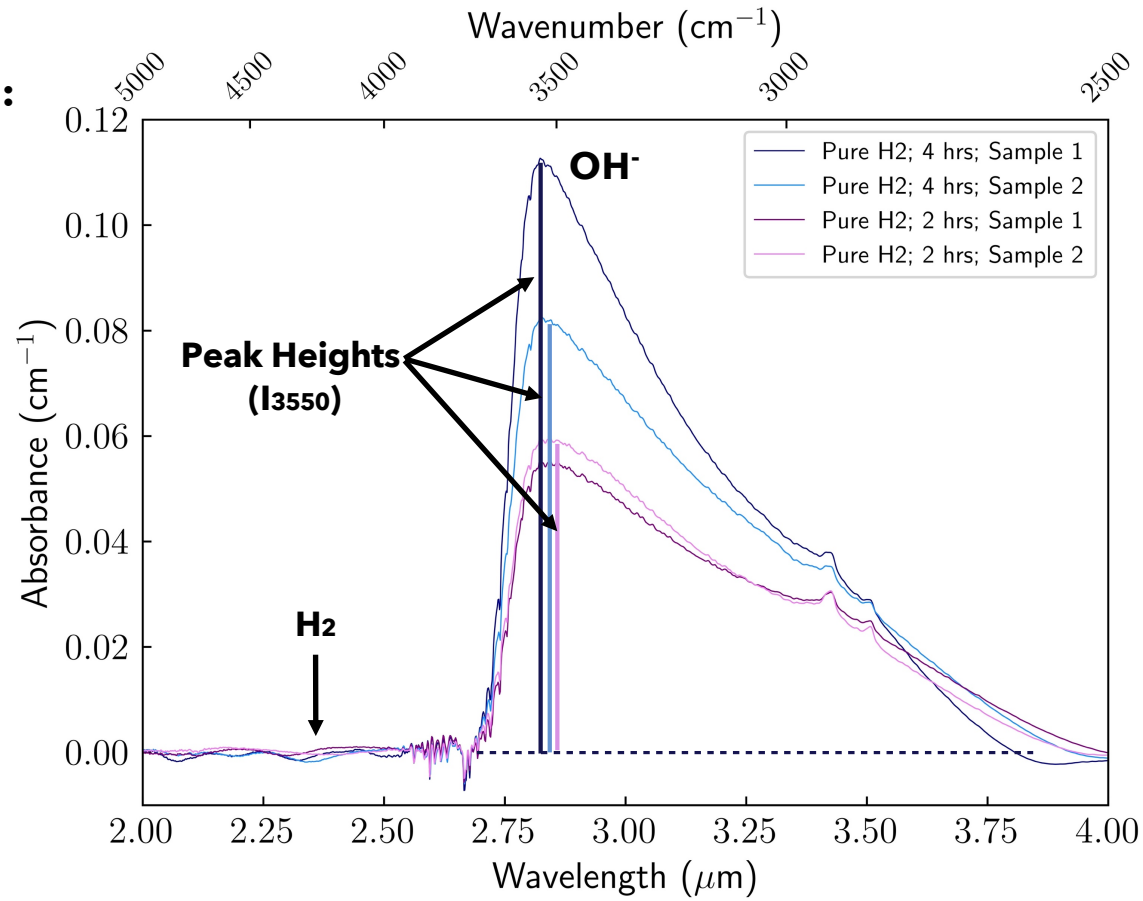
H_2 Solubility Experiments: Spectral Analysis

Quantifying Dissolved H_2 Concentration:

Beer Lambert Law:

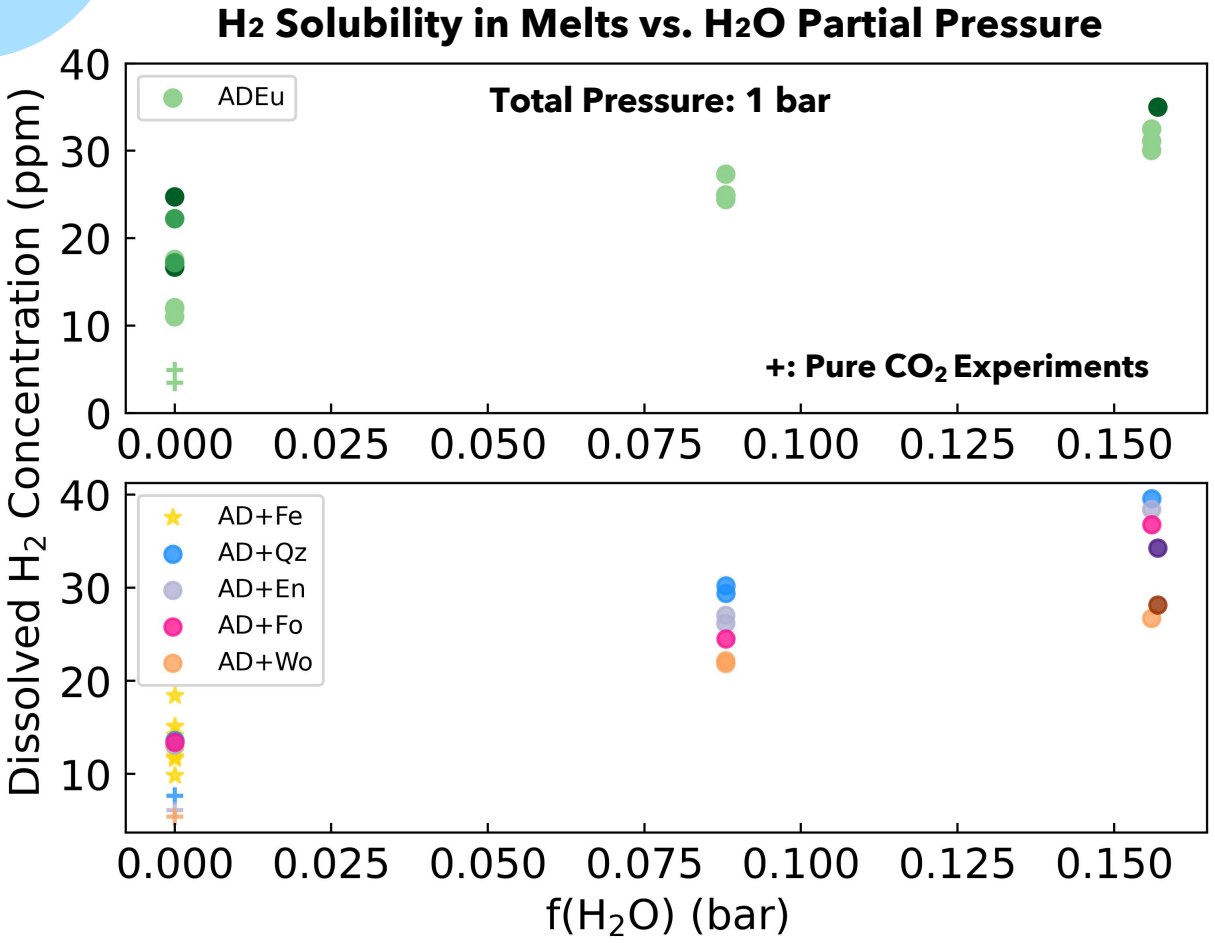
$$[H_2]_{(ppm)} = 10^6 \frac{I_{3550} M(H_2)}{d\rho\epsilon_{3550}}$$

- I_{3550}: Absorption peak heat at 3550 cm^{-1}
- $M(H_2)$: Molar mass of H_2
- d: sample thickness (m)
- ρ: glass density at glass transition temperature (T_g = 700.5 °C) (ρ avg. ~2744 kg/m^3)
- ε: Molar absorption cross section for 3550 cm^{-1} band (Fitted as a function of melt composition, on avg. ~6.0 m^2/mol)



Thompson et al. 2024 (in prep.)

H_2 Solubility Experimental Results



Anorthite-Diopside Eutectic (ADEu)

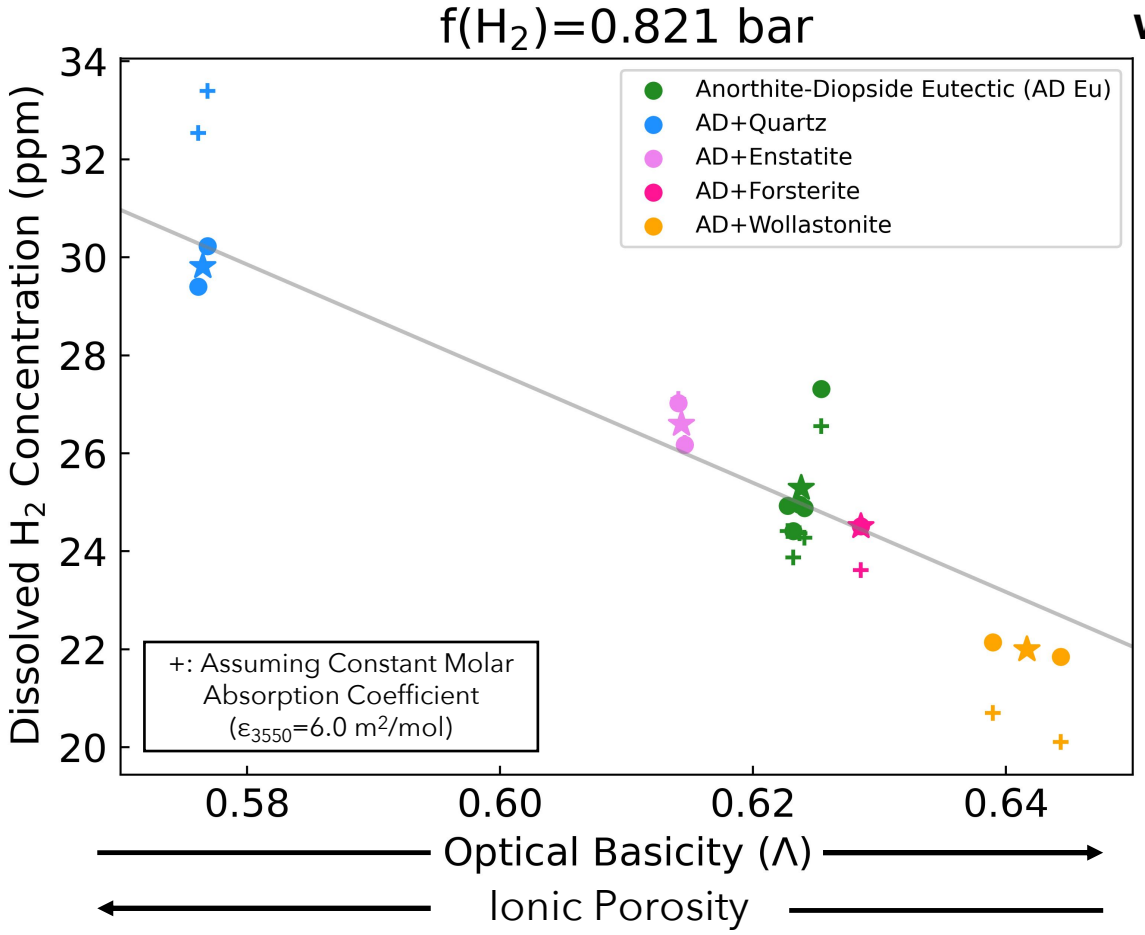
- 1400 °C
- 1475 °C
- 1550 °C

Additional Melt Compositions

- AD+Quartz (1400 °C)
- AD+Enstatite: 1400 °C, 1550 °C
- AD+Forsterite (1400 °C)
- AD+Wollastonite: 1400 °C, 1550 °C
- AD+Fe (1400 °C; Various Proportions of Added Iron: 10, 20, 30 wt. %)

Thompson et al. 2024 (in prep.)

H_2 Solubility vs. Melt Composition



Ways to Characterize the Melt Composition:

- **Degree of Polymerization**: Measure of how interconnected the silicate network is (i.e., how the Si-O tetrahedra link within the network)

  → Optical Basicity: Higher value indicates less interconnected, less viscous melt

$$\Lambda = \frac{\sum_i \chi_i m_i \Lambda_i}{\sum_i \chi_i m_i}$$

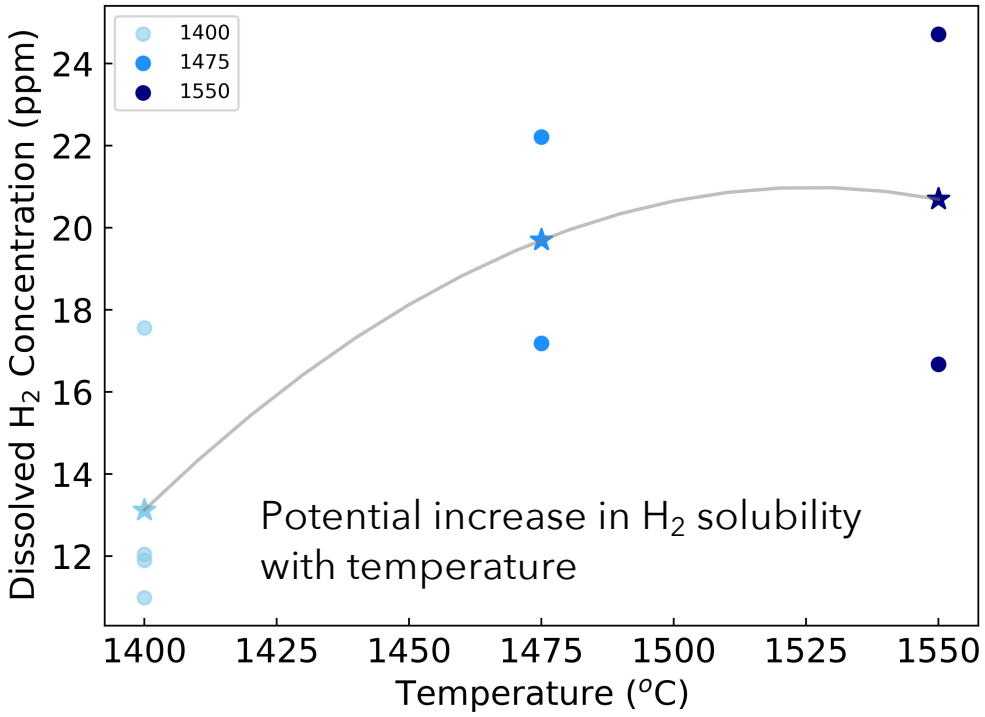
Where:
χ_i = Mole fraction of oxide i
m_i = Number of oxygen atoms of oxide i
Λ_i = Optical basicity of oxide i

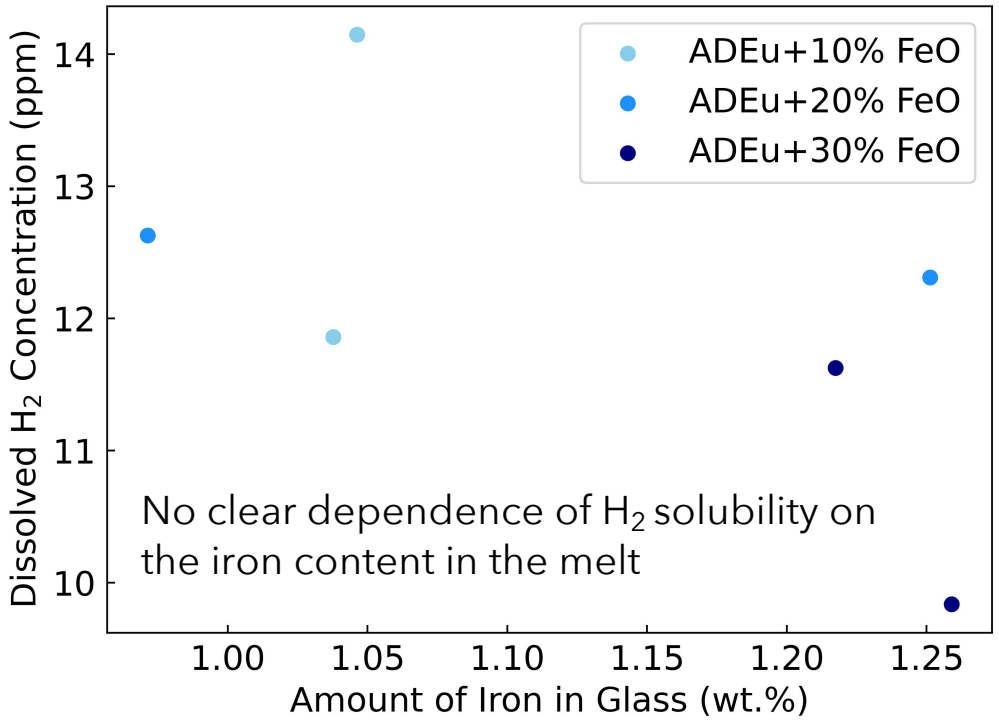
- **Ionic Porosity**: Measure of the amount of free space between ions in the melt (i.e., how open the structure is)

Thompson et al. 2024 (in prep.)

Effect of Temperature and Iron on H_2 Solubility

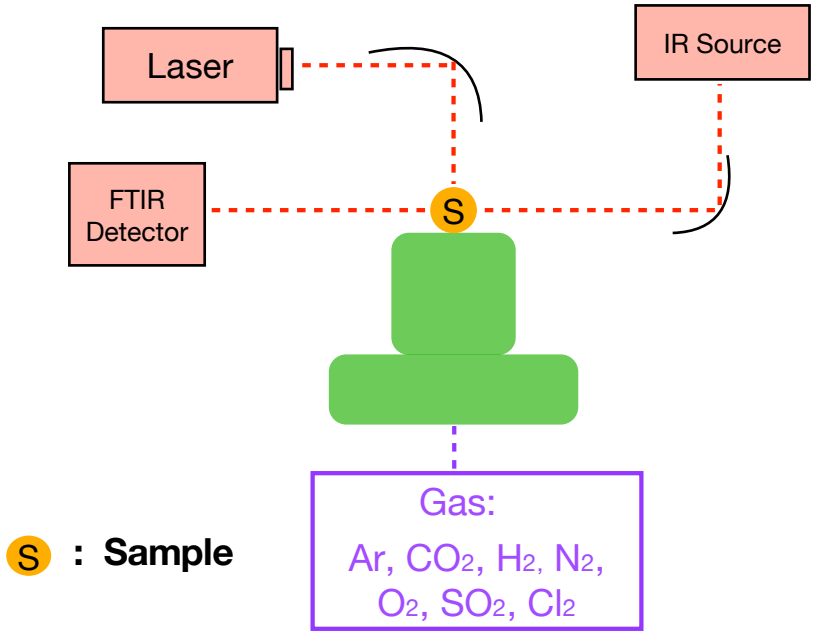
Melt Composition Base = Anorthite-Diopside Eutectic
$f(H_2)$ = 1 bar





Thompson et al. 2024 (in prep.)

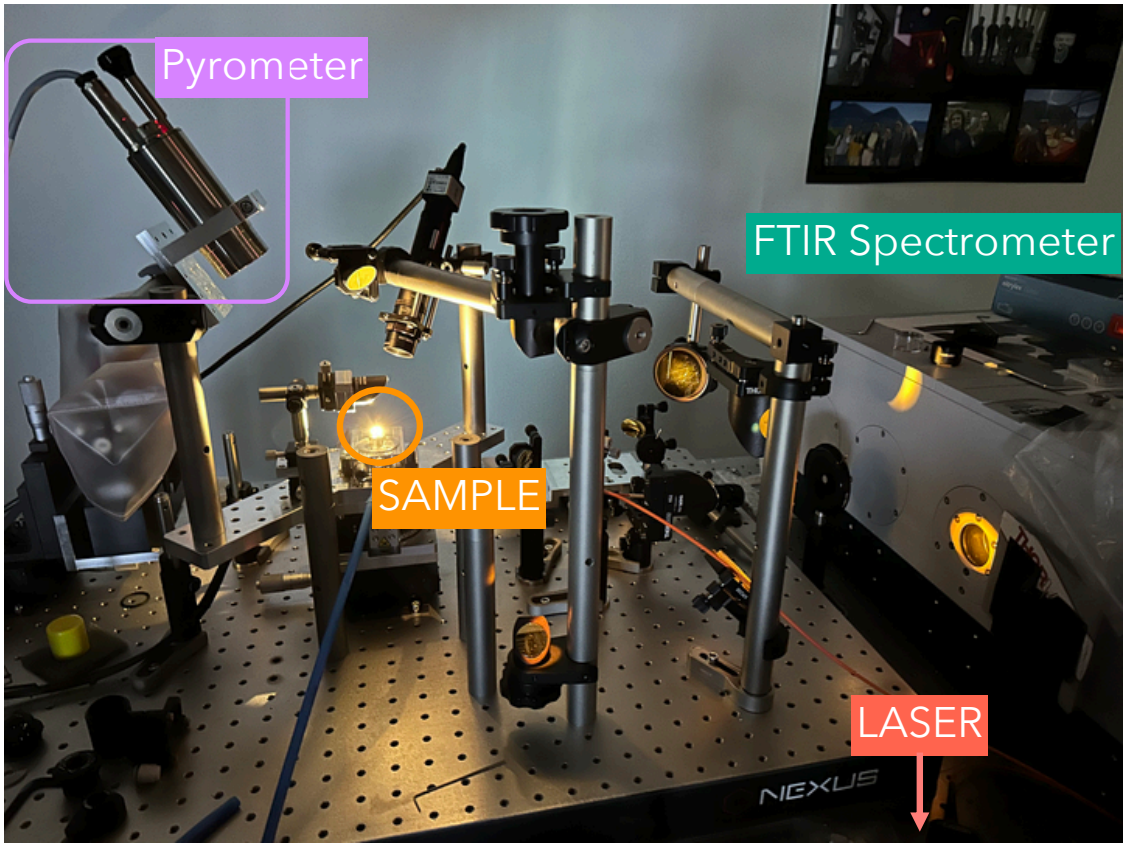
Volatile Solubility and Outgassing Experiments with the Aerodynamic Laser Levitation Furnace + FTIR



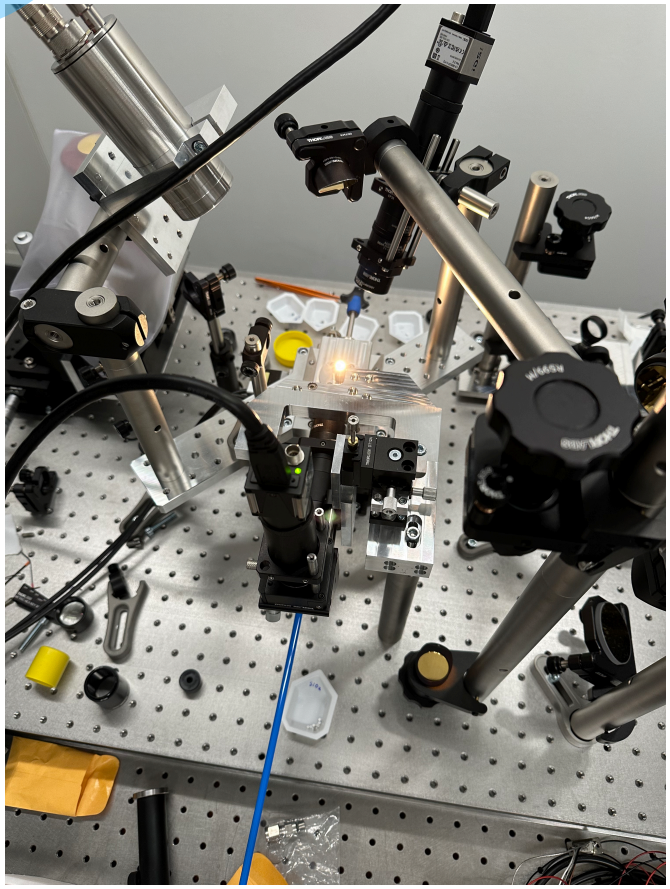
S : Sample

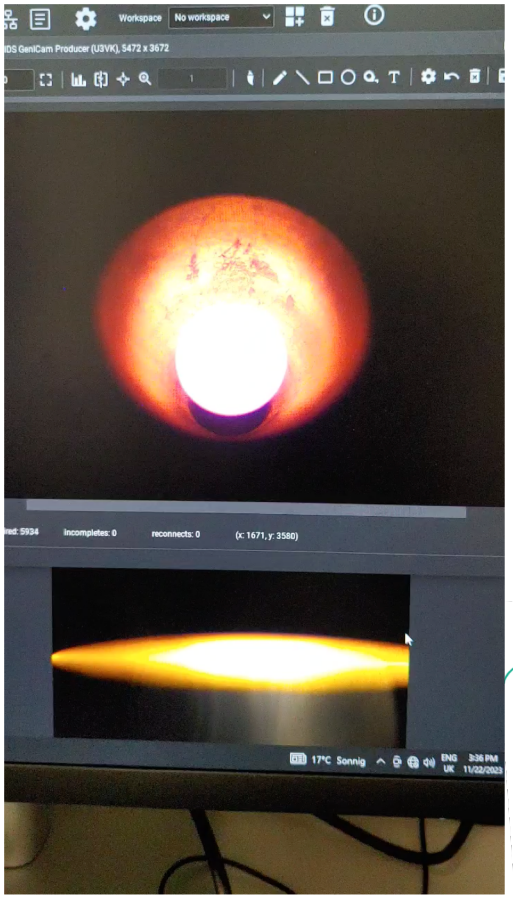
Temperature: 1450 - 2500 °C (and even higher!)

Pressure: 1 bar



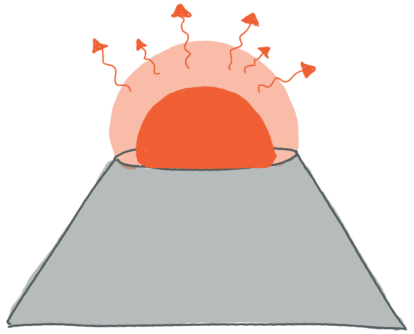
Aerodynamic Laser Levitation Furnace + FTIR



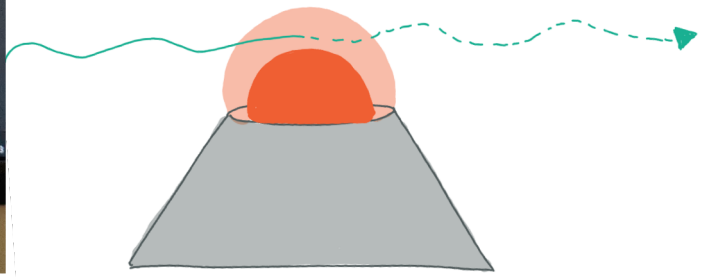


In-Situ Spectroscopy Measurements

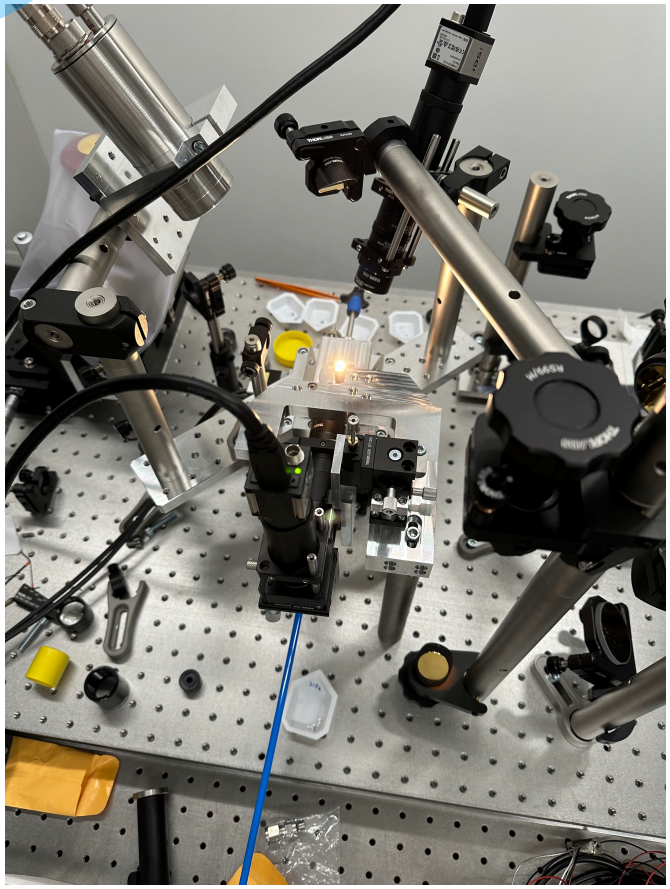
Emission Spectra

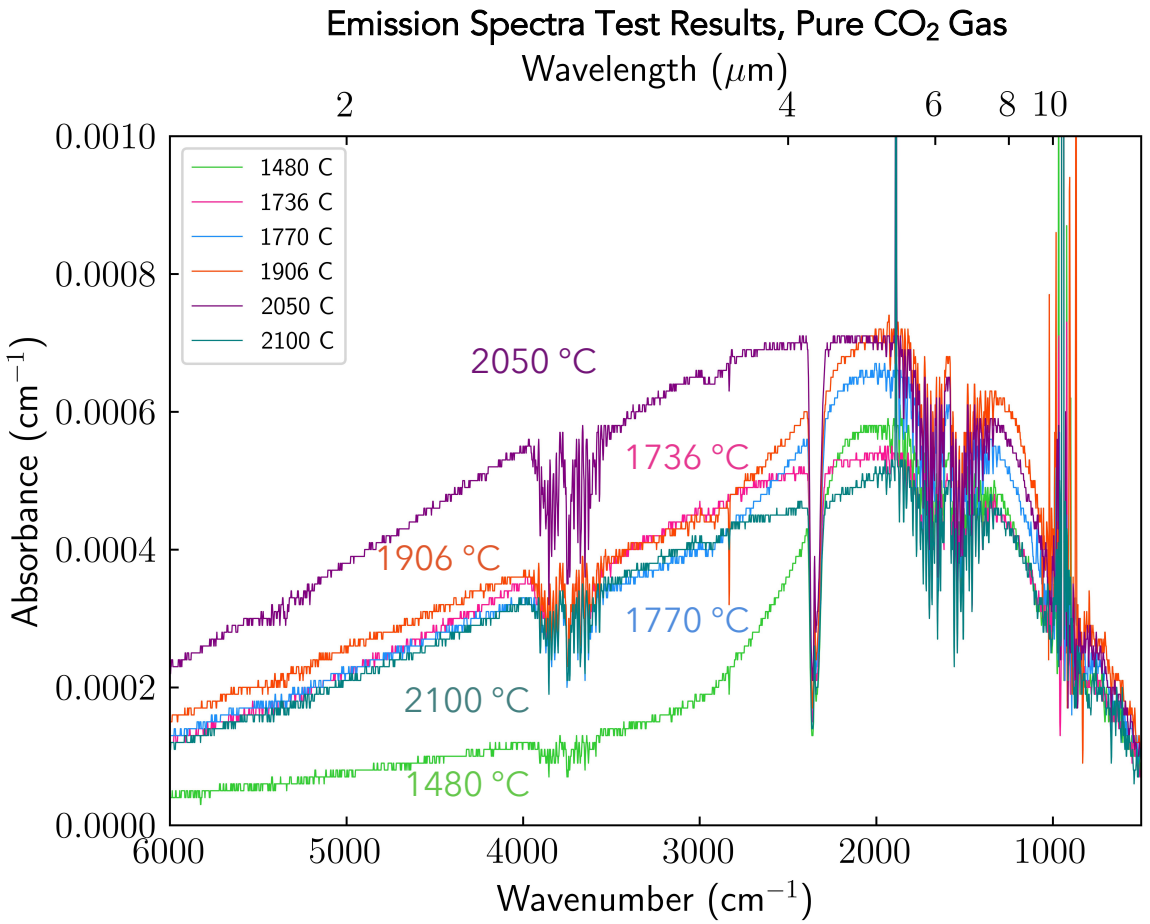


Transmission Spectra



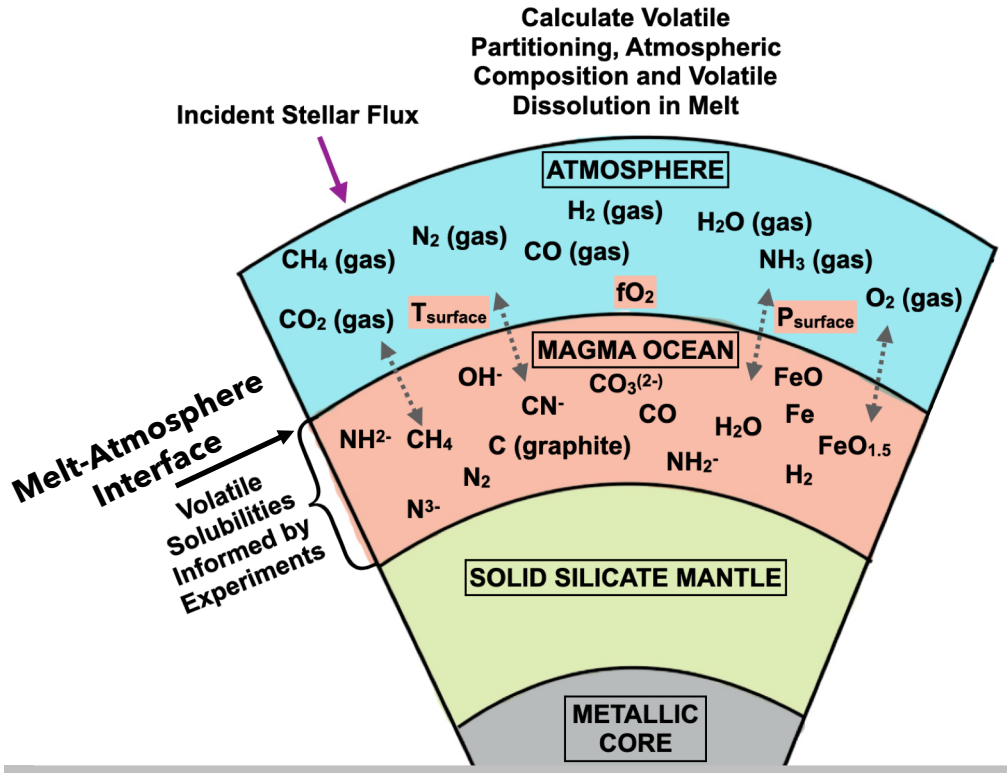
Aerodynamic Laser Levitation Furnace + FTIR





Atmodeller: Volatile Partitioning Code between Planetary Atmospheres and Interiors

Volatile speciation between melt and atmosphere is governed by composition, equilibrium chemistry between the gas species and their solubilities in the melt

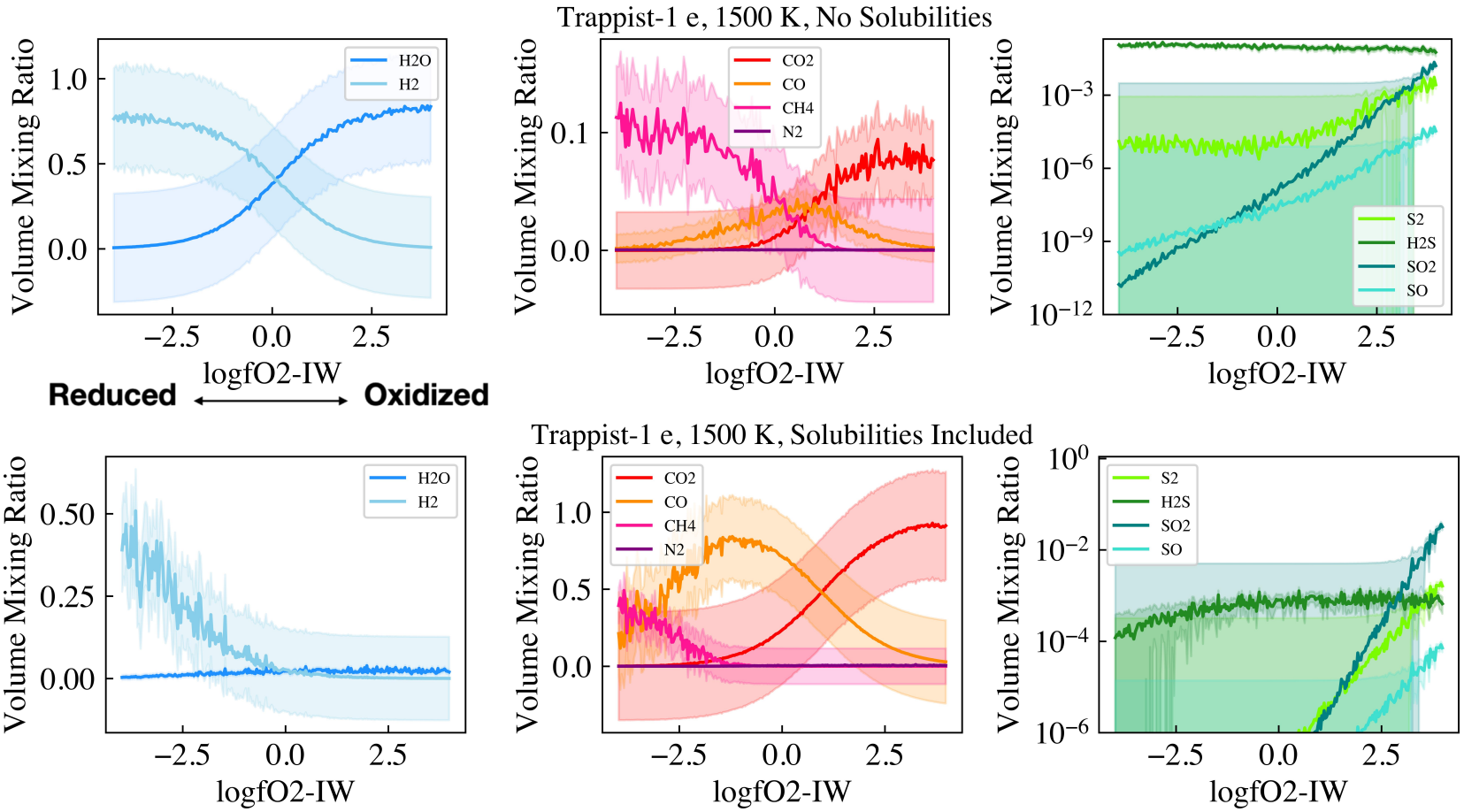


Atmodeller:

- Computes chemical equilibrium conditions at the melt-atmosphere interface
- Includes:
  - Condensed phase thermodynamics
  - Effects of (compositional-dependent) volatile solubilities in the melt
  - Gas non-ideality at high pressures (~kbar/GPa) (i.e., real gas equations of state)

Bower, Thompson et al. 2024, In Prep.

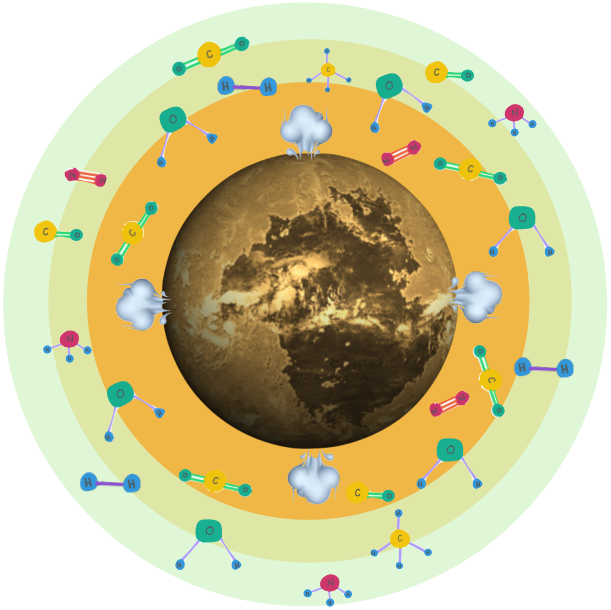
Atmodeller: Effect of Solubilities on Atmospheric Composition



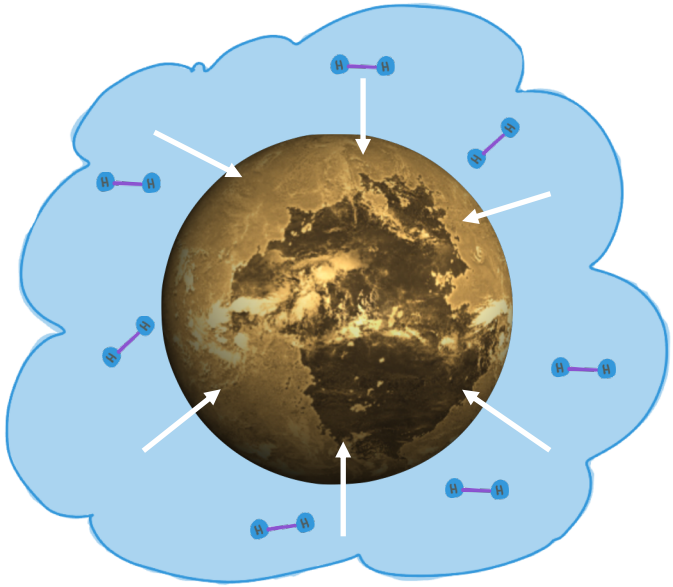
Bower, Thompson et al. 2024, In Prep.

Key Take-Aways

Magma planet atmospheric compositions depend on:
- **Rocky material that composes planet**
- **Solubilities of major gas species in the magma**

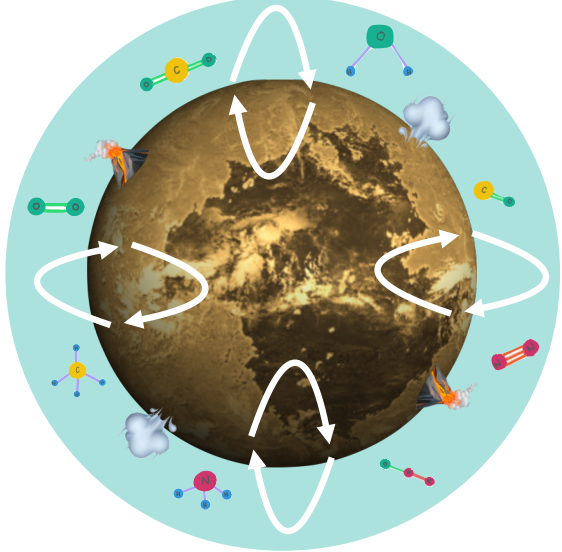


- **At 1 bar, H_2 dissolves in silicate melts as OH and solubility depends on melt composition (and maybe T)**
- **We need more experimental data on volatile partitioning between interior and atmosphere for diverse planetary melts**



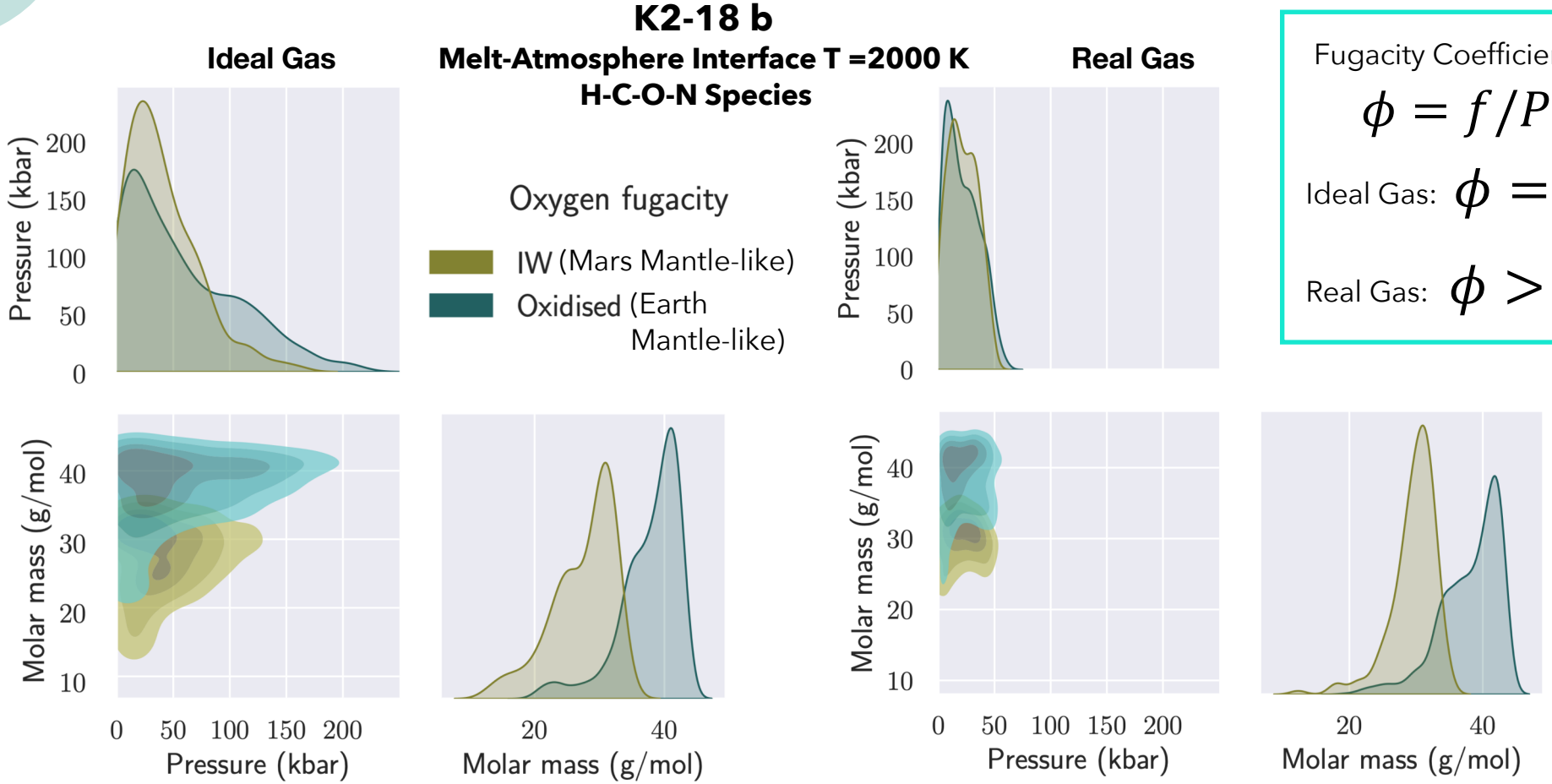
***Atmodeller*: Flexible framework to chemically connect planetary interiors and atmospheres**

- **The volatile inventory in the atmosphere is not necessarily representative of the interior**



Extra Slides

Atmodeller: Sub-Neptunes, Non-Ideality at High Atmospheric Pressures



Fugacity Coefficient

$$\phi = f/P$$

Ideal Gas: $\phi = 1$

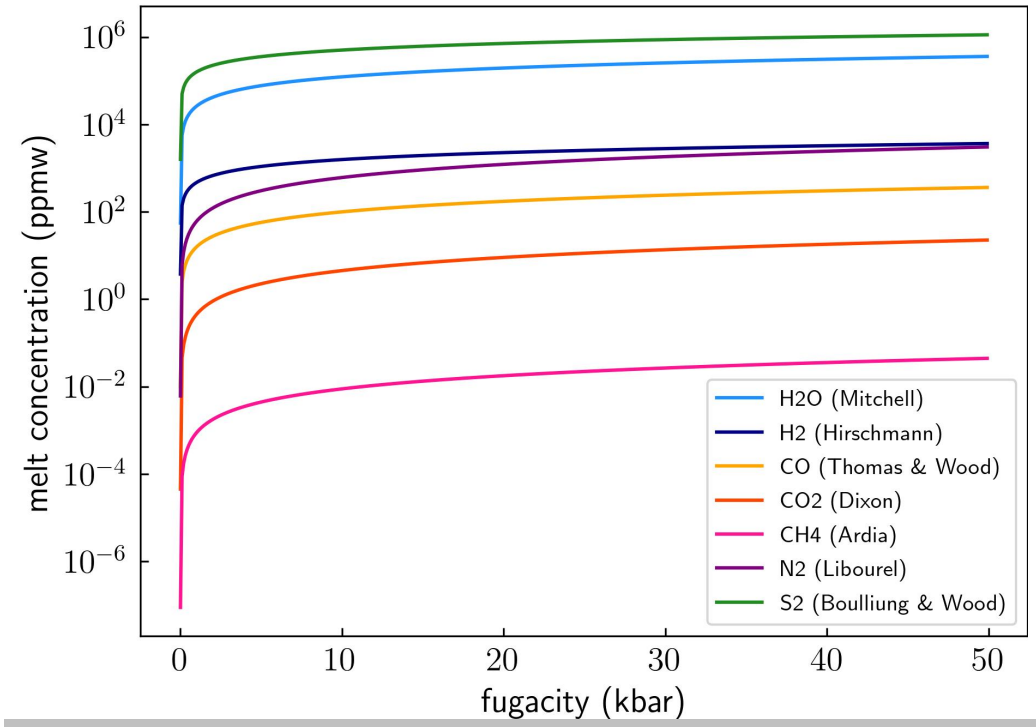
Real Gas: $\phi > 1$

Bower et al., In Prep.

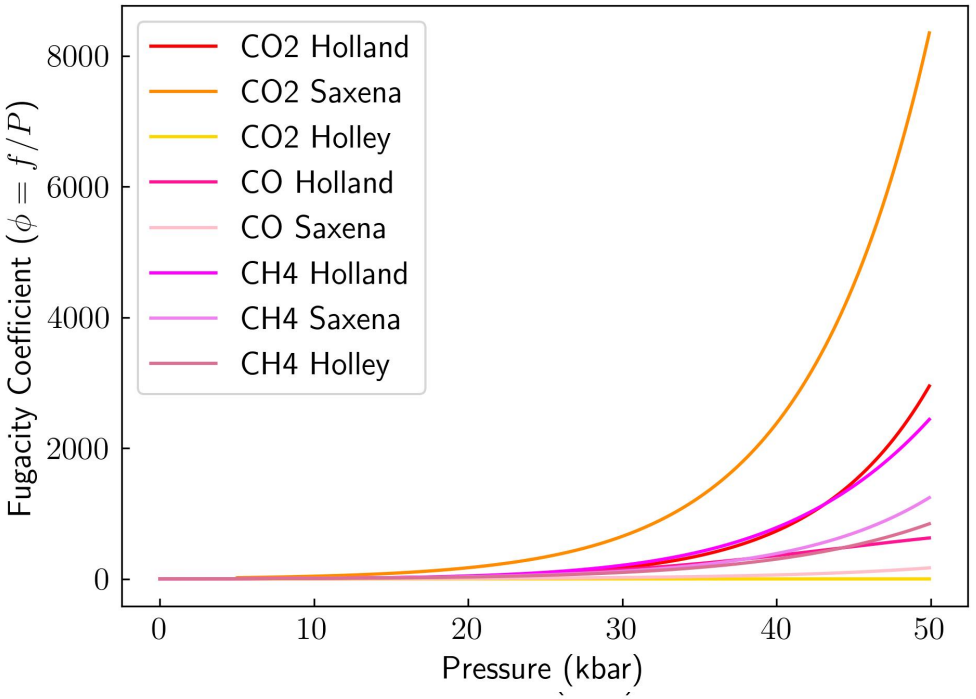
Atmodeller: Library of Solubility Laws and Real Gas Equations of State

Add your solubility laws and equations of state!

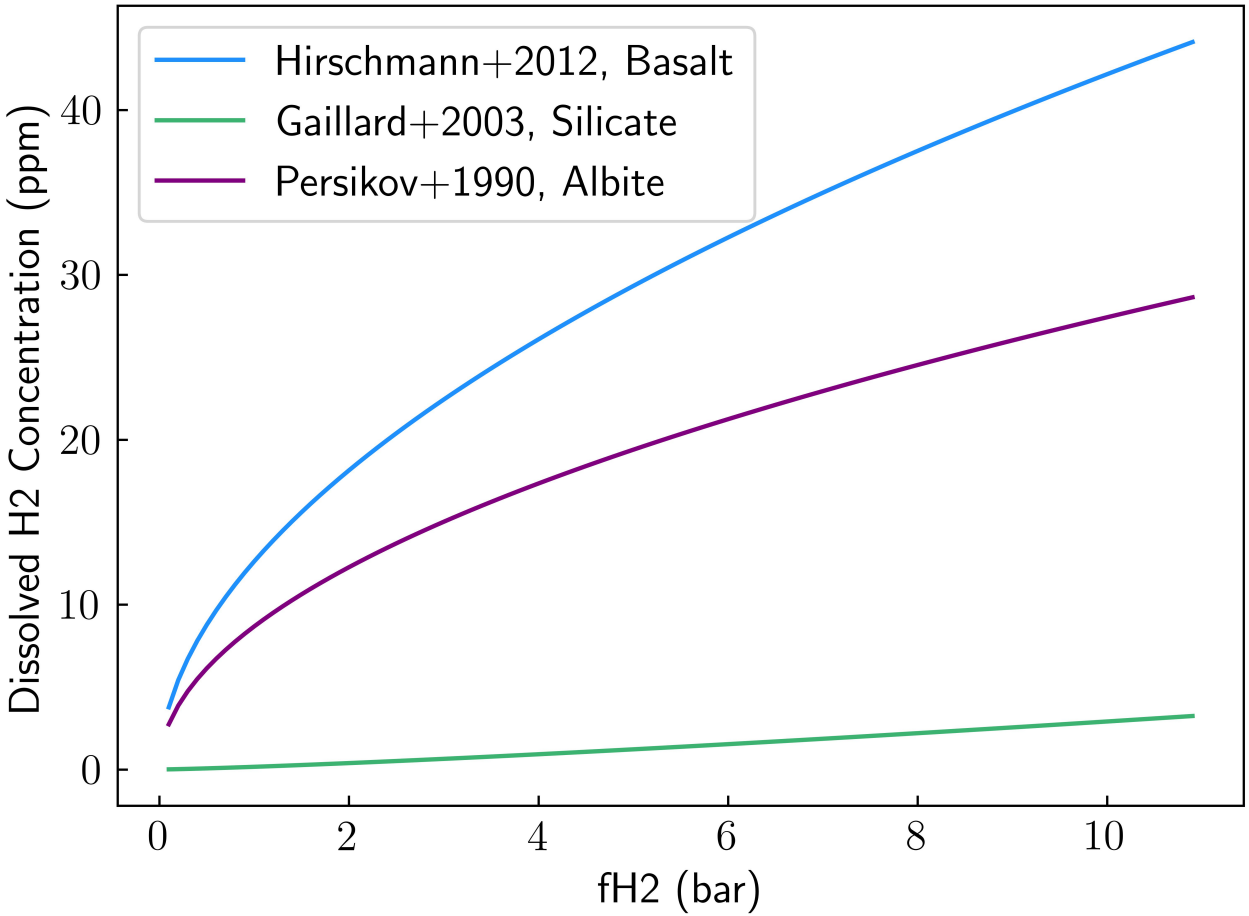
Solubility Laws for Various Melt Compositions
(e.g., Basalt, Andesite, Peridotite, Rhyolite)



Real Gas Equations of State



Bower et al., In Prep.



$$[H_2](ppm) = 10^{(0.524*\log_{10}(f_{H_2})+1.}$$

$$H_2(ppm) = 8.67\sqrt{f_{H_2}}$$

$$[H_2](ppm) = 0.163 f_{H_2}^{1.252}$$