FNRS Astronomy Contact Group
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Unravelling the Chemistry of Sub-Neptune Exoplanets from a Multi-Disciplinary Approach

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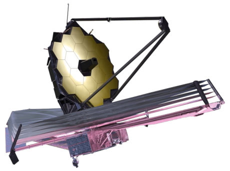
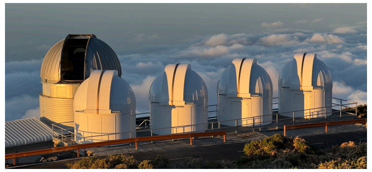
Exoplanet Science in the 2020s and beyond

The Characterisation Era. *Photometry to Spectroscopy*

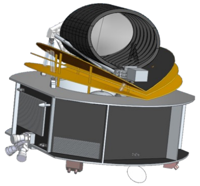
TESS (2018)



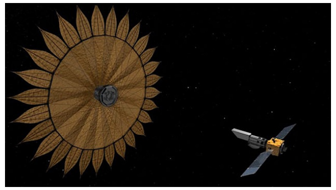
JWST (2021)



MARVEL (2025)



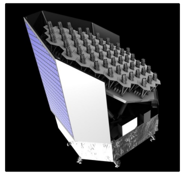
ARIEL (2029)



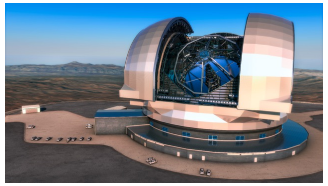
HWO (concept)

CHEOPS (2019)

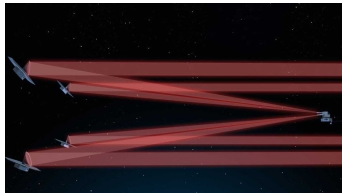
VLT(I) Asgard/NOTT
GRAVITY+
ESPRESSO (HARPS-successor)



PLATO (2026)

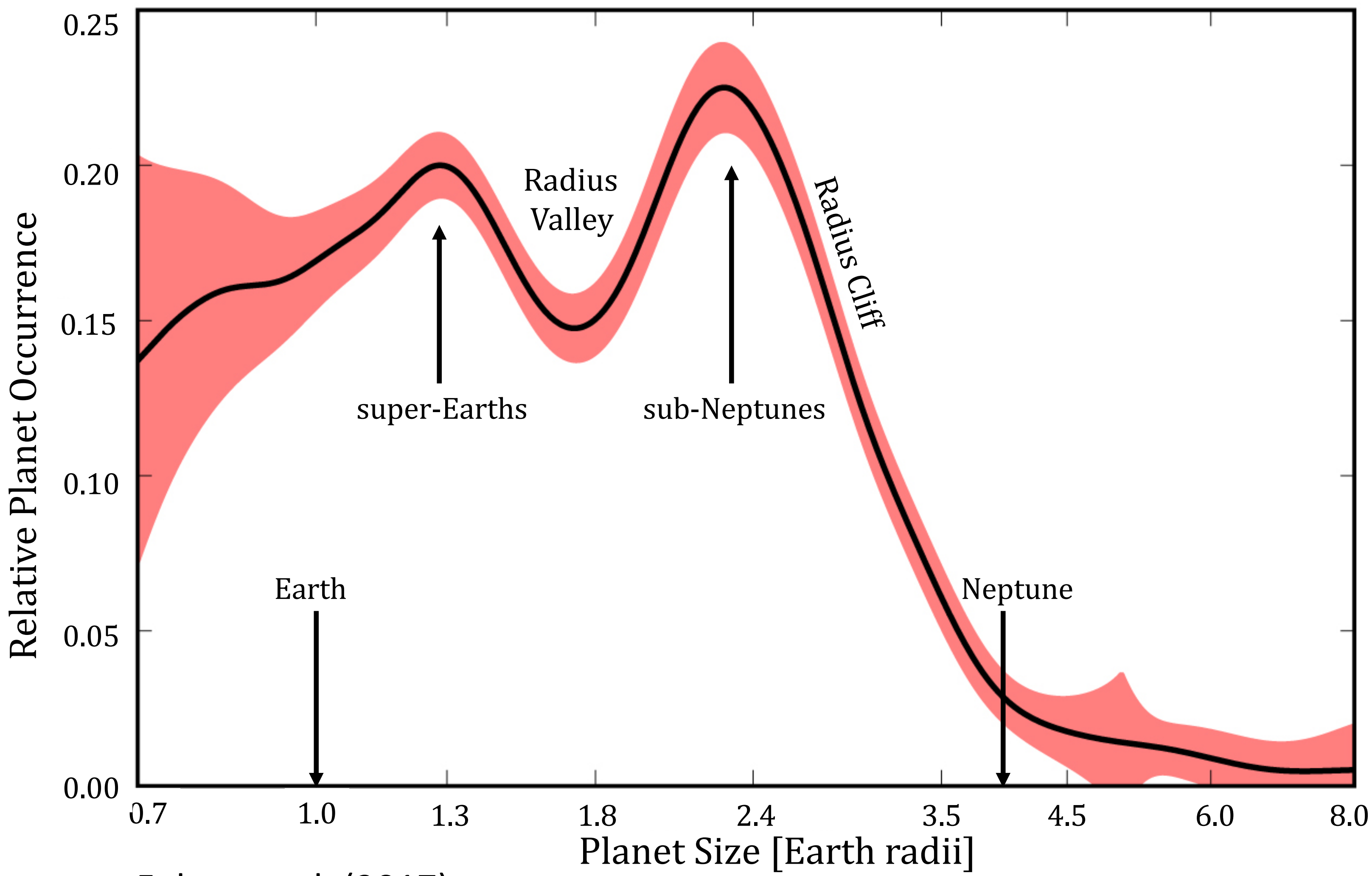


ELT (2029)



LIFE (concept)

What is the Composition of Most Common Exoplanets?

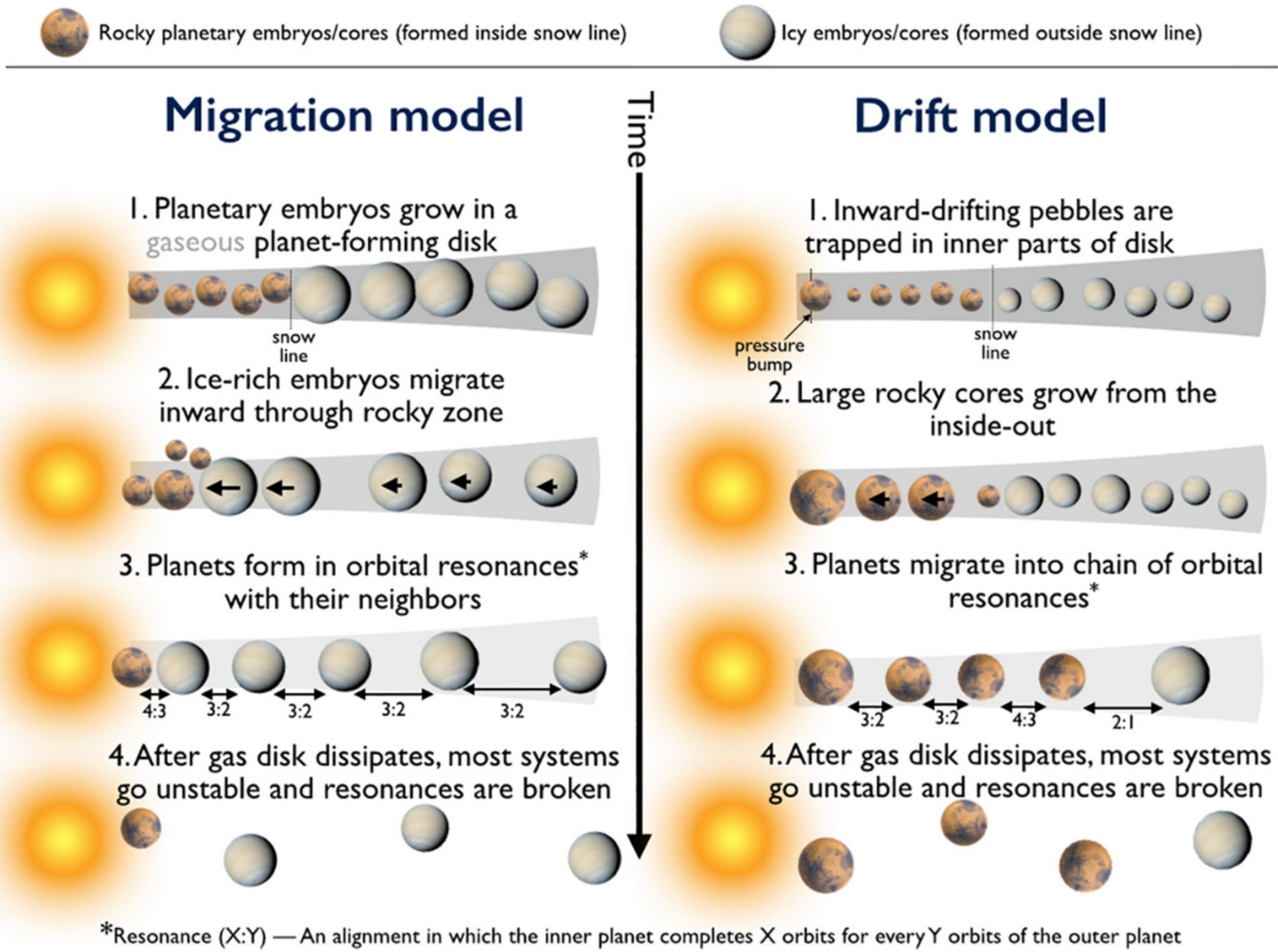


Fulton et al. (2017)

No Super-Earths and Sub-Neptunes in the Solar System

Embryo migration model favours volatile-rich planets

Pebble drift model favours volatile-poor planets



Bean et al. (2021)

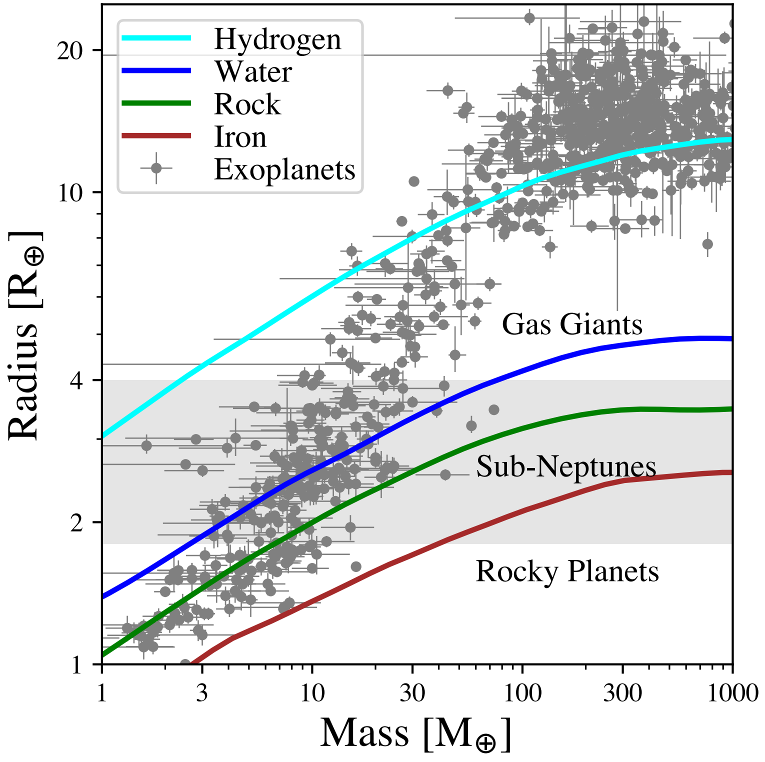
see also Burn et al. (2024)

First Insights into Exoplanet Composition

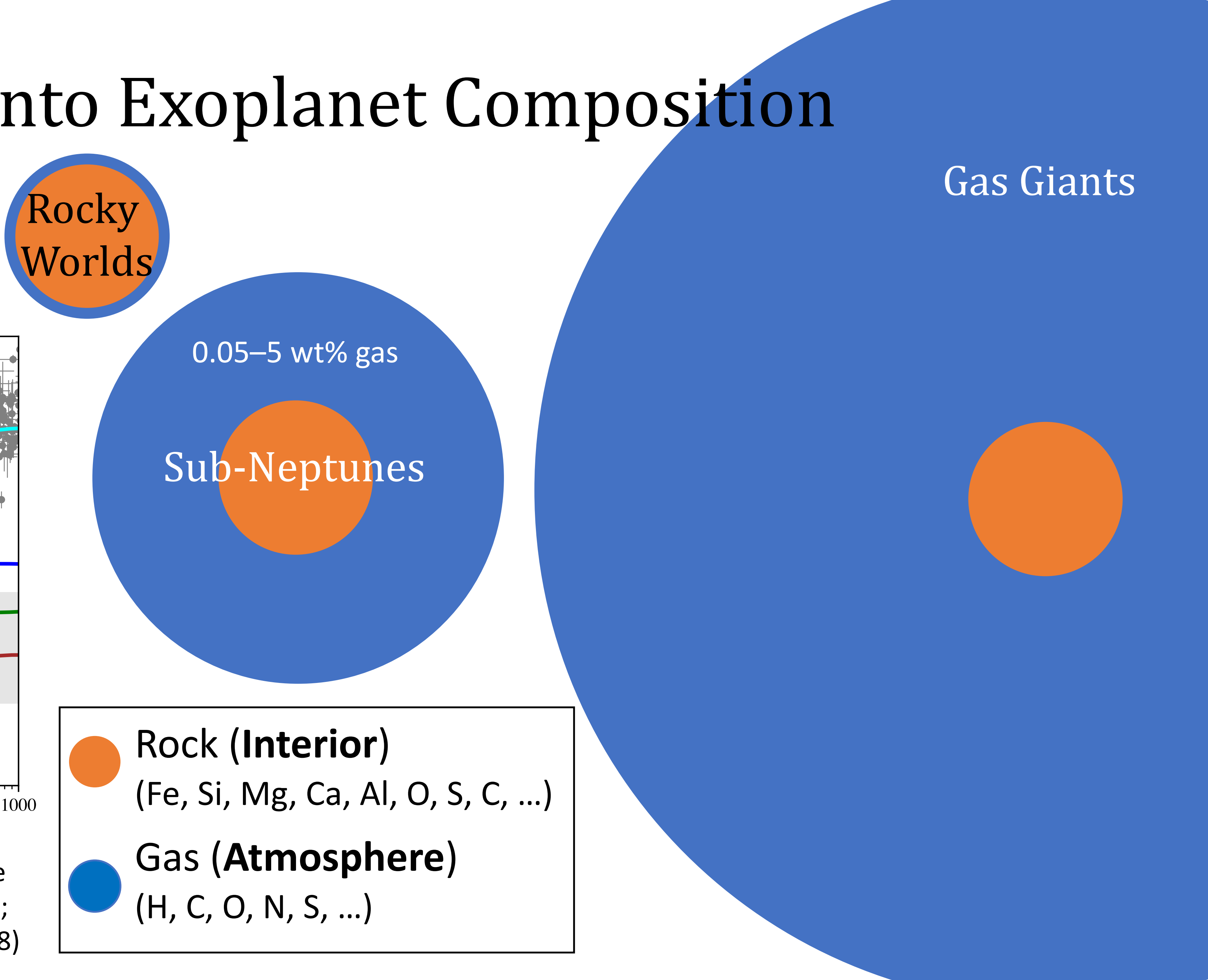
Mass and Radius

↓

Planet Bulk Composition



Data: NASA/Caltech Exoplanet Archive
Equations of state: Seager et al. (2007); Hakim, Rivoldini, Van Hoolst et al. (2018)

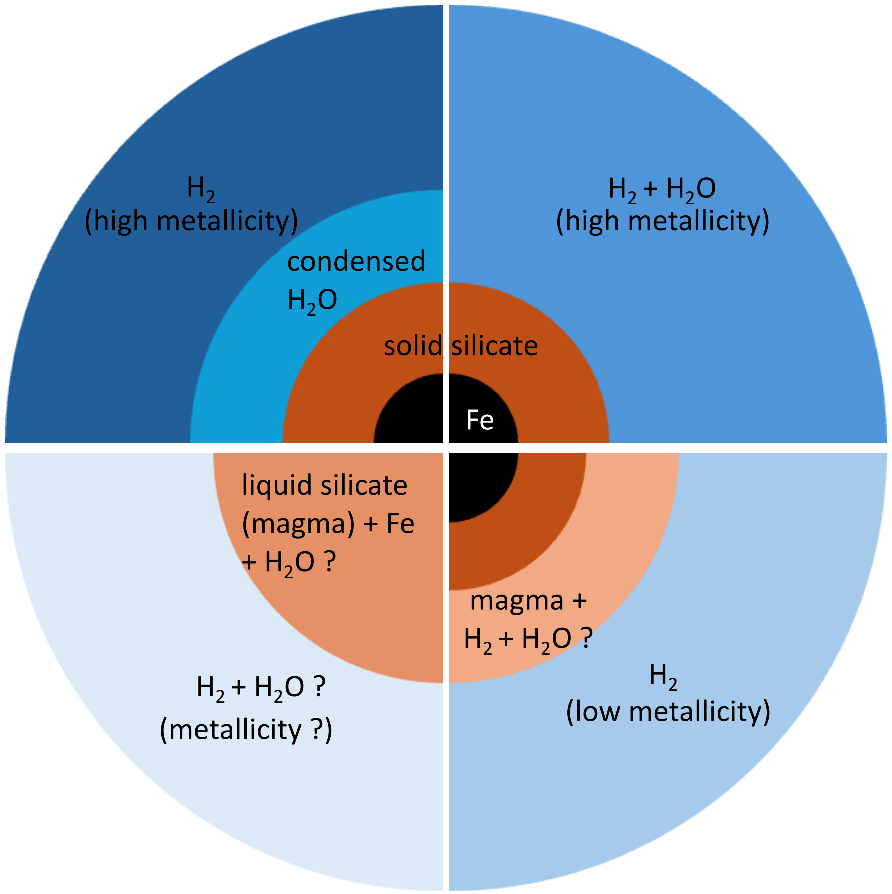


Rock (**Interior**)
(Fe, Si, Mg, Ca, Al, O, S, C, ...)

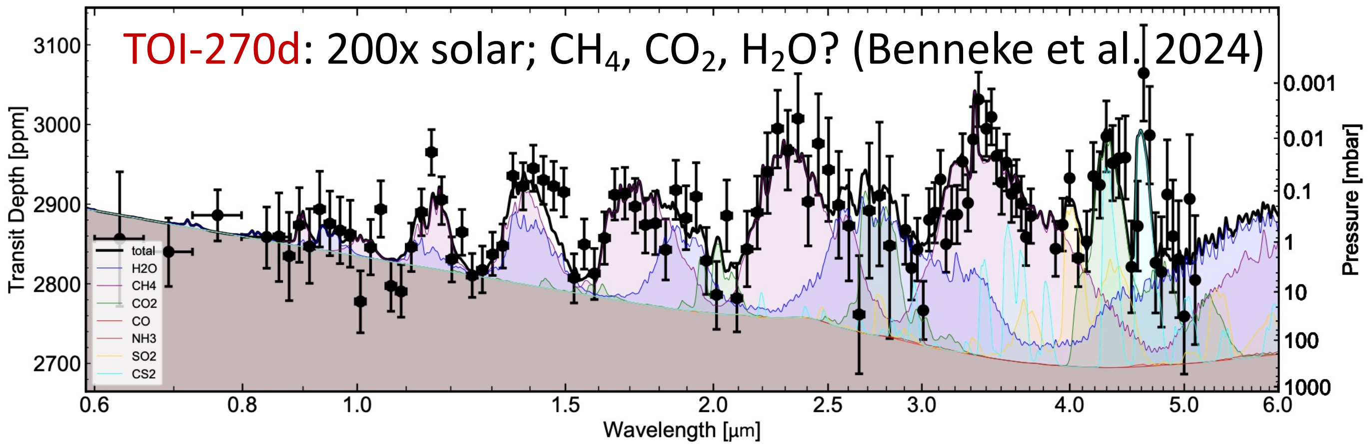
Gas (**Atmosphere**)
(H, C, O, N, S, ...)

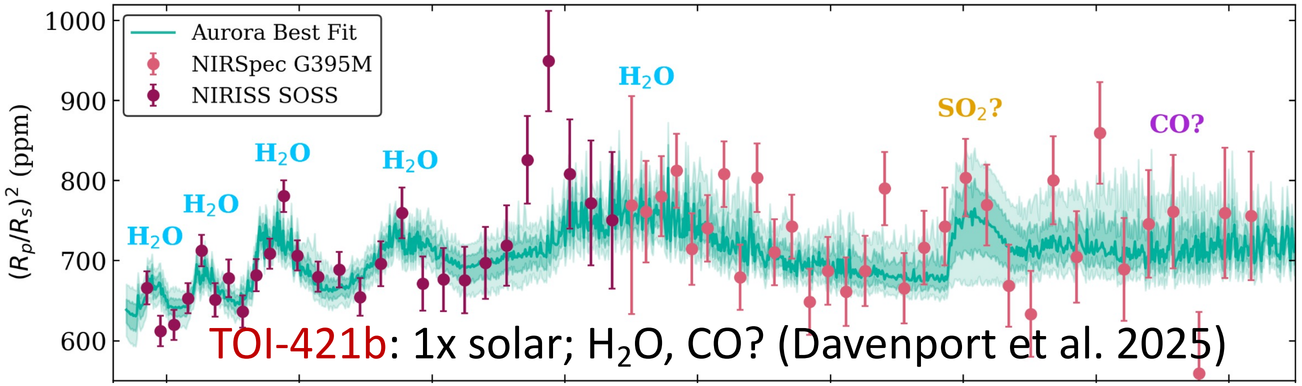
Atmospheric Constraints

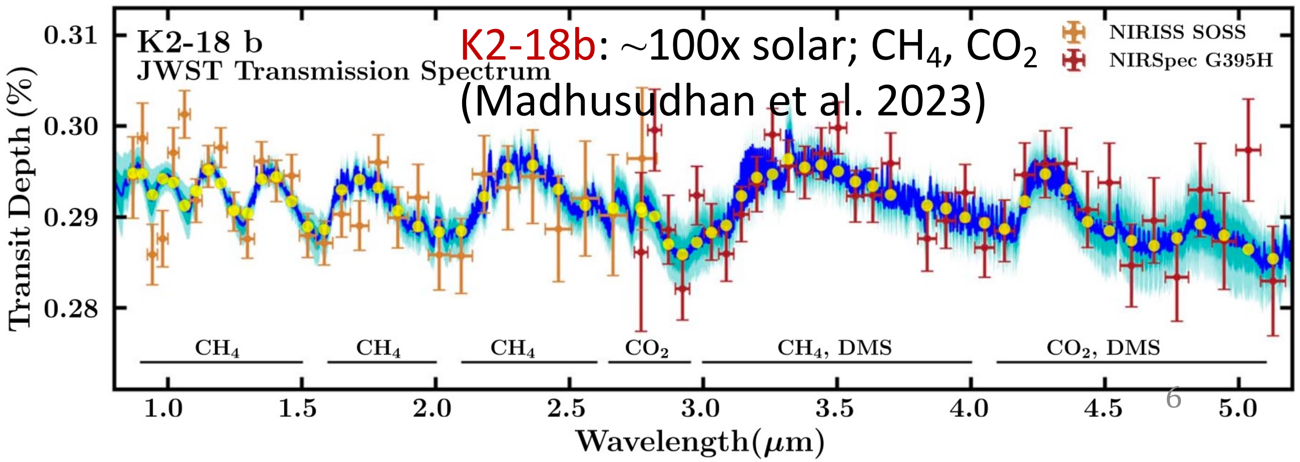
JWST cannot reveal the composition of deeper layers



Atmospheric metallicity of 1x – 100x solar

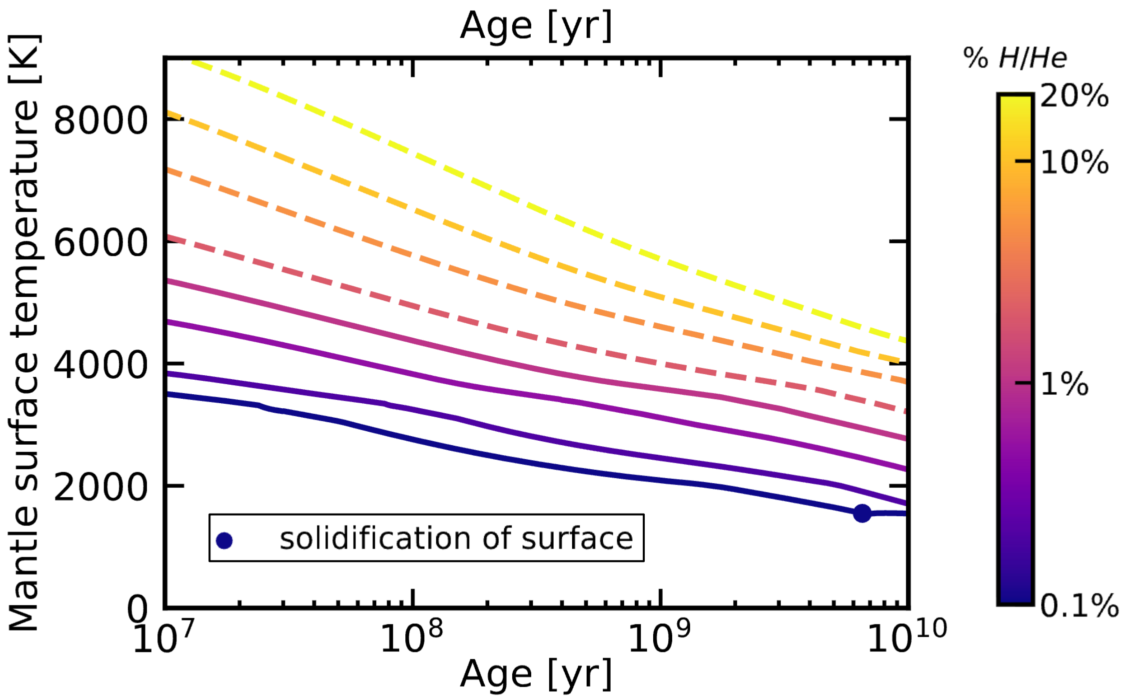






Theoretical Predictions

Magma ocean lifetime exceeds 1 Gyr



Tang et al. (2025); see also Vazan et al. (2018)

H_2-rich envelope dissolves in magma

Chachan & Stevenson (2018)

H_2 exhibits non-ideal (real) gas behaviour

Kite et al. (2019)

Magma and envelope react

Schlichting & Young (2022)

Magma and envelope produce SiH_4 and SiO

Misener et al. (2023); Charnoz et al. (2023)

H-C-N-O-bearing gases also dissolve in magma and exhibit real gas behaviour

Tian & Heng (2024)

SiO (5-6 **μ**m) and SiH_4 (4.5 **μ**m) are observable

Zilinskas et al. (2023); Ito et al. (2025)

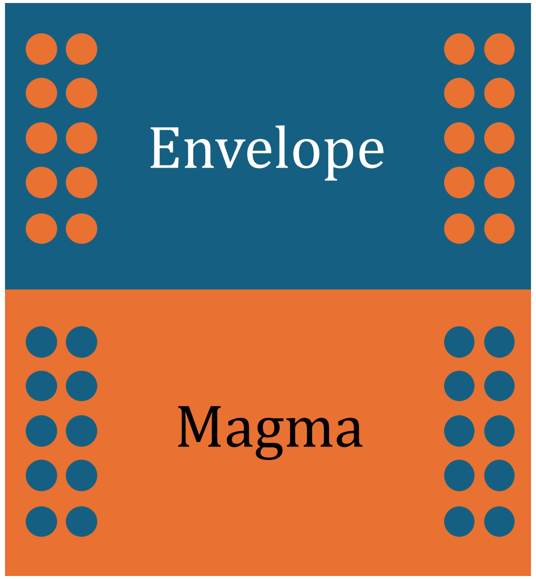
Magma–Envelope Coupling = Exchange

Volatile Element Budget from Metallicity

+

Refractory Element Budget from Metallicity and Mantle Melt Budget

=



Python 3.10+

github.com/ExPlanetology/atmodeller

Bower, Thompson, Hakim et al. (2025)

Gas – Gas Reactions

Magma – Gas Reactions

Gas Solubility in Magma

Real Gas Behaviour

Lack of Thermochemical Data

Gas – Gas Reactions	→	Equilibrium constants
Magma – Gas Reactions	→	Phase relations
Gas Solubility in Magma	→	Gas solubility constants
Real Gas Behaviour	→	Equations of state

- Experimental validity for limited pressures/temperatures
- Data missing for certain species
- Little or no data on miscibility of magma and hydrogen

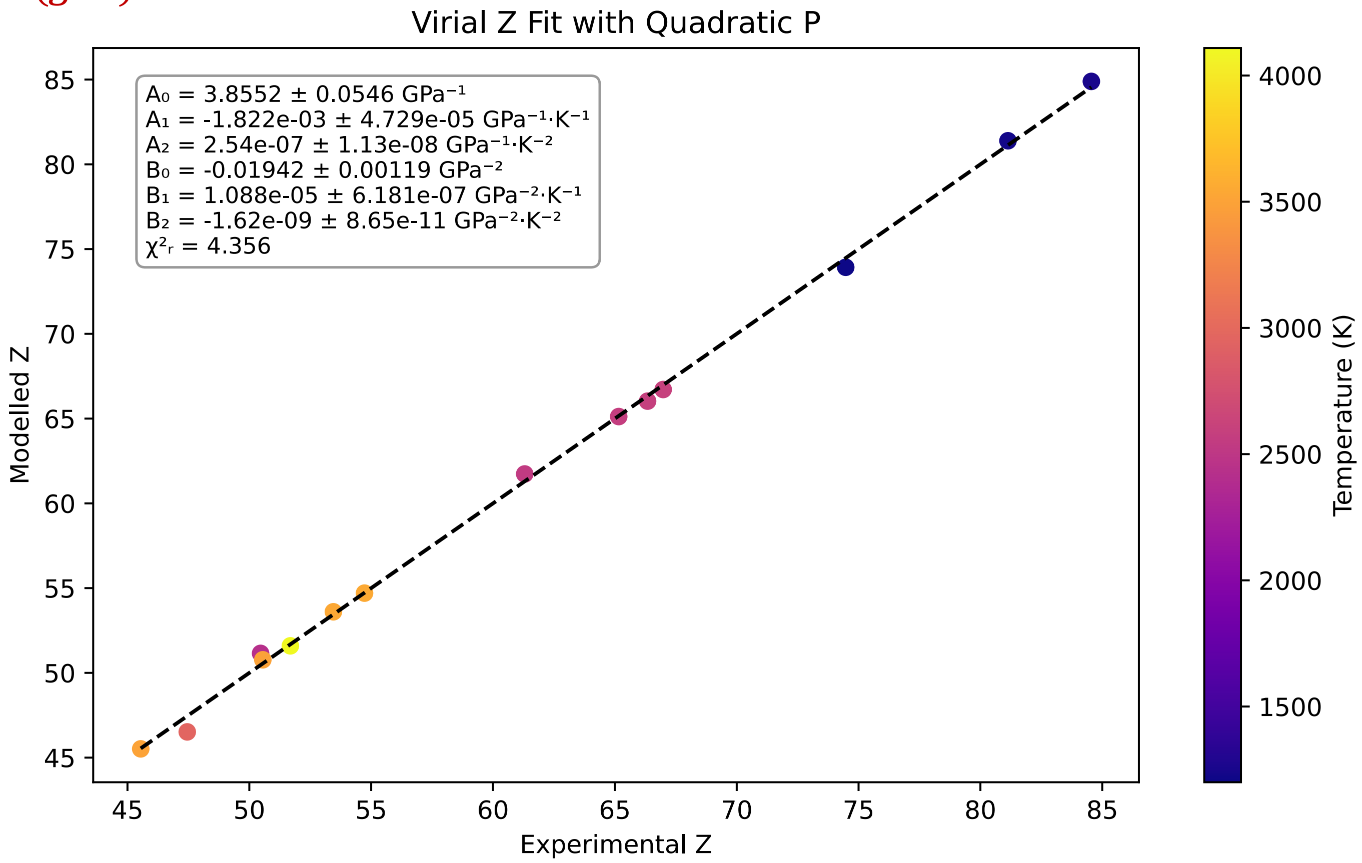
New Real Gas Equation of State of SiH_4

$$SiO_{2(magma)} + 4H_{2(gas)} \rightleftharpoons SiH_{4(gas)} + 2H_2O_{(gas)}$$

Second-order virial equation fit to experimental data on silane (P < 138.7 GPa = 1387 kbar, Wang et al. 2018)

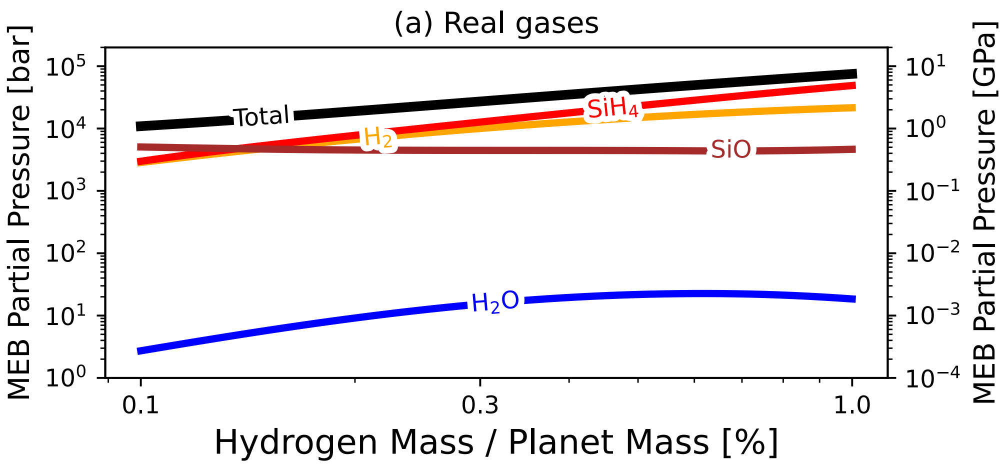
Compressibility of SiH_4

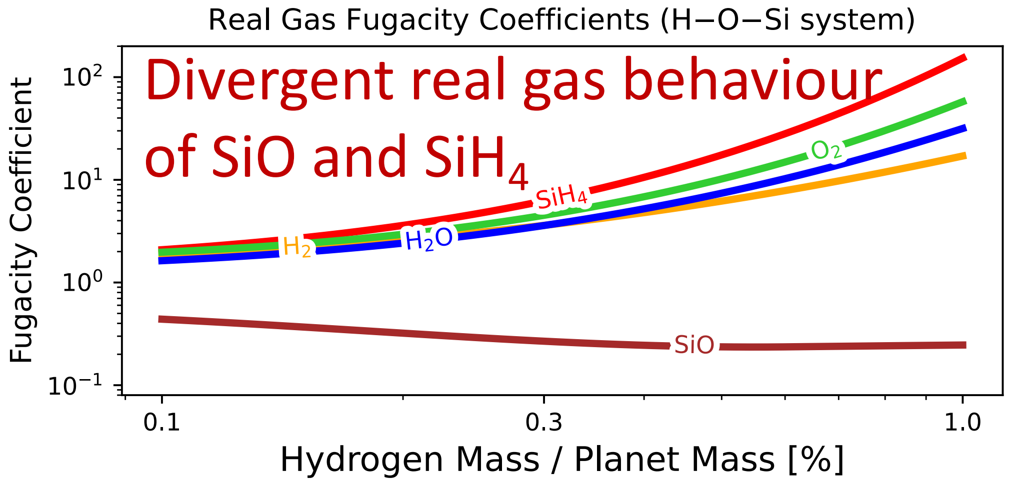
$$Z = \frac{PV}{RT}$$



Hakim et al. (2025, in review)

MEB Partial Pressures : Ideal v/s Real



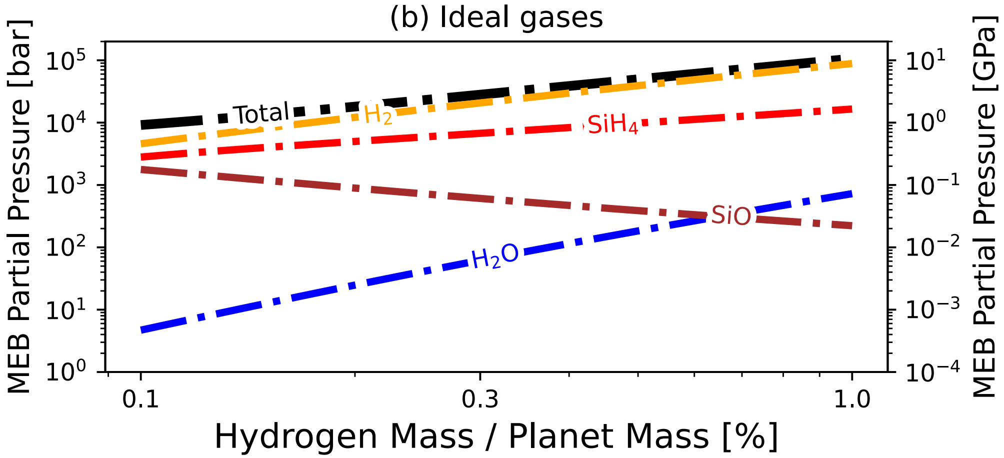


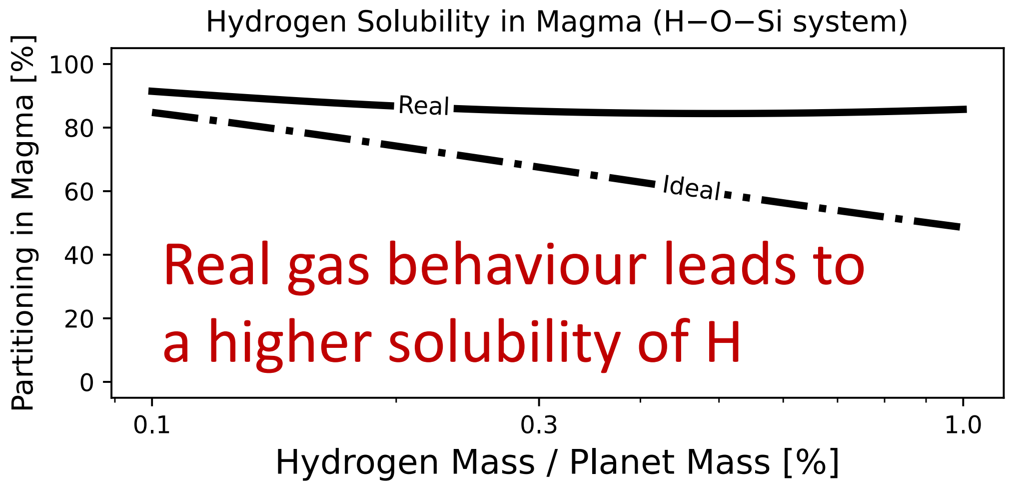
partial pressure

fugacity

$$f = \boldsymbol{\Phi}\, P$$

fugacity coefficient

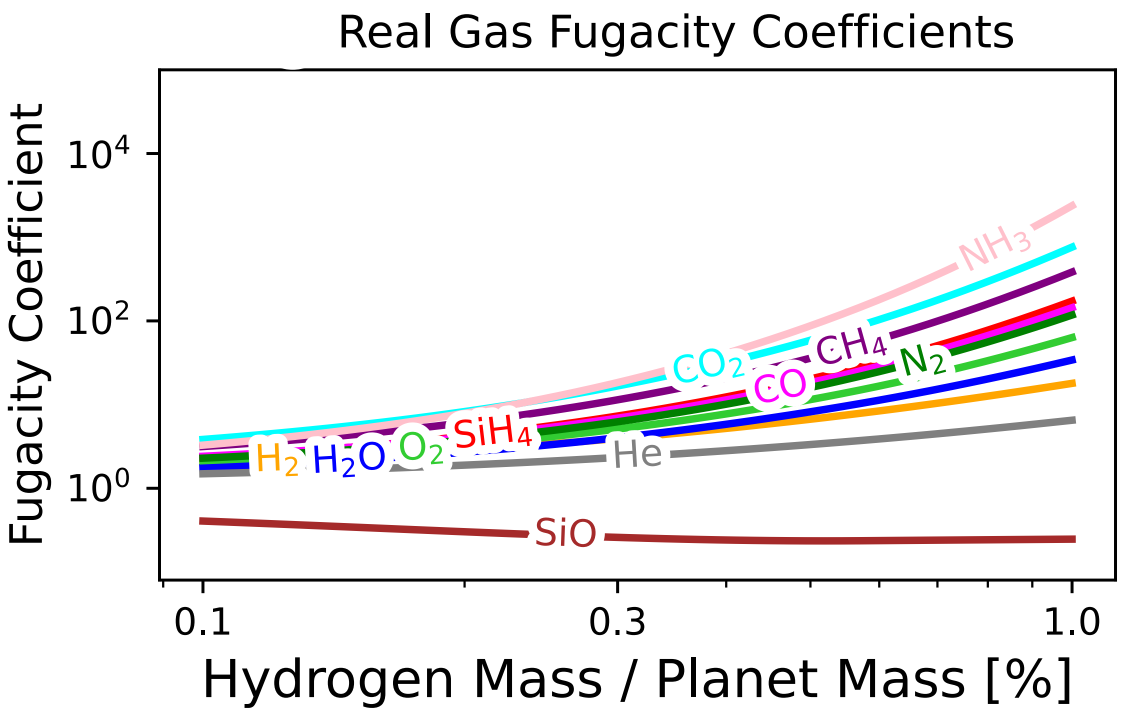


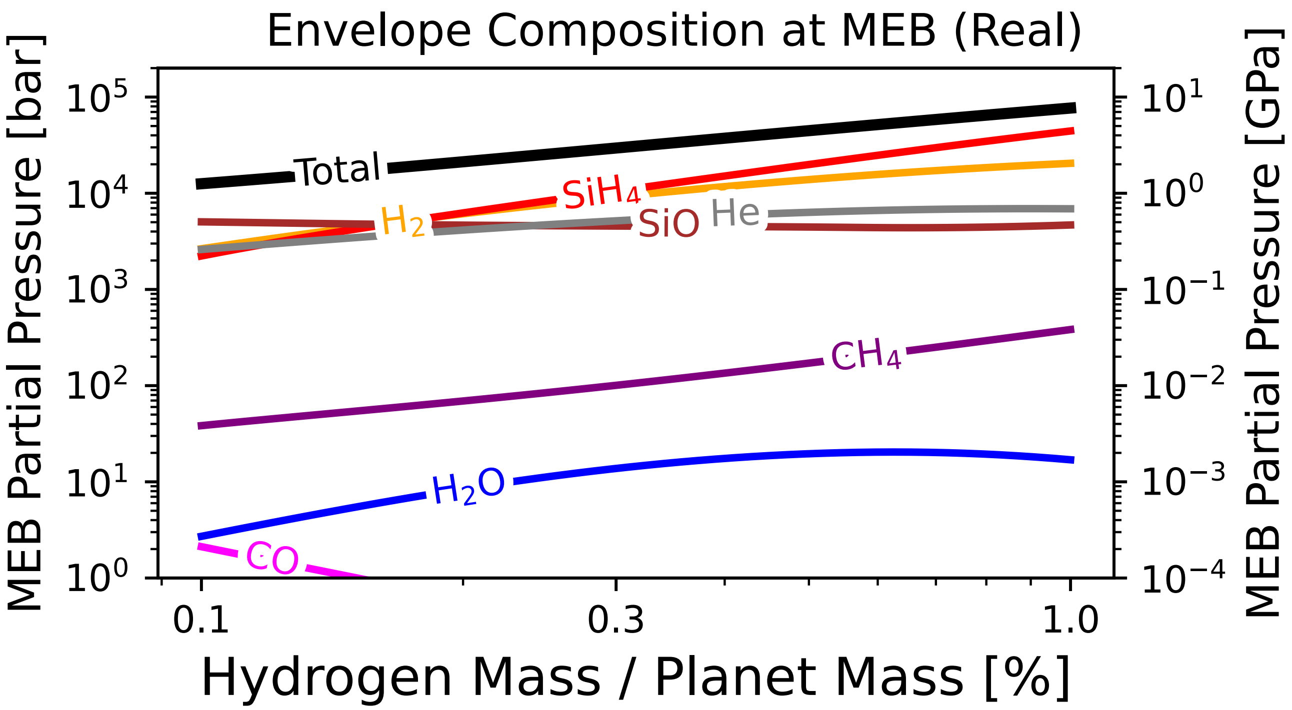


MEB = Magma–Envelope Boundary

Hakim et al. (2025, in review)

Depletion of H_2/He and Enhancement of SiO



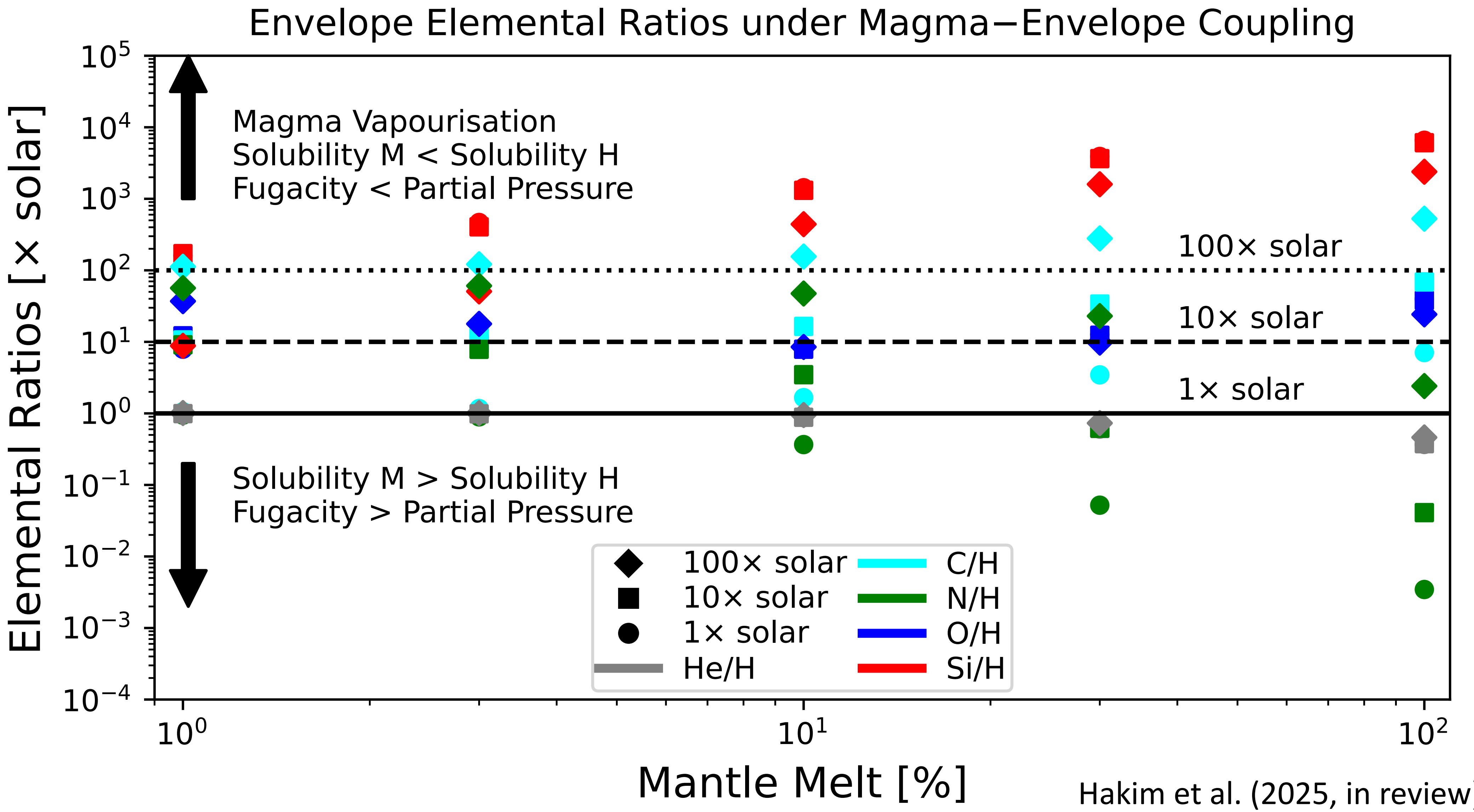


All gases exhibit strong non-ideal effects

Si-bearing gases are important at the magma-envelope boundary

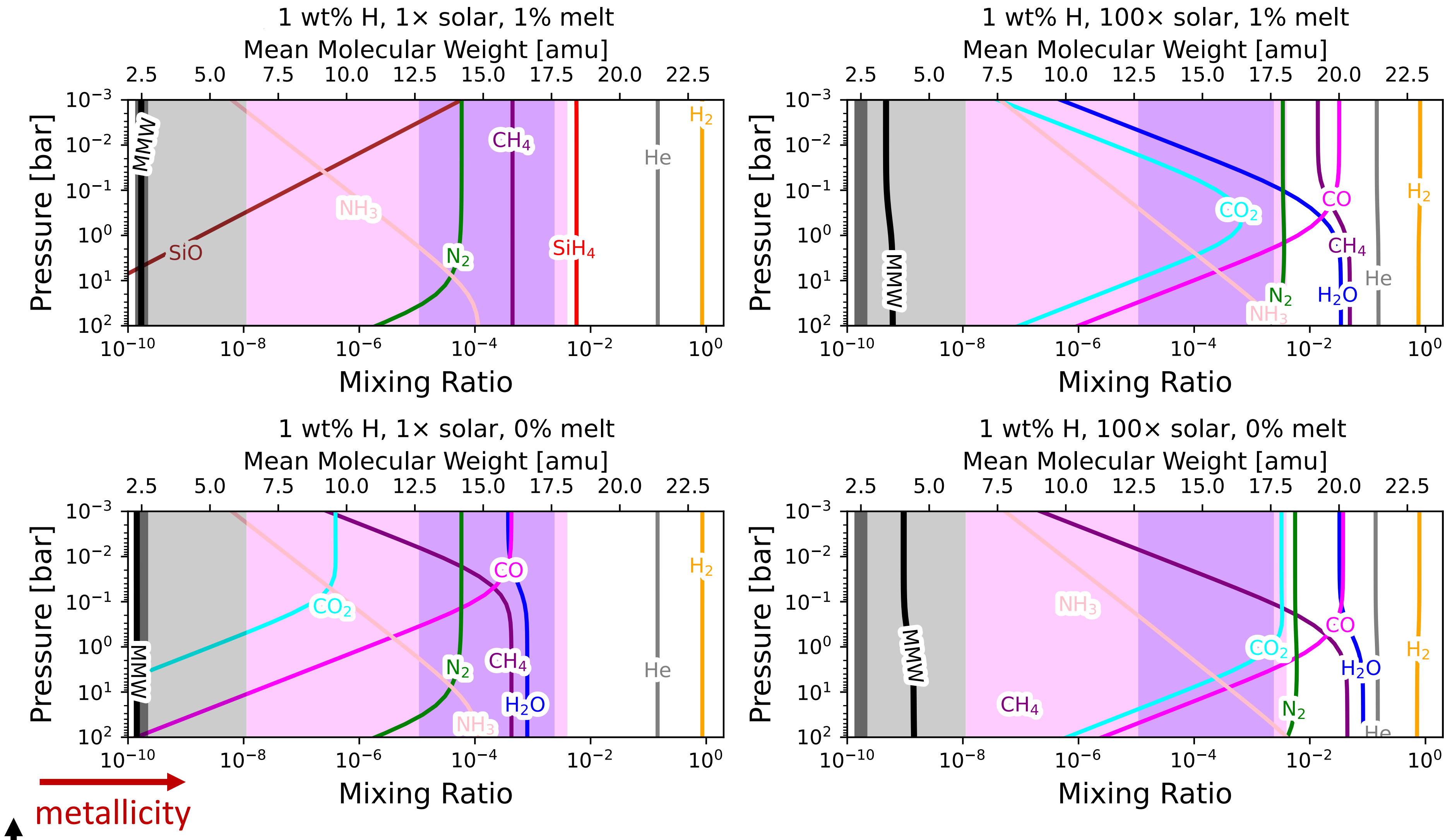
Hakim et al. (2025, in review)

Chemical Abundances Diverge from Nebular



Hakim et al. (2025, in review)

Silane–Methane Competition in TOI-421b ?



High mantle melt fraction and low accreted gas metallicity favour silane over methane

Observations are consistent with 1x solar – 0% melt

100x solar – 1% melt can also explain observations

Hakim et al. (2025, in review)

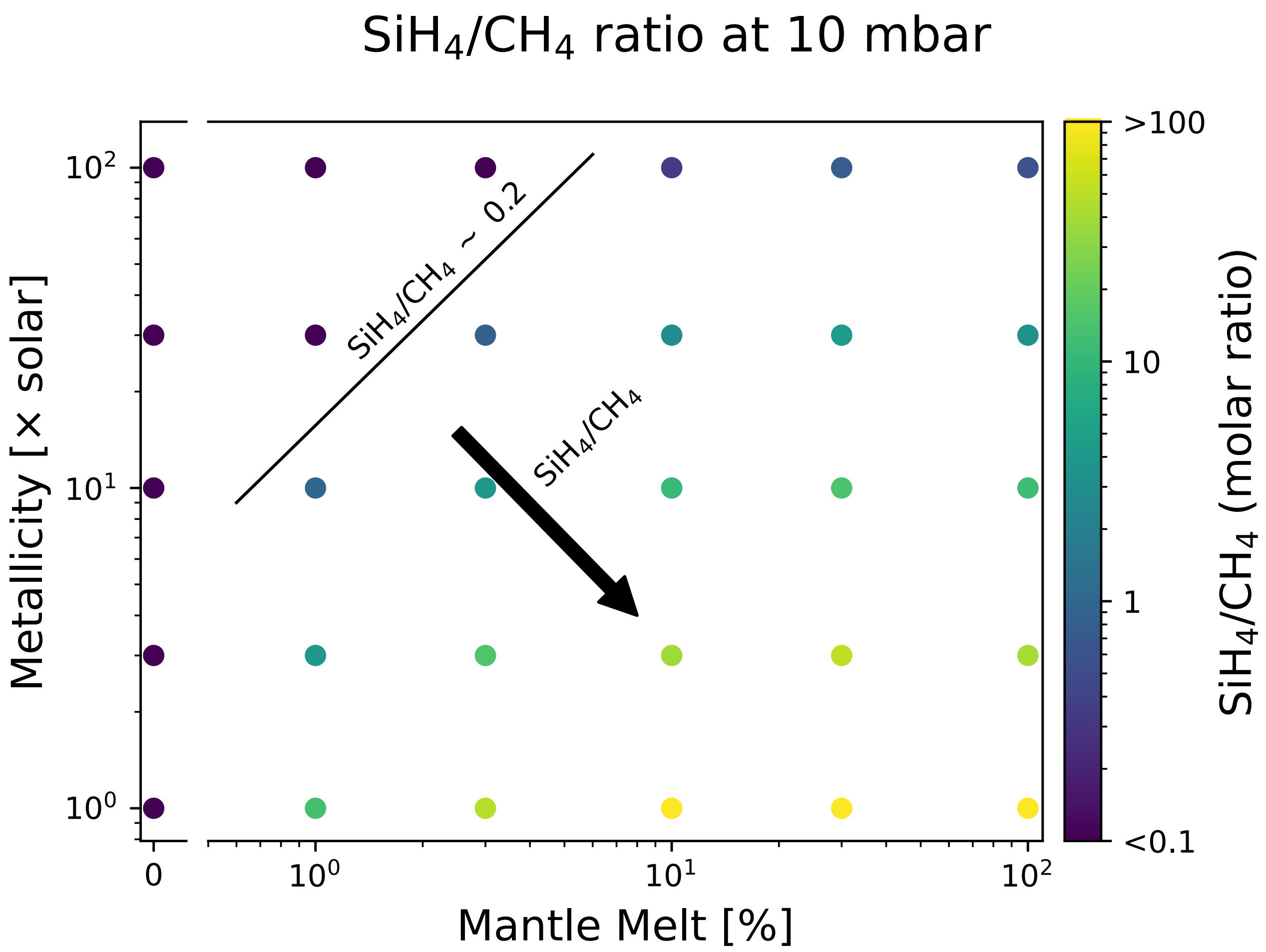
Silane/Methane (Si/C ratio) as a Diagnostic of Metallicity and Mantle Melt Fraction

- Magma-derived Si and envelope-derived H

$$SiO_{(gas)} + 3H_{2(gas)} \rightleftharpoons SiH_{4(gas)} + H_2O_{(gas)}$$

- Envelope-derived C and envelope-derived H

$$CO_{(gas)} + 3H_{2(gas)} \rightleftharpoons CH_{4(gas)} + H_2O_{(gas)}$$



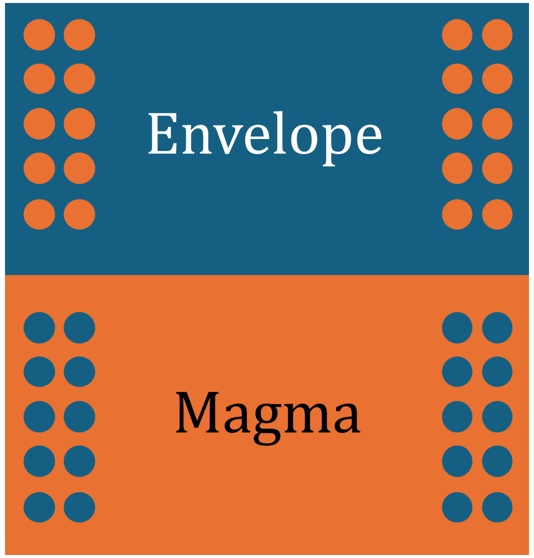
Hakim et al. (2025, in review)

Take Away Messages

- Atmosphere chemistry with gas solubility and real gas behaviour, including a new EOS of SiH_4 (also SiO)
- Elemental abundances in the envelope diverge from those of accreted gas metallicity (not considered by retrievals yet)
- Silane–methane competition (Si/C ratio) could be a diagnostic of accreted gas metallicity and mantle melt fraction
- Need new thermochemical data on the stability of phases at extreme pressures and temperatures

A Multi-Disciplinary Approach on Interior–Atmosphere Coupling of Sub-Neptunes

Models



Luka Vranckx

Anjana Shaju

ROYAL OBSERVATORY OF BELGIUM

KU LEUVEN

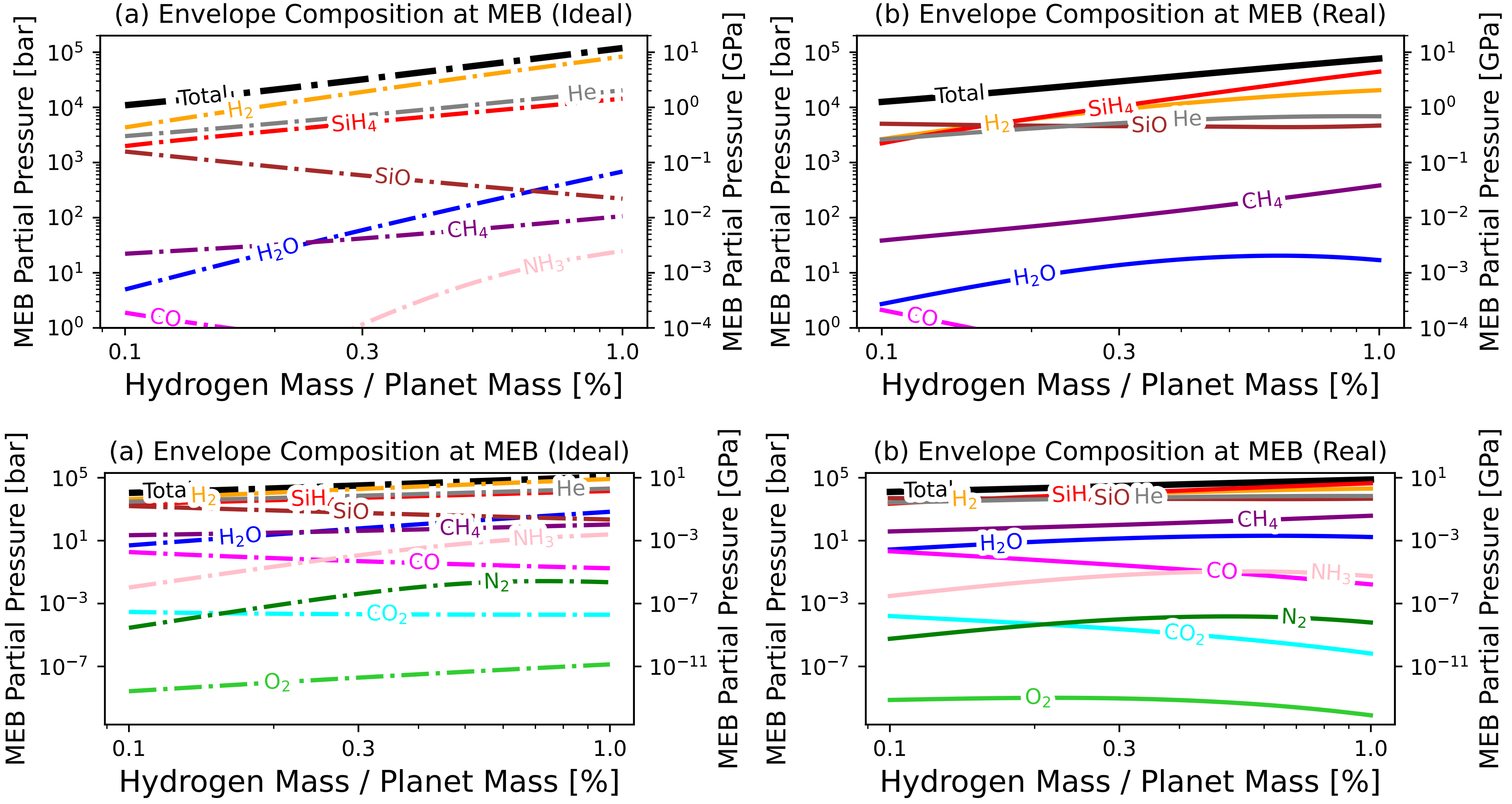
fwo Research Foundation Flanders
Opening new horizons

Lab Experiments

Multi-Anvil (O. Namur)

Thank You

Depletion of H_2/He and Enhancement of SiO

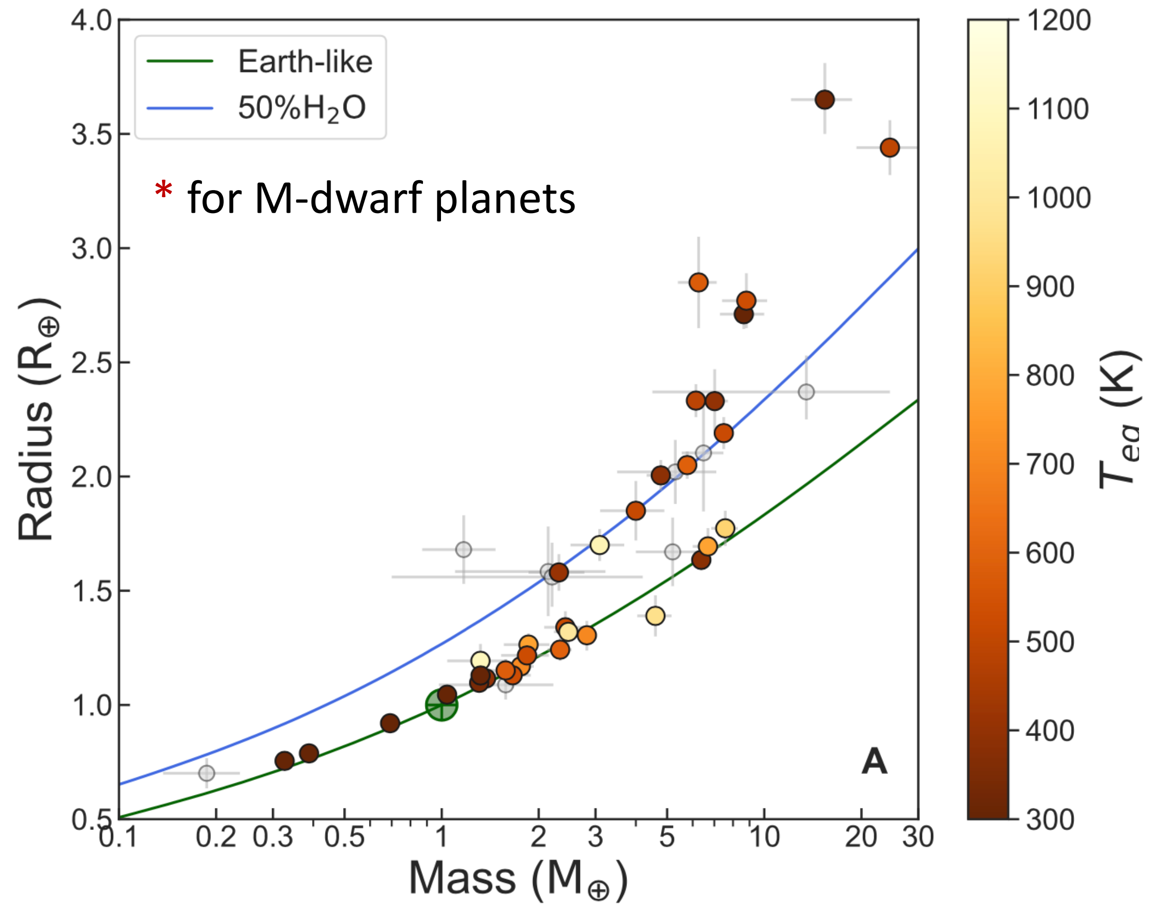


Full Range

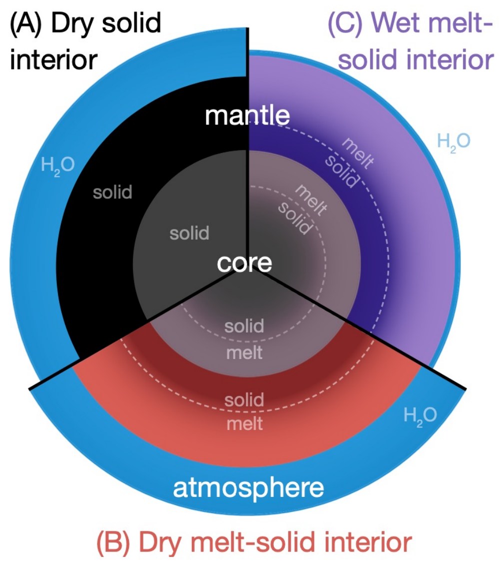
Hakim et al. (2025, in review)

M-R Data Are Degenerate: Water-rich?

Mass-radius measurements point to dry and wet exoplanet populations*

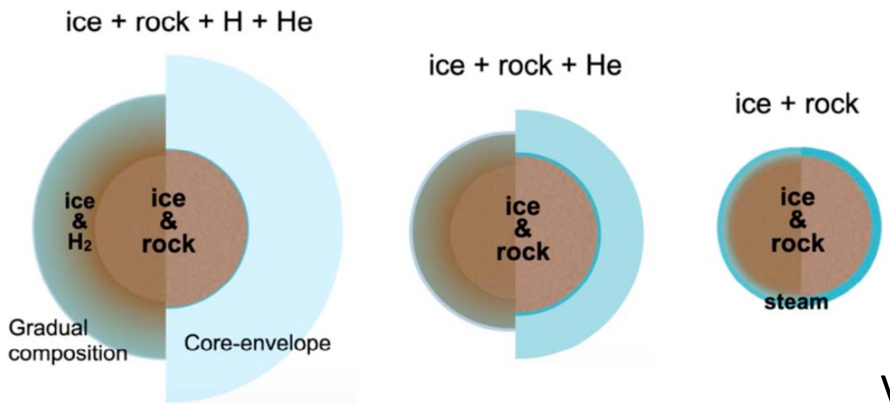


Luque & Pallé (2022) Sci



Dry/wet mantle models lead to a difference of up to 16% in radius

Dorn & Lichtenberg (2021) ApJL
see Kite et al. (2020);Bower et al. (2022)



Hydrogen and rock can be miscible at high pressures

Vazan et al. (2022)
Young et al. (2025)

Sub-Neptunes could contain 0.01–1 wt% H_2 and < 10 wt% water