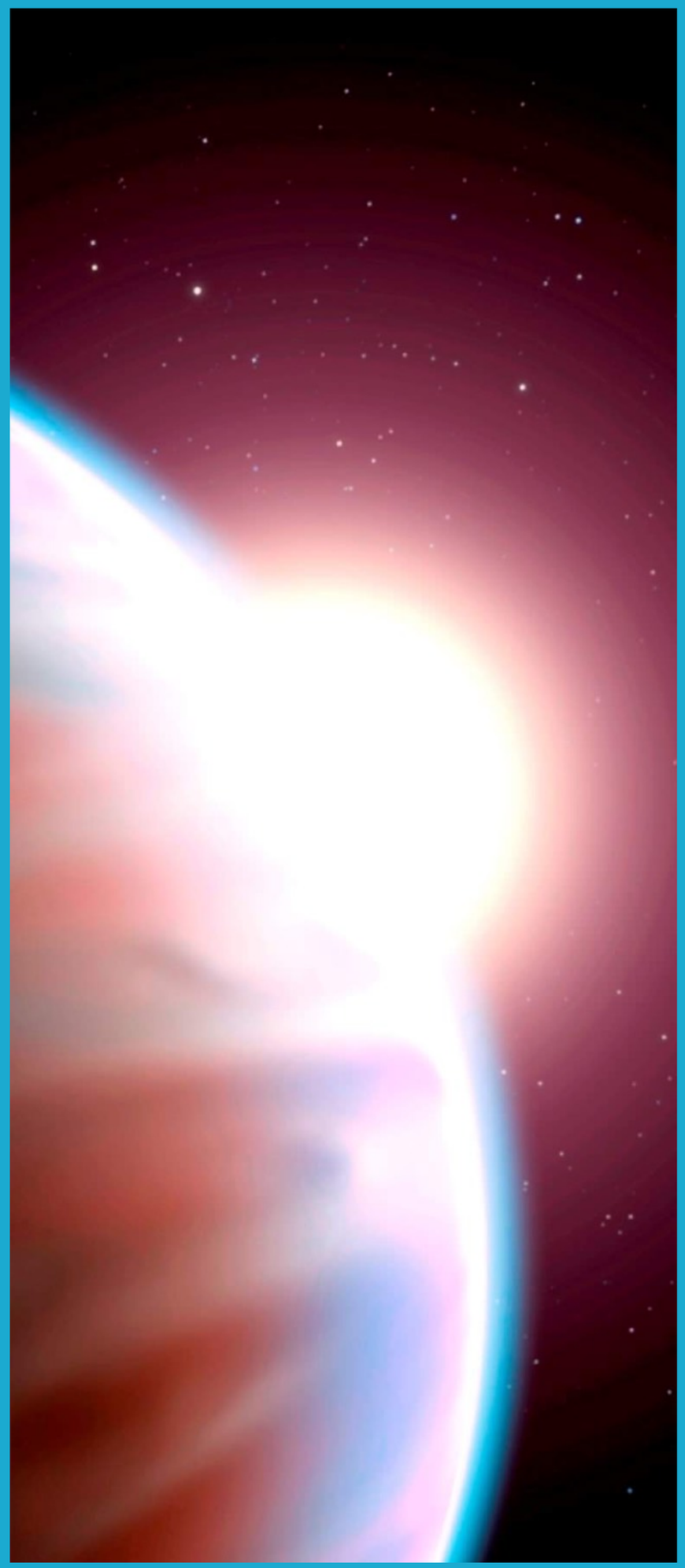

UNDERSTANDING THE CHEMICAL COMPOSITION OF EXOPLANET ATMOSPHERES

Olivia Venot, Yamila Miguel
& the Chemistry Working group: Robin Baeyens, Jérémy Bourgalais, Benjamin Fleury, Yuichi Ito, Yui Kawashima, Karan Molaverdikhani, Julianne I. Moses, William Pluriel, Pascal Tremblin, Franck Selsis, Mantas Zilinskas,
Ludmila Carone, Nathalie Carrasco, Quentin Changeat, Leen Decin, Masahiro Ikoma, Jérémy Leconte, Paul Mollière, Vivien Parmentier, Giovanna Tinetti, Shang-Min Tsai, Tiziano Zingalès

ARIEL Chemistry Working group

- An understanding of the chemistry in exoplanet atmospheres is crucial to get a proper interpretation of ARIEL observations

- In the ARIEL ChWG we explore potential atmospheric compositions and the impact of diverse physical processes on such chemical species

- Today we will present only a selection of the work of the ARIEL ChWG

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Hydrogen-dominated planets
Effect of horizontal mixing

- Tidally-locked planets might have big day-night temperature gradients, and thus, their chemical composition could also vary.
  ➠ Important variation of emission spectra with orbital phase

- However, horizontal winds can transport chemicals in the atmosphere from one side to another (quenching), thus reducing the chemical gradient.
  ➠ Less variation of emission spectra with orbital phase

- Questions: which planets might have variations of composition with phase? Which ones have a chemical composition horizontally quenched?
  ➠ 2D models for a grid of warm-Neptunes : 500 K < T_{eff} < 2500 K
  metallicity : 1, 10, 100, 1000 x solar.

PT grid from 2D-ATMO (P. Tremblin)
chemical models of J. Moses

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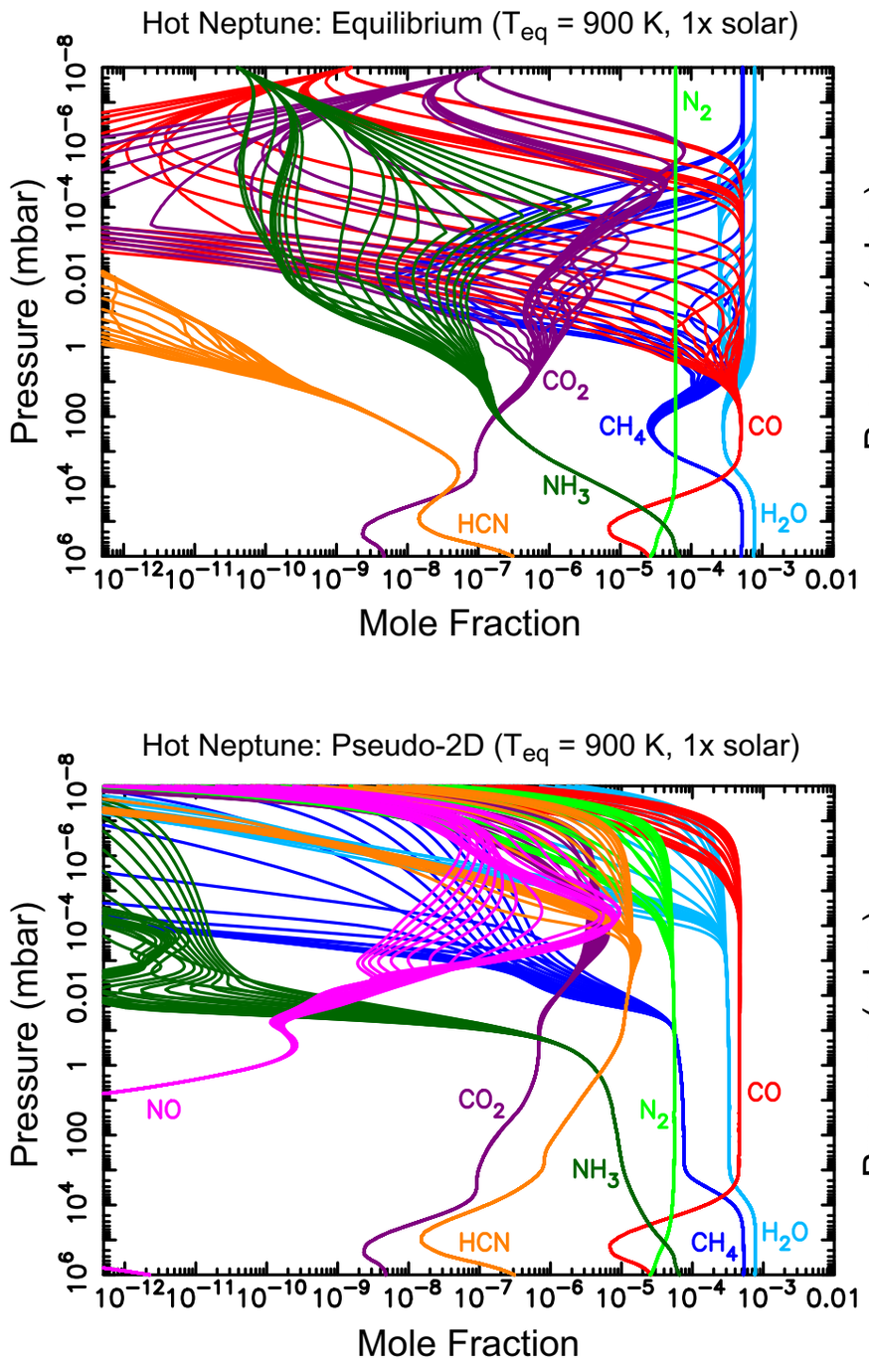
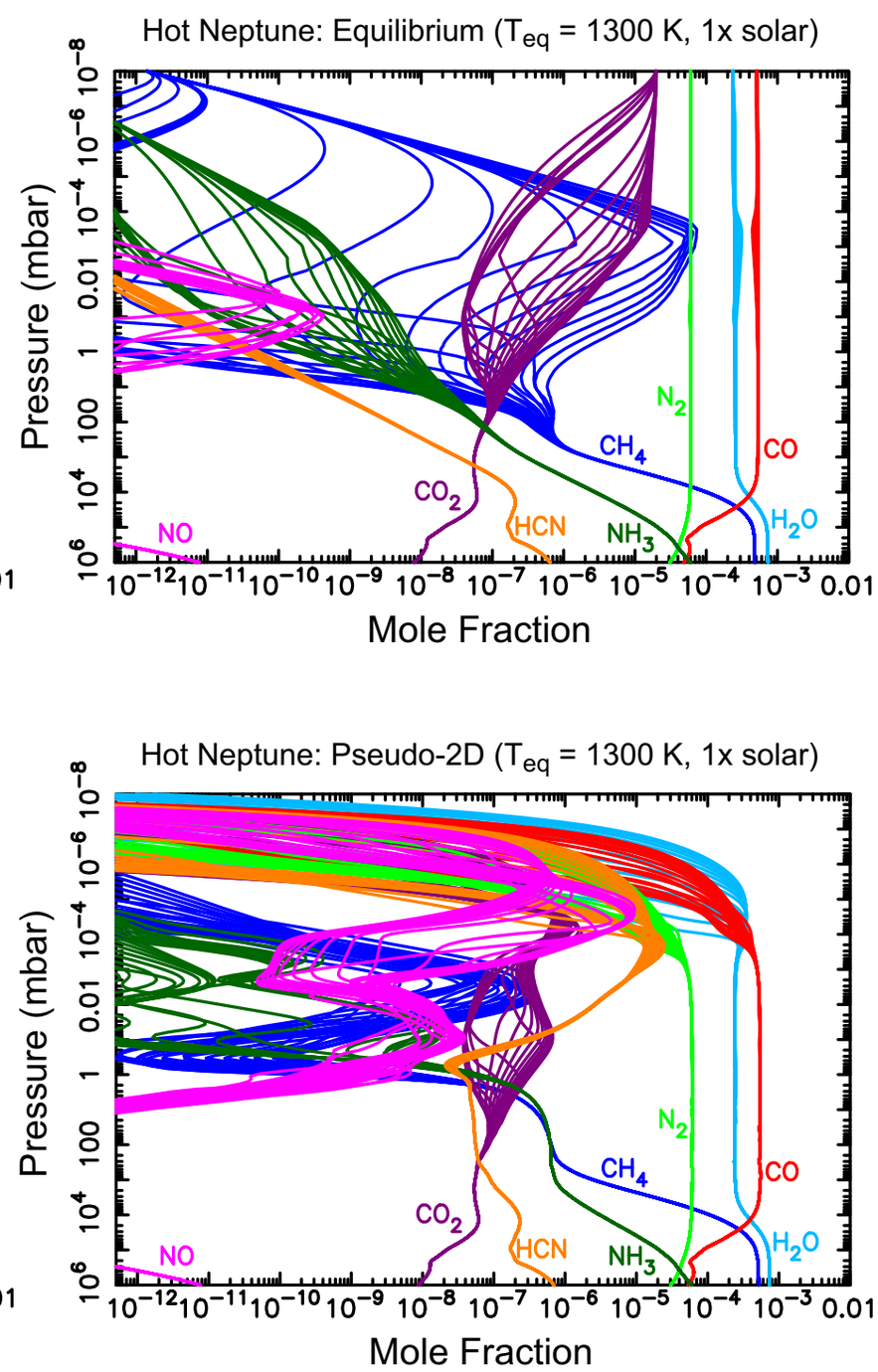
Hydrogen-dominated planets

Effect of horizontal mixing

Chemical composition

- photolysis, vertical and horizontal mixing affect the chemical composition.
- globally, we see an homogenisation of abundances with longitude, but still some variations at high altitude





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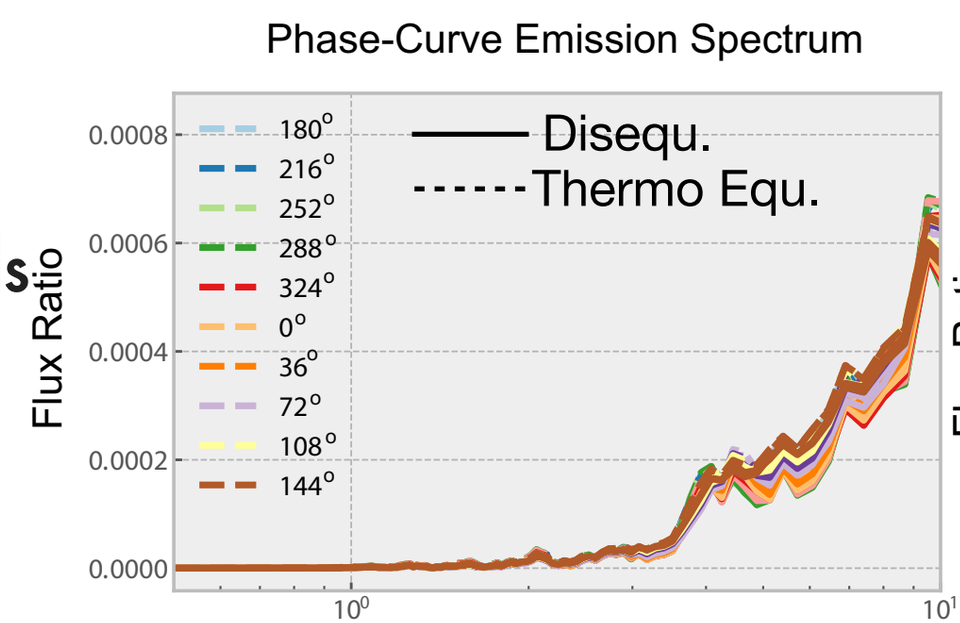
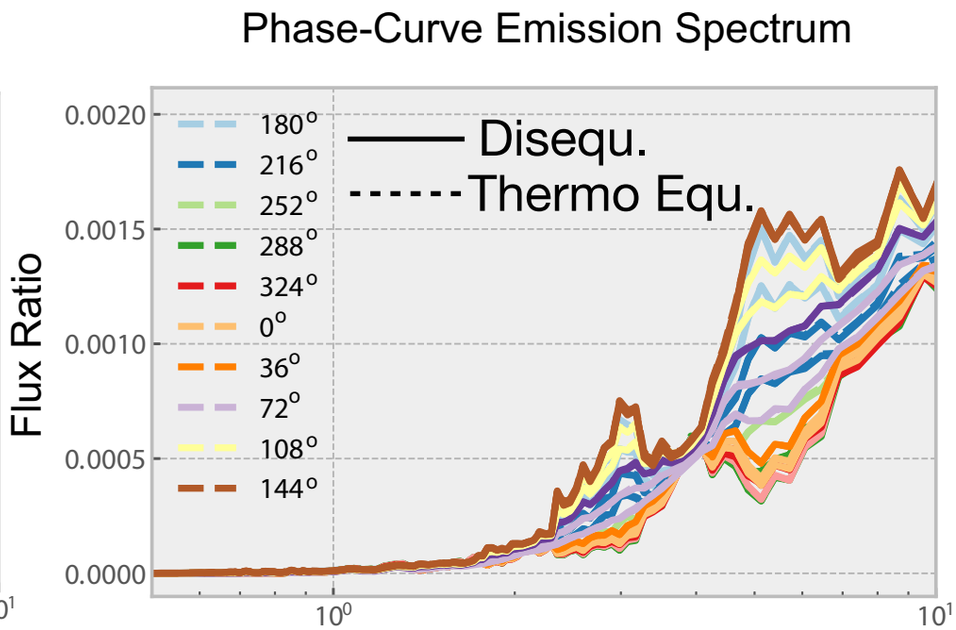
Hydrogen-dominated planets

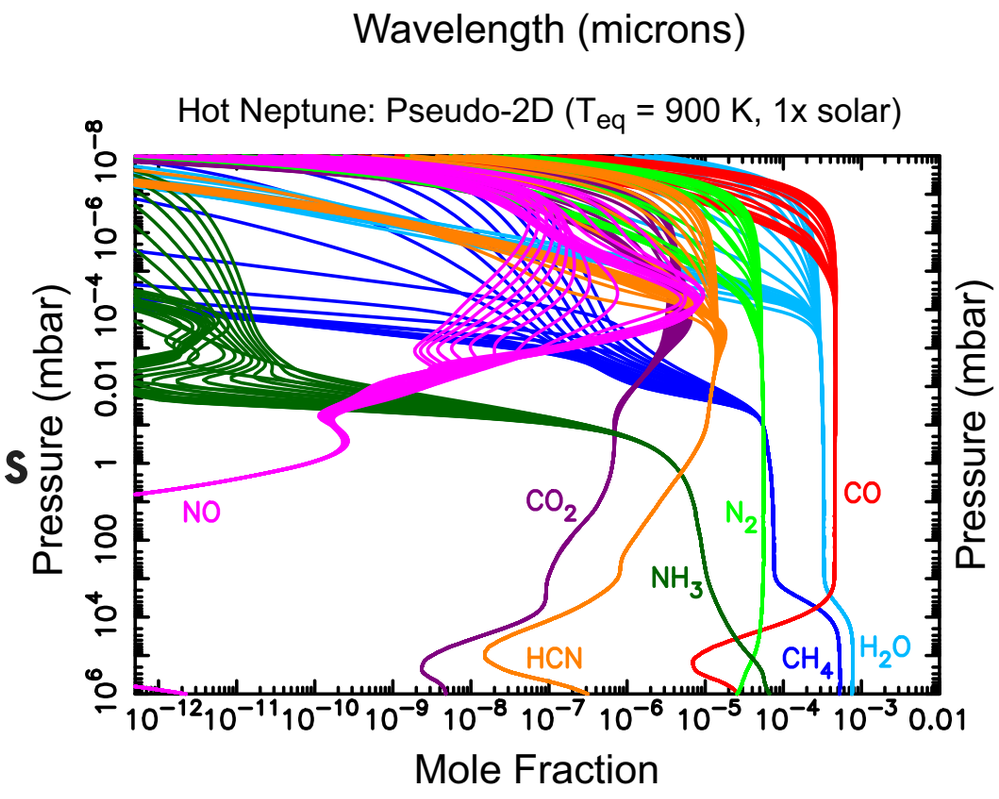
Effect of horizontal mixing

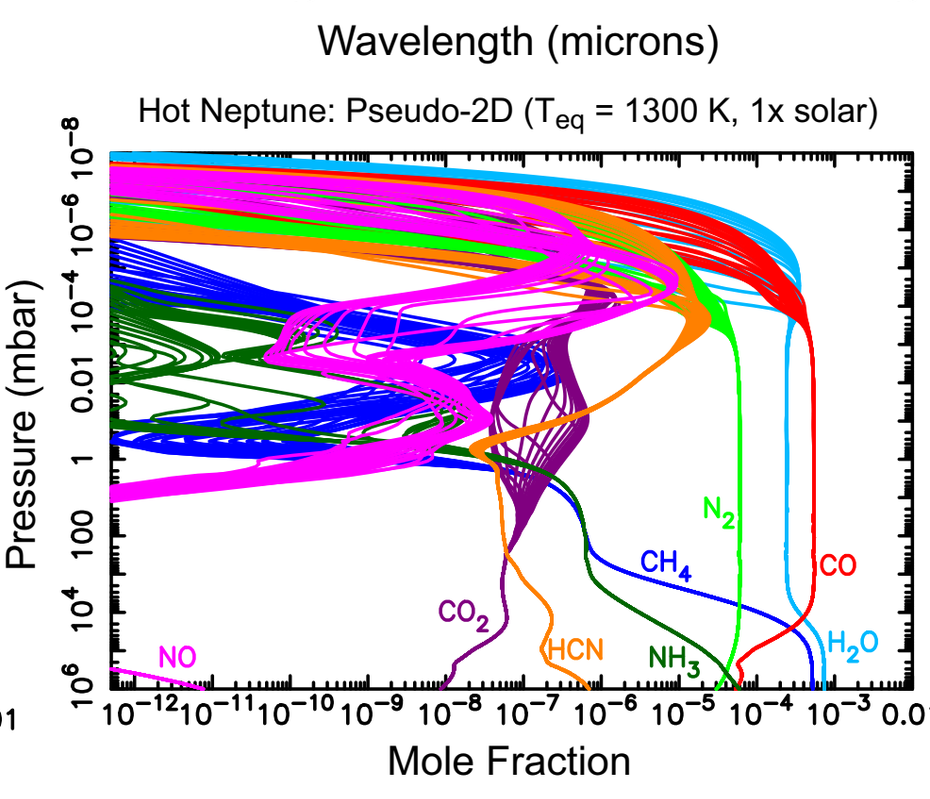
Phase curves:

- similar between equilibrium and disequilibrium models because:
  - the low pressures do not contribute much to the emission spectra
  - the dominant active species (H_2O, CO) show only minor differences between eq. and diseq. models
- variations due to differences of temperature









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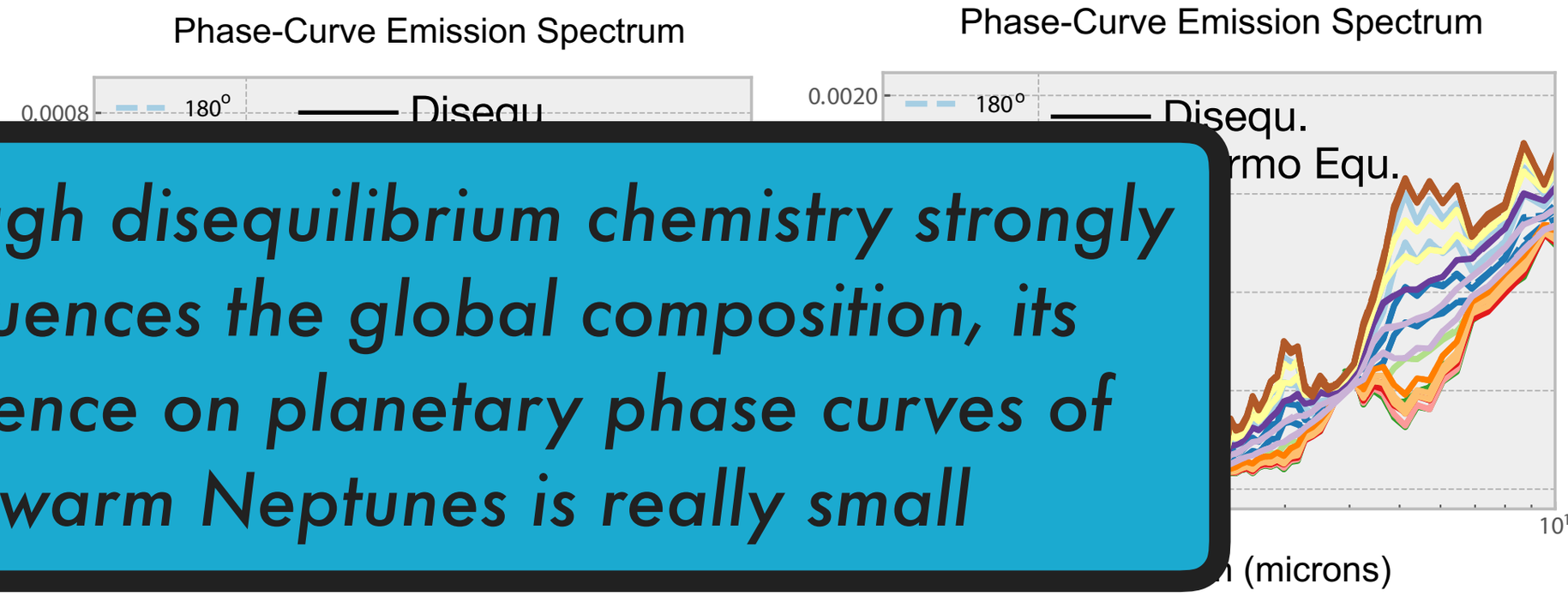

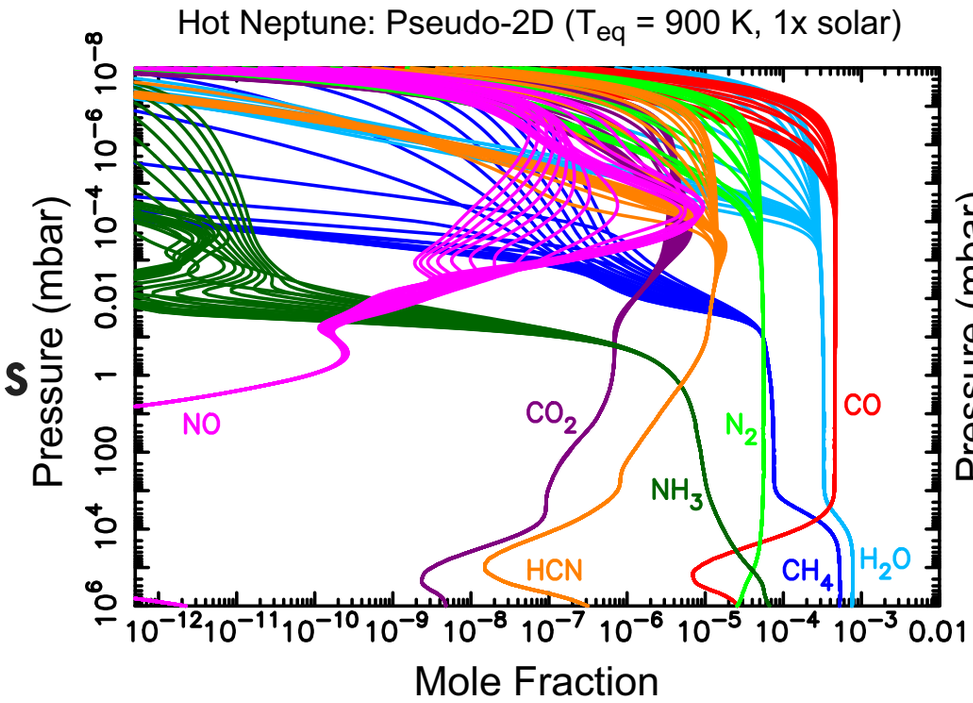

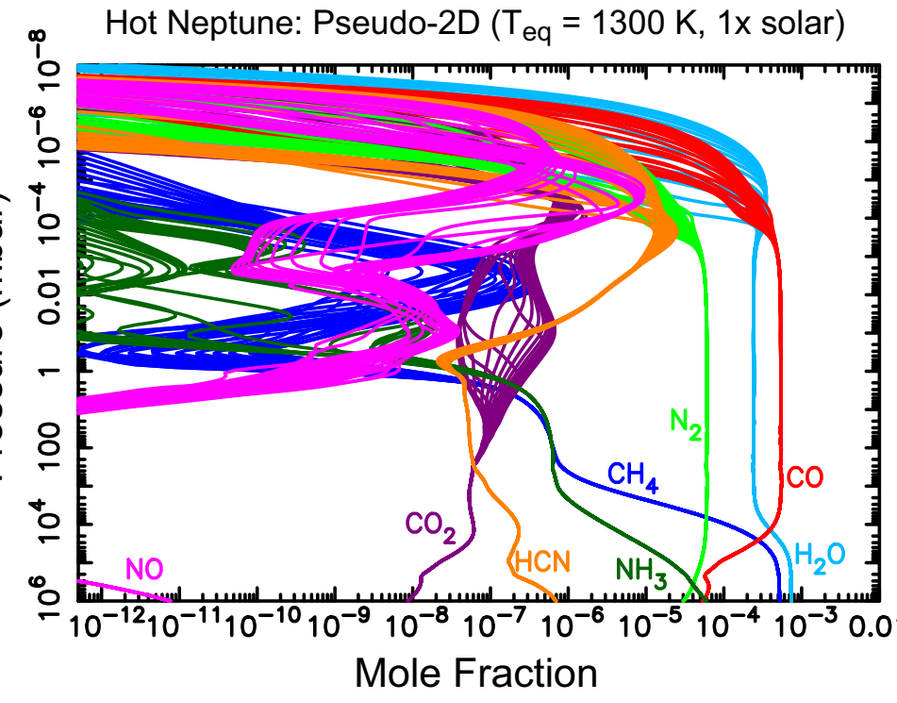

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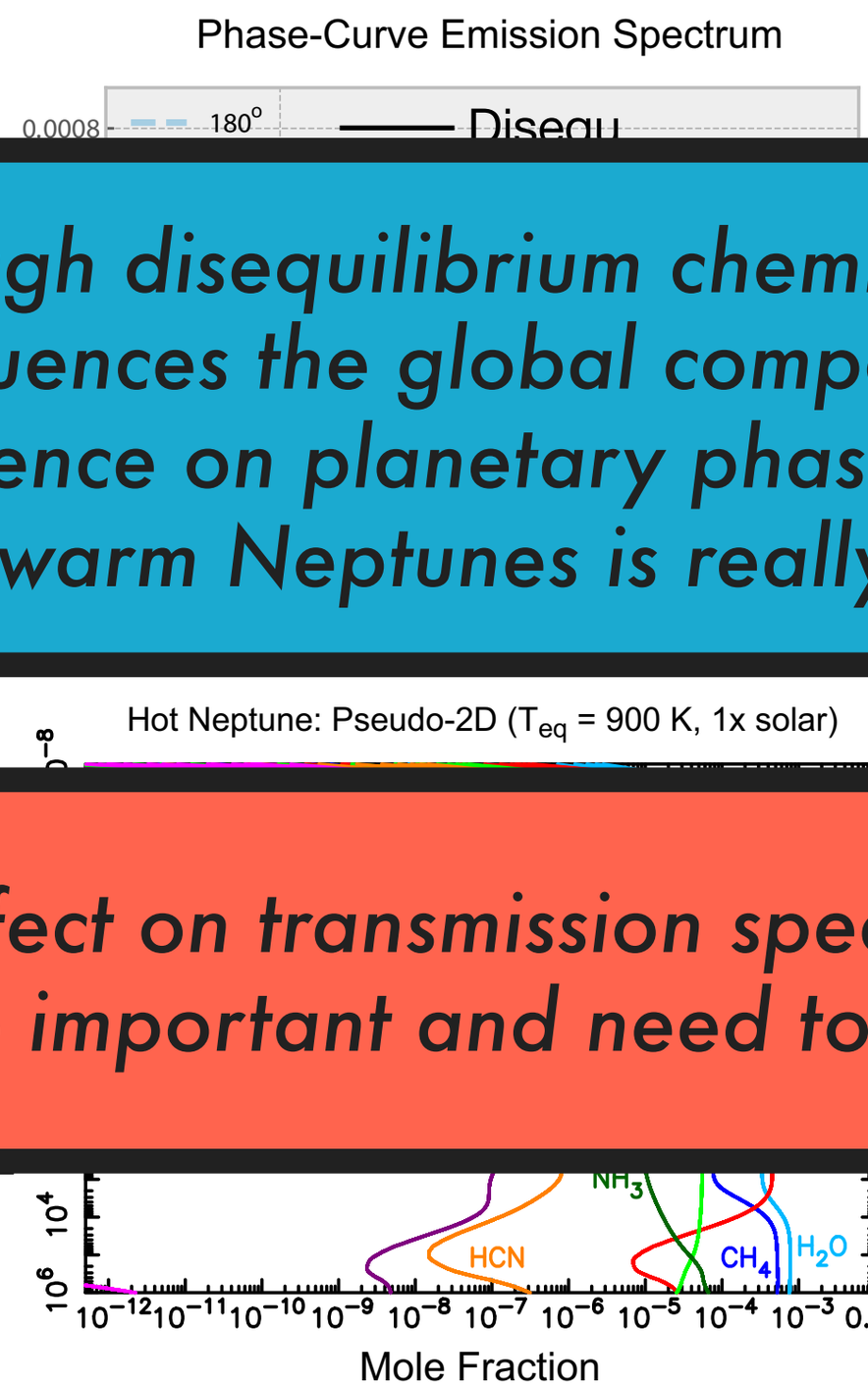
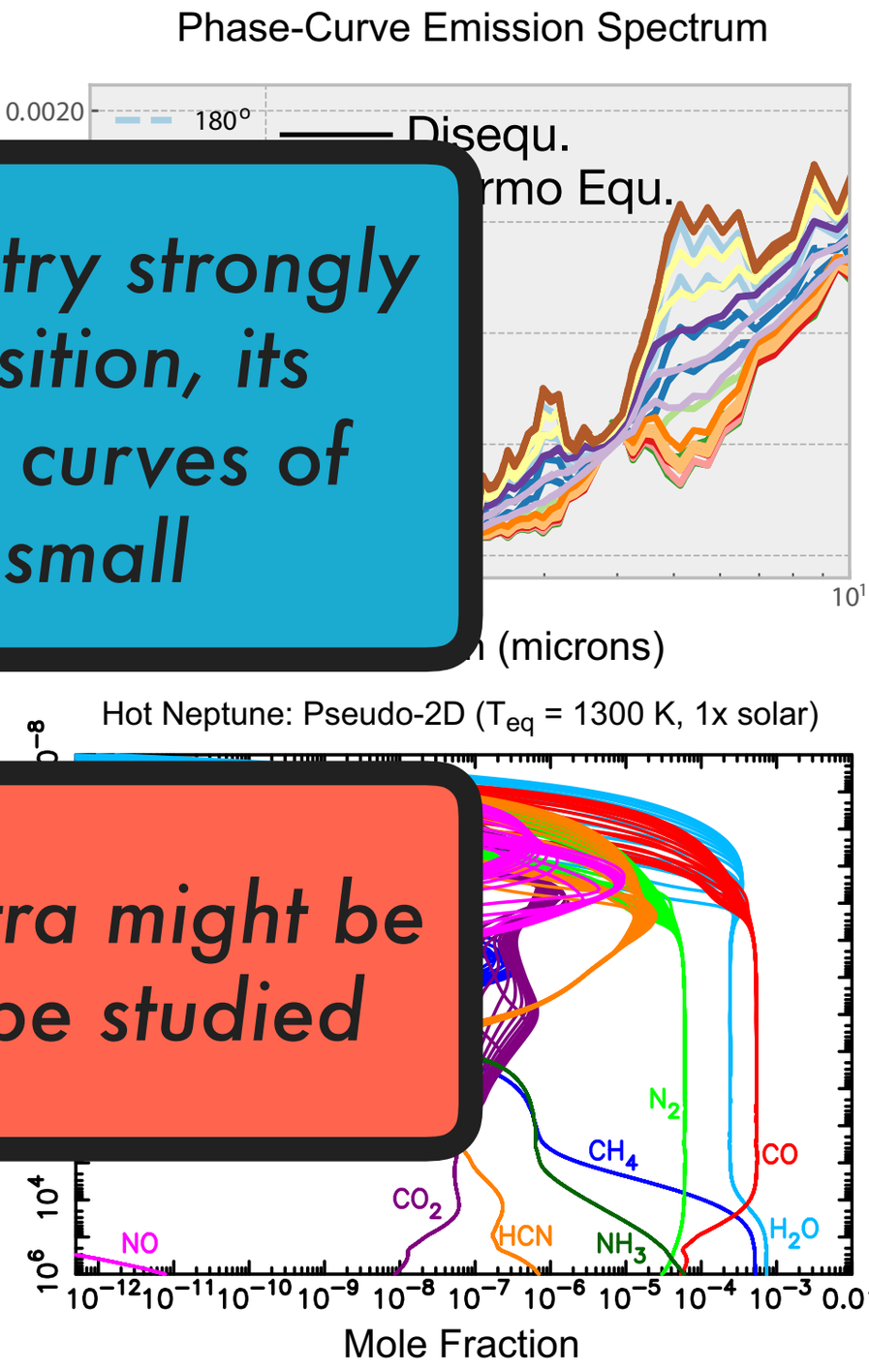
The effect on transmission spectra might be more important and need to be studied





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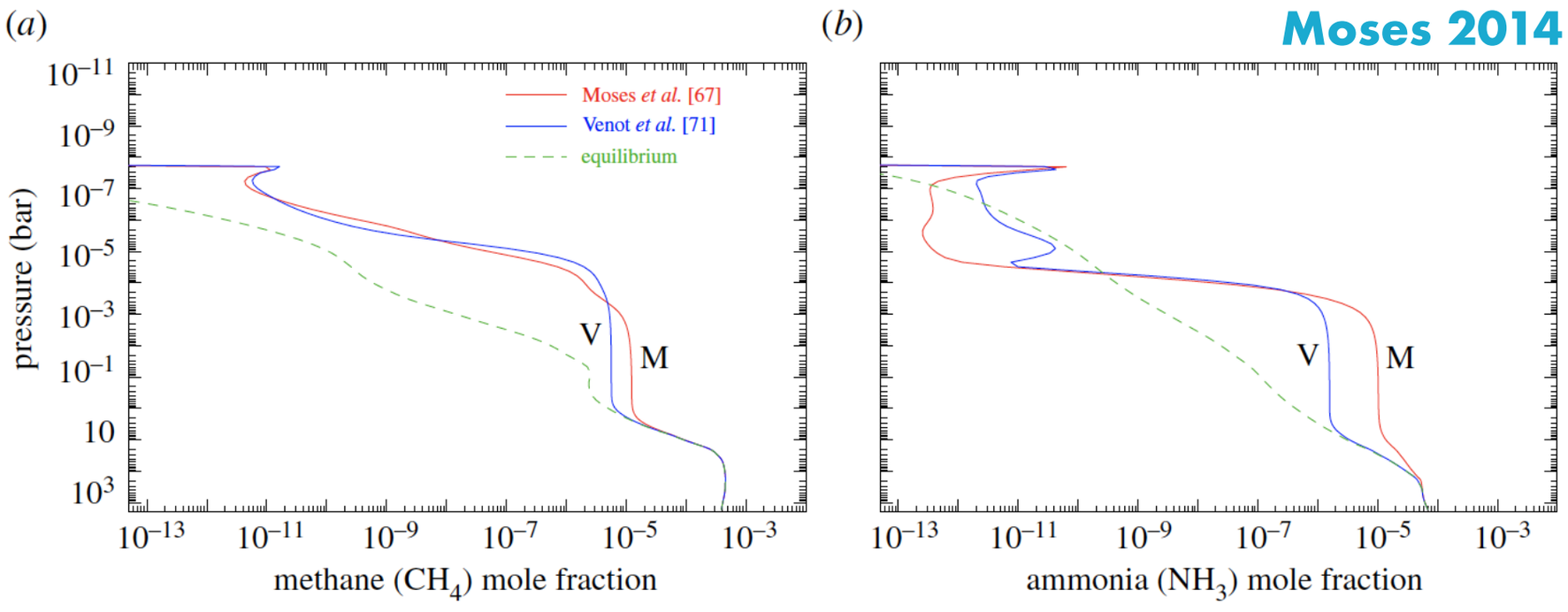
Importance of chemical scheme

Update of Methanol chemistry

- The chemical scheme is one of the most important ingredients in kinetic models
- The list of reactions and the associated rates adopted are not always consensus and are sometimes subject to debate.
- In particular, methanol's reactions could be at the root of differences between Venot et al. (2012) and Moses et al. (2011)



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- In particular, methanol's reactions could be at the root of differences between Venot et al. (2012) and Moses et al. (2011)
- Venot+2020 has revised Venot+2012 's network, in particular methanol (CH_3OH) sub-scheme, using recent combustion studies

➠ *New scheme*: *108 species and 1906 reactions*

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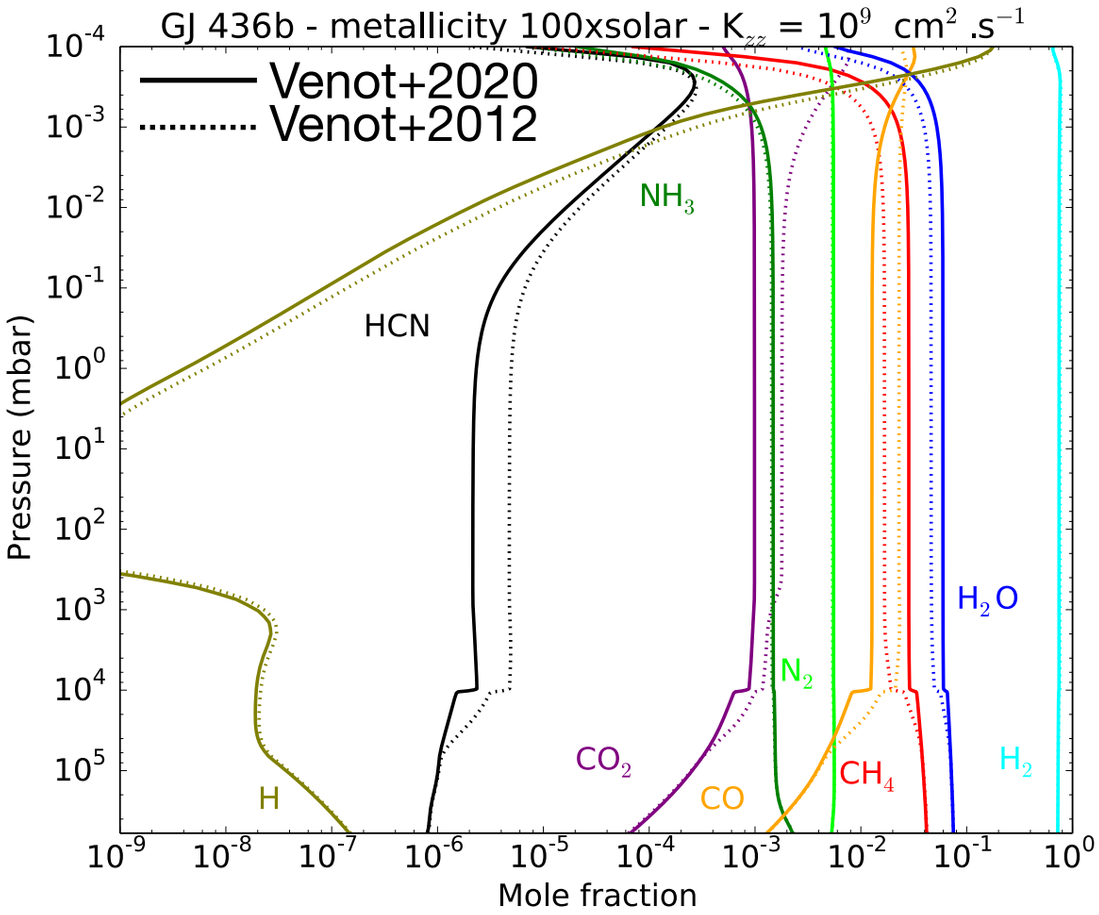
Importance of chemical scheme

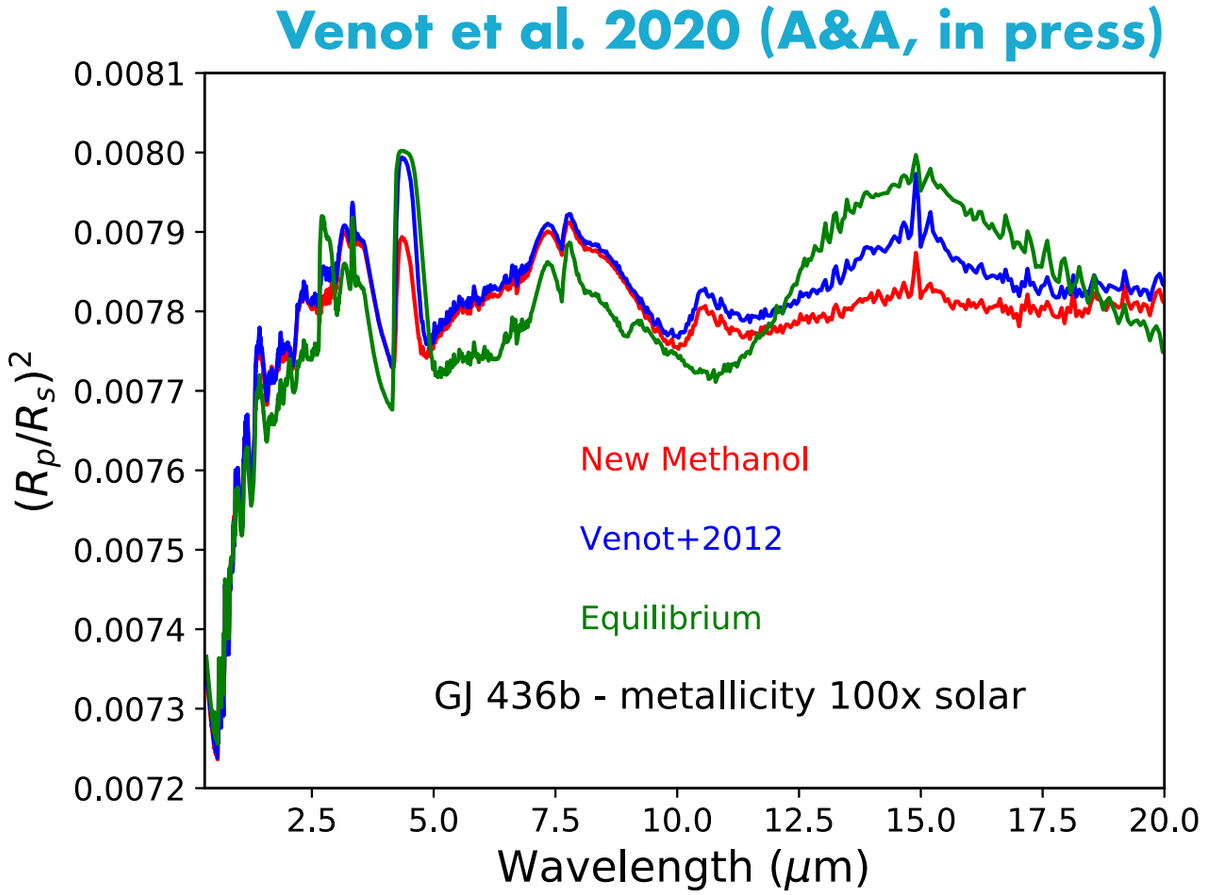
Update of Methanol chemistry

- Minor effect on hot Jupiters's atmospheres, but significant for warm Neptunes



- Quenching of CO and CH_4 happens deeper
- Can lead to a change of the main C-bearing species

- Impact on transmission spectra (CO_2 bands @4.5 and 15μm)
- Such departures up to 100 ppm are largely above ARIEL error bars



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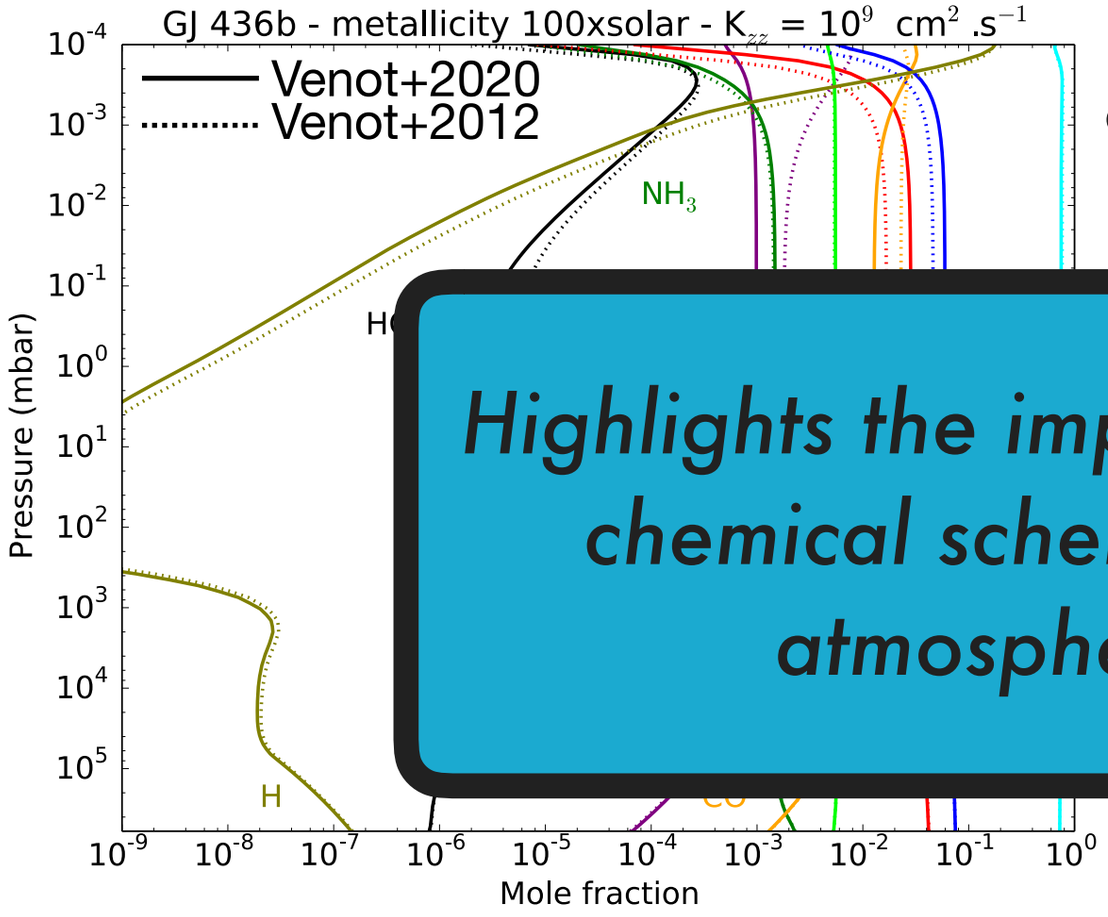

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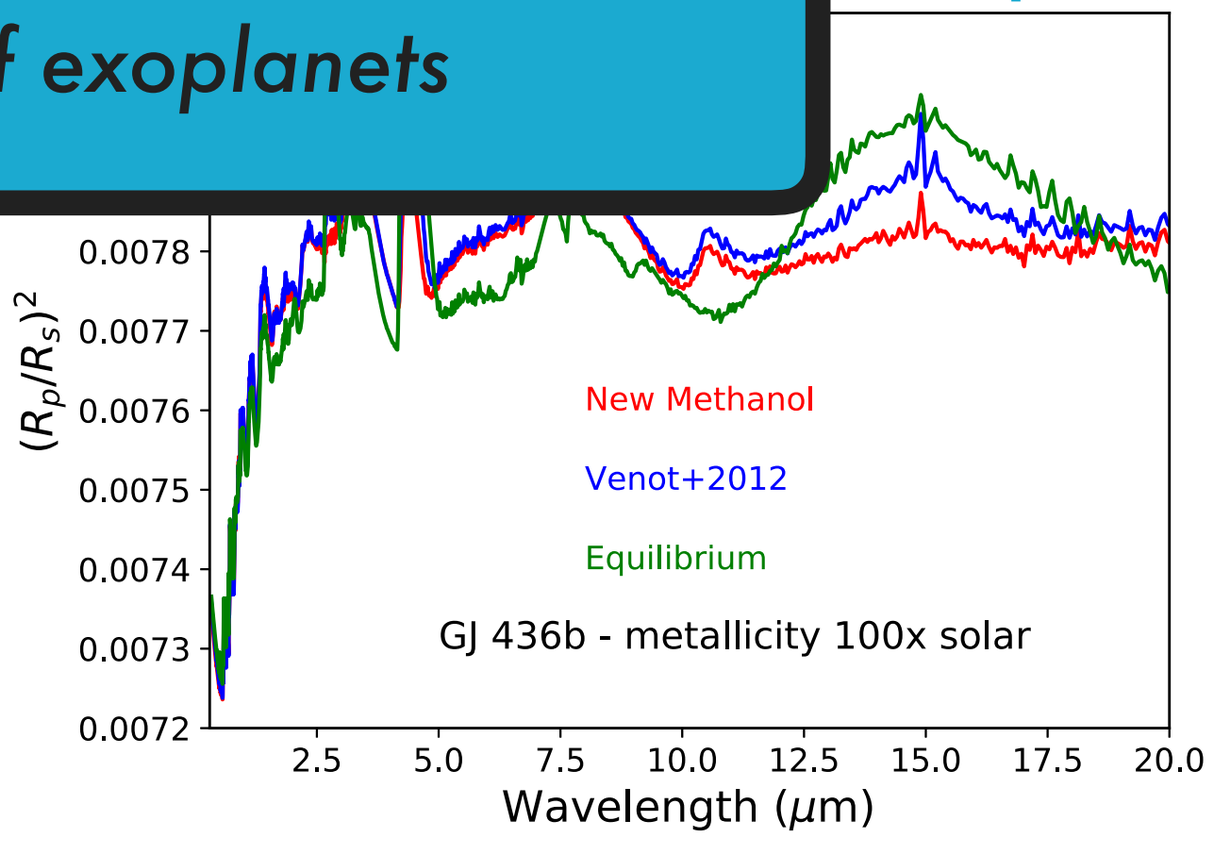
Highlights the importance of using reliable chemical schemes to understand the atmosphere of exoplanets



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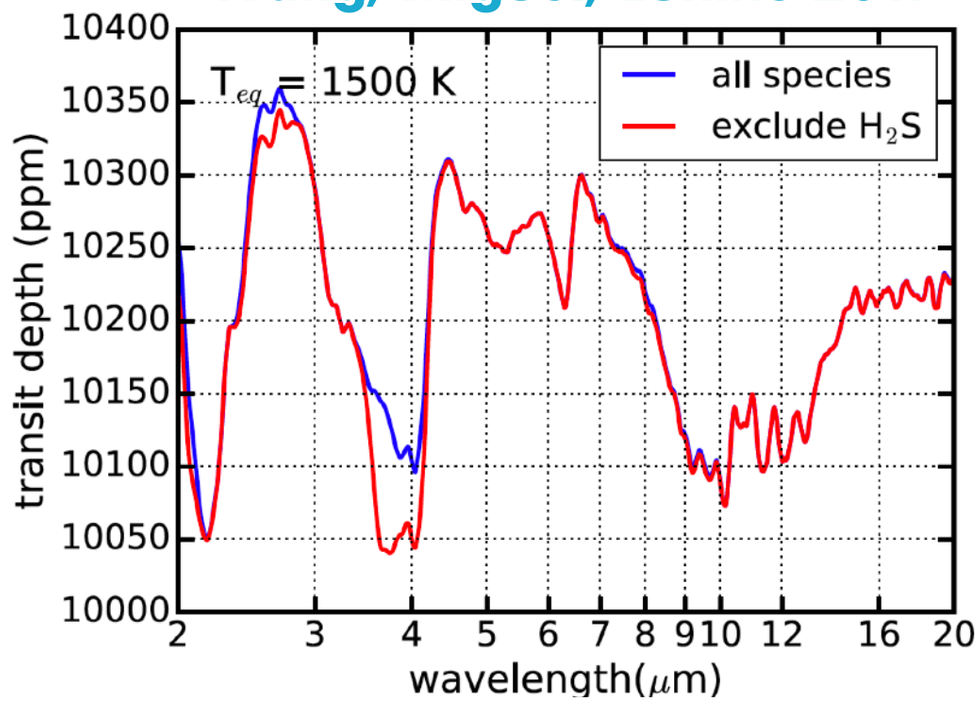
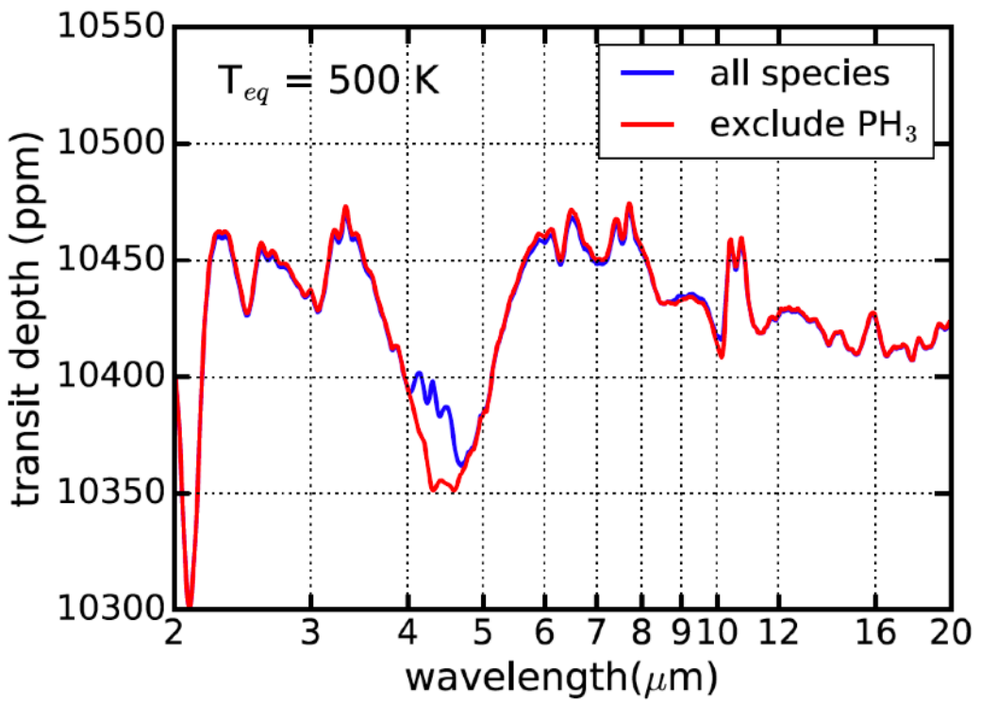
Importance of chemical scheme

Sulfur and Phosphorous Species

- P and S ignored in most chemical schemes
- Wang+2017 studied relevance of S- and P-species in M_{Jup}-planets with 500K<Teq< 2000K.
- Main species PH_3 and H_2S, have deep features on emission and transmission spectra.
- H_2S can be more abundant than NH_3 for planets with T_{eq} > 1000 K
- Feature of PH_3 (@4.5μm) relevant for planets with T < 500 K
- Features of H_2S (@2.8 and 4μm) relevant for planets with high T (1500 K)

Wang, Miguel, Lunine 2017





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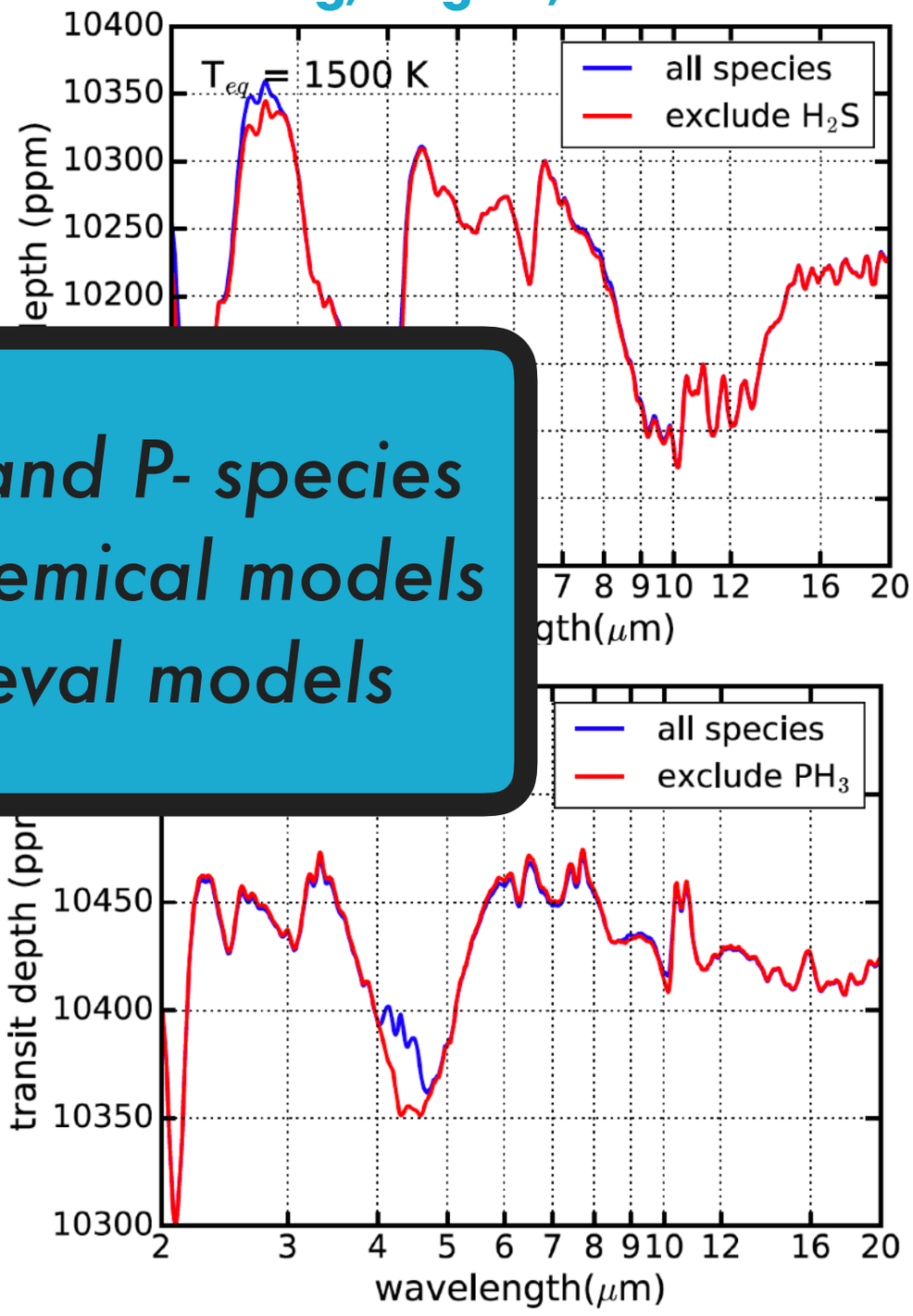
Shows the importance of S- and P- species that should be included in chemical models but also forward and retrieval models

Wang, Miguel, Lunine 2017



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Key Points

Hydrogen-dominated Atmospheres

- Disequilibrium chemistry strongly influences the global composition, but the influence on planetary phase curves of warm Neptunes is rather small. The influence on transmission spectra might be studied further.
- Using reliable chemical schemes is paramount to understand the atmosphere of exoplanets atmospheres
- S- and P- species are important and should be included in all models used to interpret observations.

Further interesting work!!

- Hazes can hide spectral features and their study will allow us to have a better interpretation of ARIEL data => *talk by Yui Kawashima*
- Carbon-rich Exoplanets with T>1200K are not in equilibrium (Lab measurements – Fleury+2019)
- A transit spectra with signatures of photochemical organic aerosols, could indicate a high C/O ratio (Lab – Fleury+2019)
- The ionic chemistry is expected to be important => *talk by Jérémy Bourgalais*
- CO_2 cross section highly depend on temperature. Proper values need to be used for correct interpretation of ARIEL measurements (Lab – Venot+2018)

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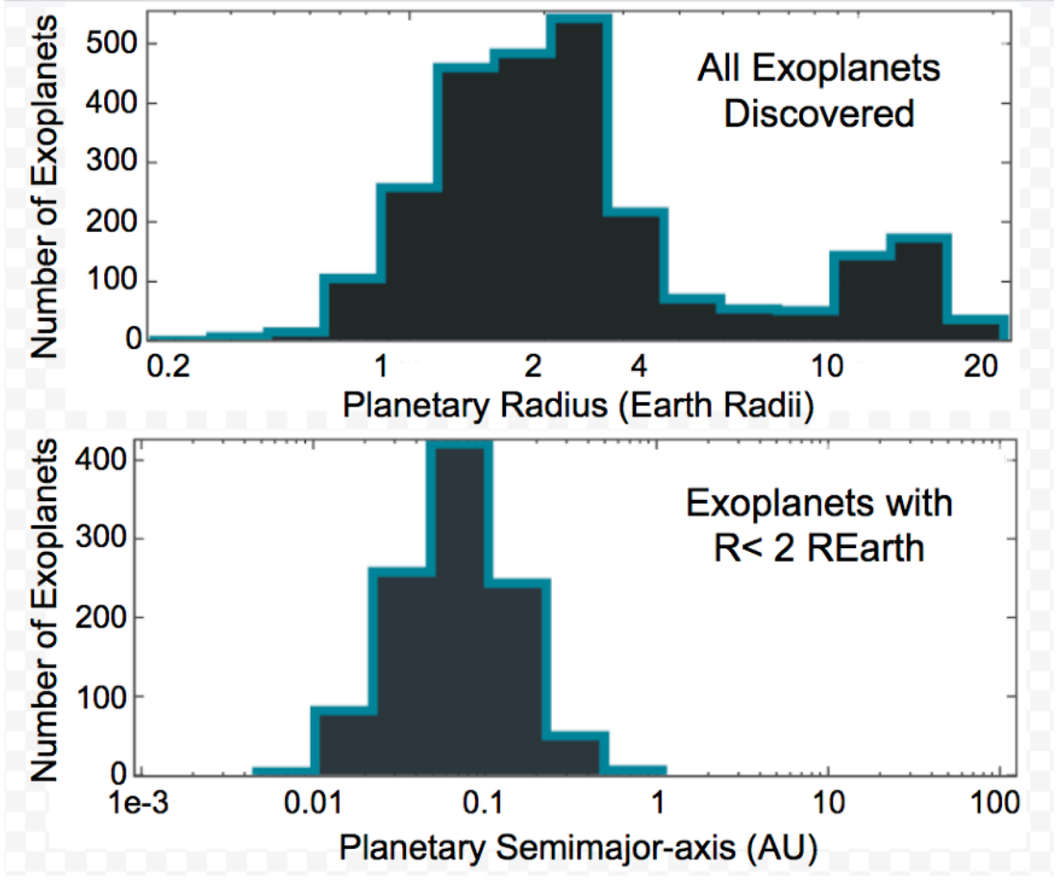
Hot Rocky Exoplanets's Atmospheres

Good targets for ARIEL!

- Rocky planets and super-Earths are the most common exoplanets found.
- Some of the hottest ones are good targets for ARIEL.
- Their atmospheric composition is difficult to predict (secondary atmospheres)



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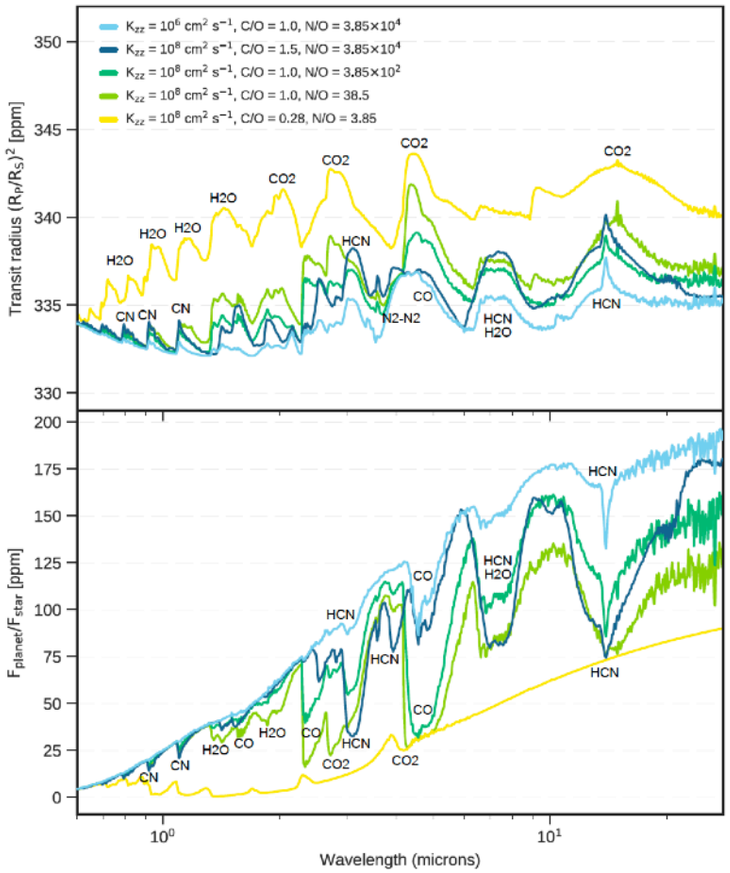
Hot Rocky Exoplanets's Atmospheres

Good targets for ARIEL!

Zilinskas+,submitted



Atmosphere from outgassing during evolution

No atmosphere

- Example: phase curves observations of 55 Cnc e point towards high-μ, potentially Nitrogen-dominated atmospheres

=>For N-dominated atmospheres: *poster by Mantas Zilinskas* (hint: features of HCN & CO -for high C/O. In atmospheres very H-depleted, features of C_2H_2 and CN)

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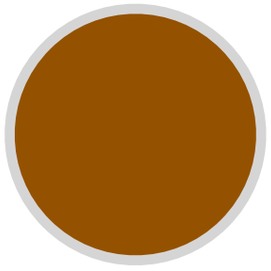
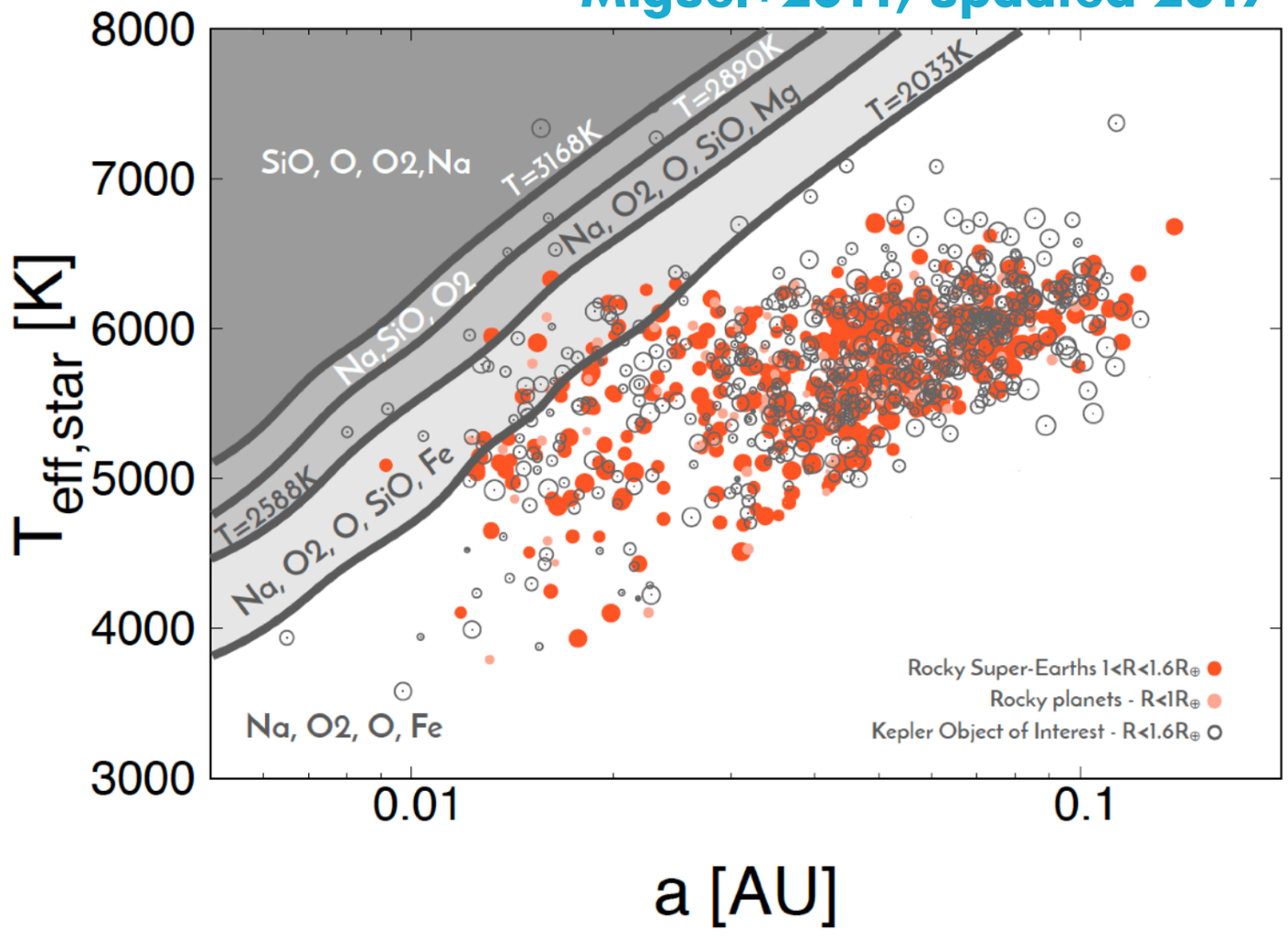
Rocky Exoplanets's Atmospheres
With Ultra Short Periods

- Some hot-rocky planets might have lost their volatiles and have an atmosphere made of vaporised magma
- Observability of hot-rocky exoplanet atmospheres => *talk by Yuichi Ito*



Thin atmosphere from vaporised magma

Miguel+2011, updated 2017



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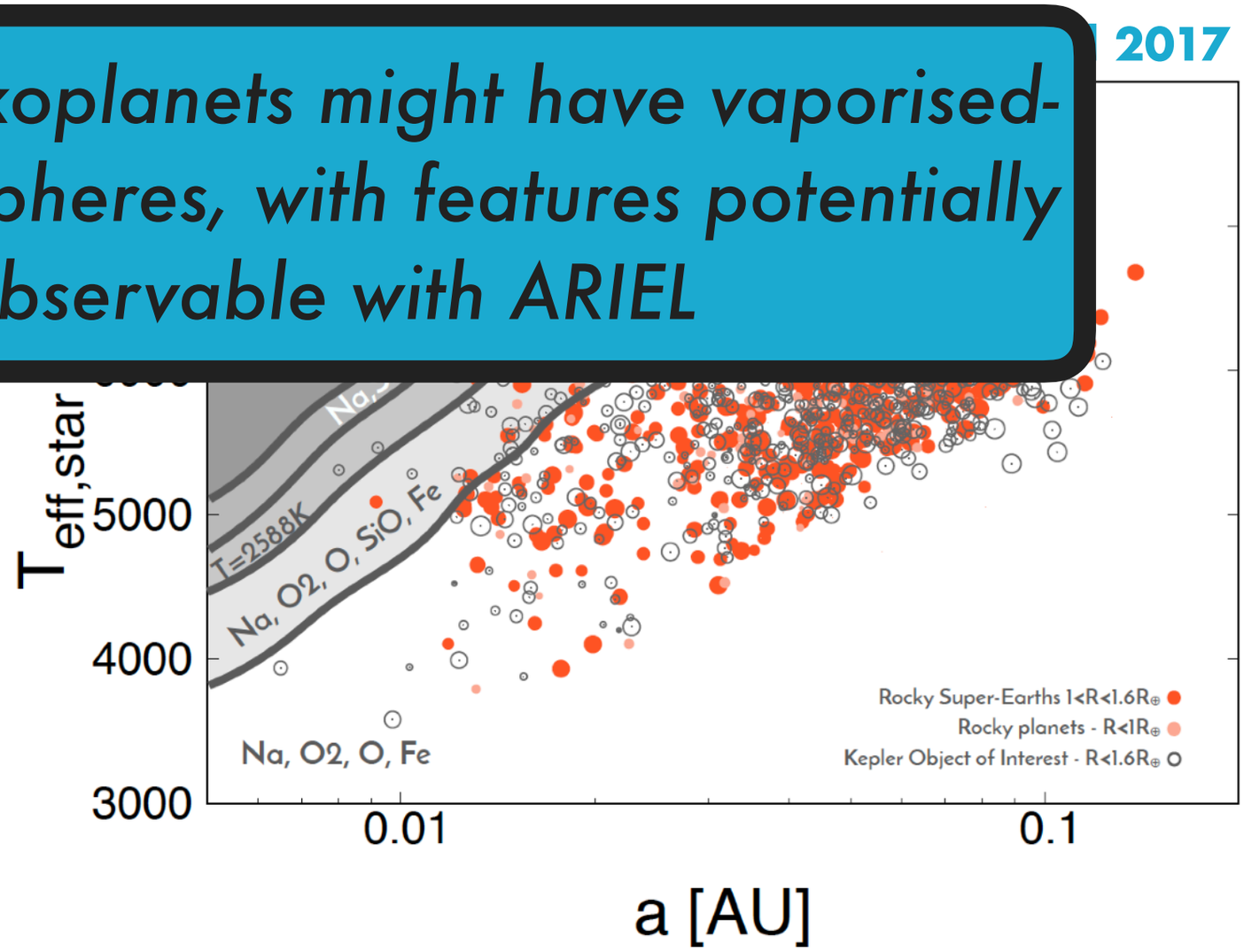
Hot-rocky exoplanets might have vaporised-rocks atmospheres, with features potentially observable with ARIEL

Thin atmosphere from vaporised magma



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Key Points

Hot Rocky Exoplanets's Atmospheres

- These are the most abundant planets found
- Atmospheres largely unknown and with a potentially high diversity
- 55 Cnc-e observations pointed towards N-dominated atmospheres, which might have features of HCN, CO (high C/O), and C_2H_2 and CN if highly depleted in H (Zilinskas+2020, sub)
- Hot-rocky exoplanets might have vaporised-rocks atmospheres.
- All these features are potentially observable with ARIEL.

- Clouds might be present in these hot-rocky exoplanet atmospheres (results by Mahapatra+2017)
- The ionic chemistry is expected to be important => *talk by Jérémy Bourgalais*

Further interesting work!!

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