Prospects for Biosignatures

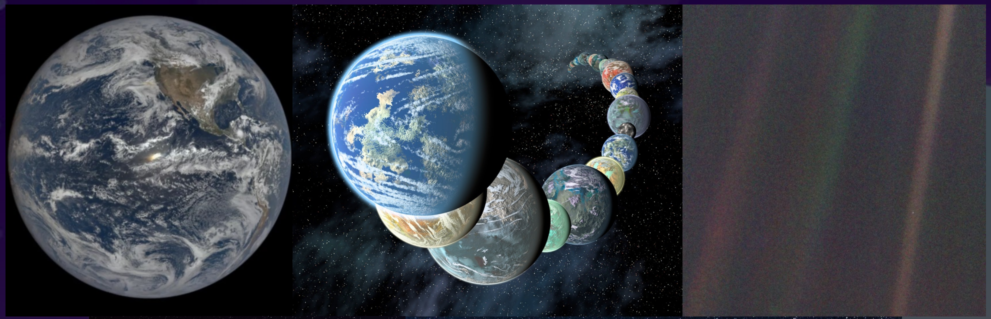
Edward Schwieterman

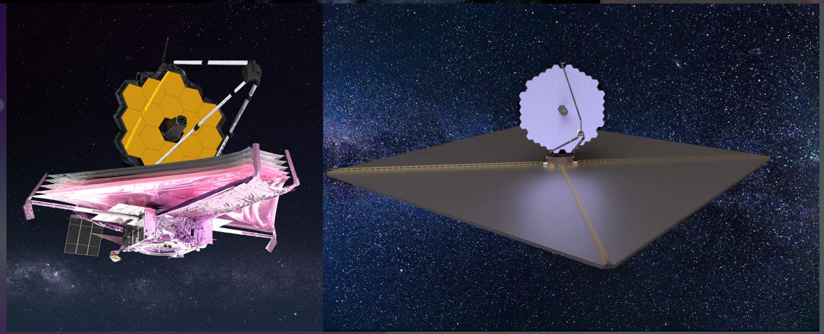
University of California, Riverside

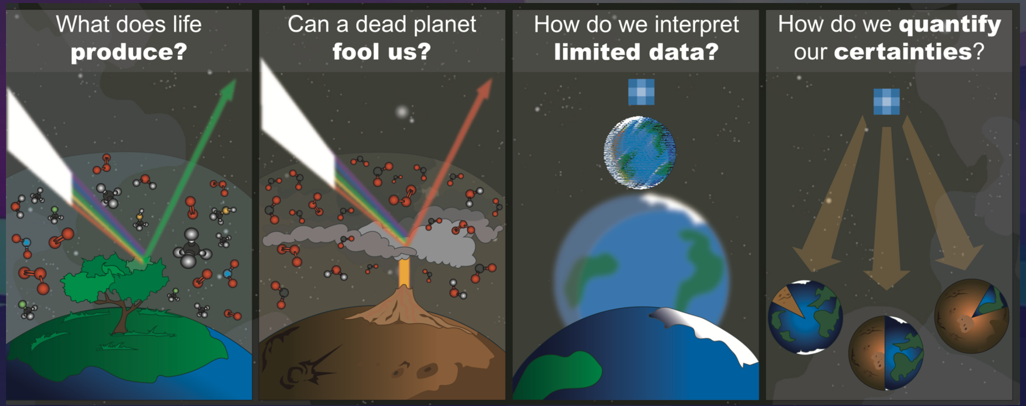
Sagan Summer Workshop 2023

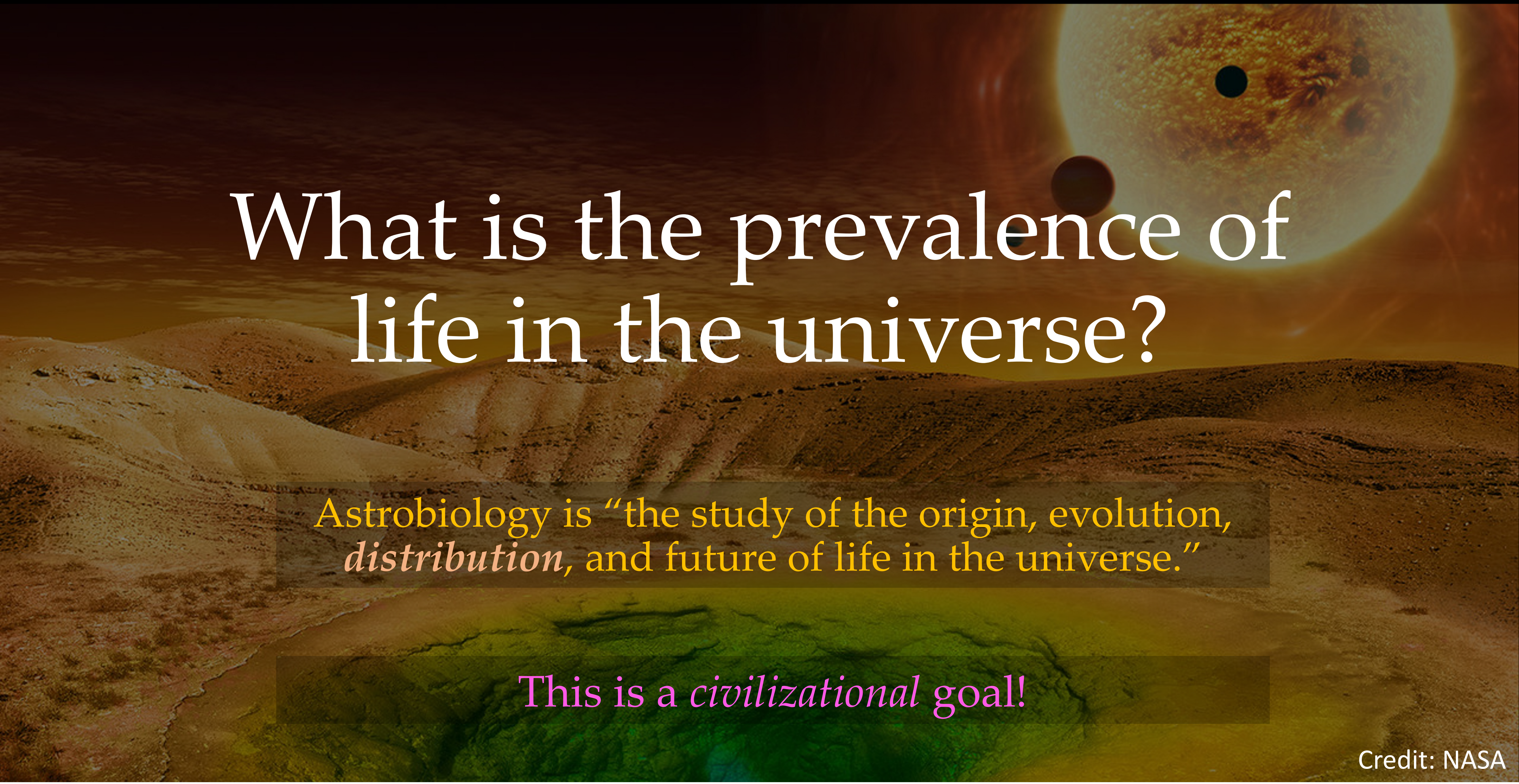
Characterizing Exoplanet Atmospheres: The Next Twenty Years

7/28/2023



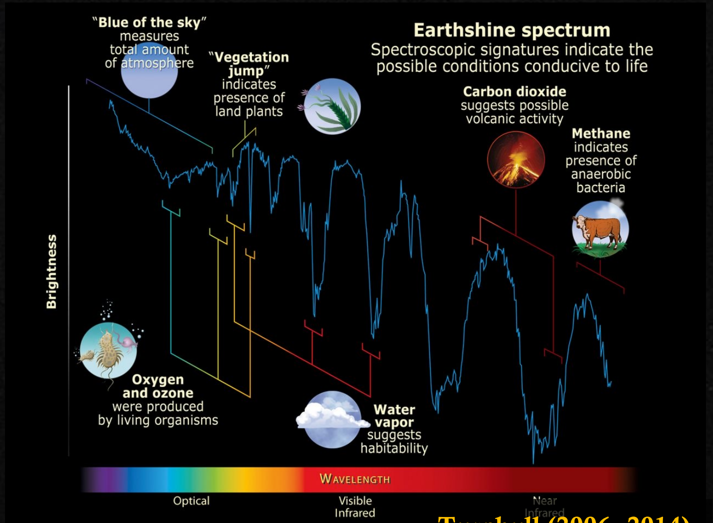




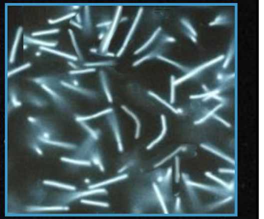

What is the prevalence of life in the universe?
Astrobiology is "the study of the origin, evolution, *distribution*, and future of life in the universe."
This is a *civilizational* goal!

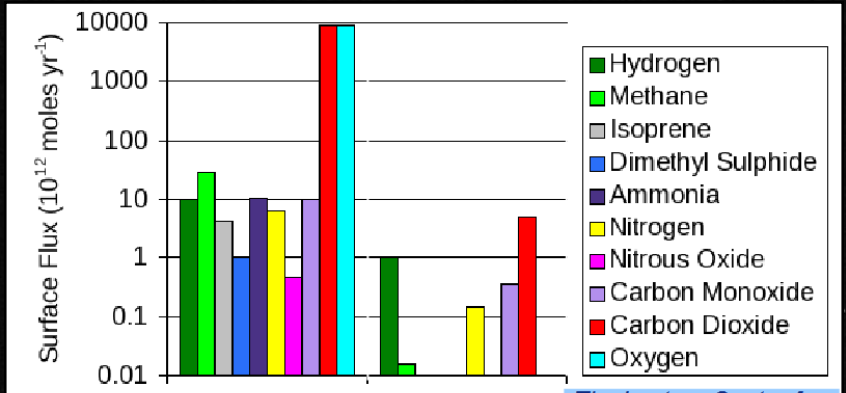
Credit: NASA

Life Is a Possible Outcome of and Influence on Planetary Evolution



Turnbull (2006, 2014)





Tim Lenton, Centre for Ecology and Hydrology

- Earth's atmospheric composition is not predictable from cosmic (—or bulk—or crustal) abundances. It does not have a "metallicity" (e.g., C:O:N).
- It has changed drastically through time, despite initial conditions, due in part to co-evolution with life and stellar factors.
- No simple abiotic outgassing + escape model can explain Earth's current atmosphere.
- Any abiotic model that could explain Earth's current atmospheric composition *is wrong*.
- The life hypothesis cannot be excluded *a priori*.

~~What is the prevalence of life in the universe?~~

How common are **planetary biospheres** in the **solar neighborhood?**

Credit: NASA

Exoplanet Biosignature: *A Remotely Detectable Indicator of Life*

- **Produced by Life**
- **~Global In Extent**
- **Produce Observable Features (line absorption)**
- **Builds up to Detectable Amounts (robust to photochemistry)**
- **Separable from Abiotic Processes (false positives)—*Given Context***

Earth-Based Approaches

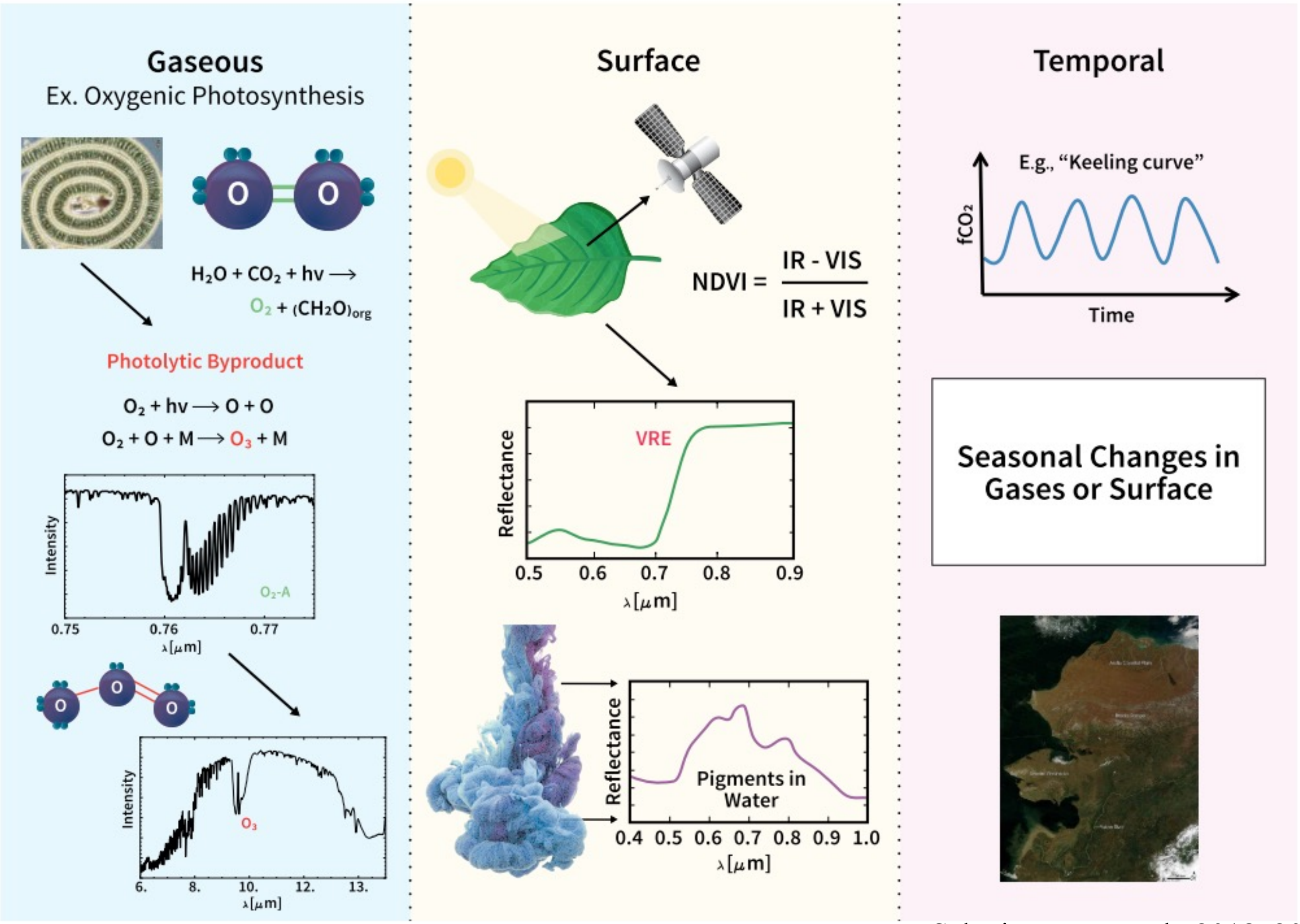
- Automatically passes first few tests (produced by life, detectable, can build up, etc.)
- Heritage of existing data and models for Earth system
- Will always have more information about Earth
- Earth through time
- **Limited by environment, composition, and historical/evolutionary contingencies**

Agnostic and Other Approaches

- Generalized Thermodynamic or Kinetic Disequilibrium
  - ”All small molecules” Approach (e.g., Seager & Bains, 2016)
- Network topologies (e.g., Wong+2023)
- Ground-up: not constrained by Earth history contingencies
- broader universe of potential signatures
- **Requires more laboratory and modeling work**

Possible Biosignatures on Terrestrial Planets

- **Atmospheric Gases:** O_2, O_3, CH_4, N_2O, DMS—$(CH_3)_2S$, DMSe—$(CH_3)_2Se$, C_5H_8, CH_3Cl, CH_3Br, CH_3SH, PH_3, NH_3, etc.
- **Surface Features:** Vegetation Red Edge (VRE), anoxygenic photosynthesis, rhodopsins, other pigments
- **Temporal Changes:** Seasonal Change in Gas (e.g., CO_2, CH_4, O_3 or Pigments)
- **Always Context-Dependent!**



Schwieterman et al., 2018, 2021

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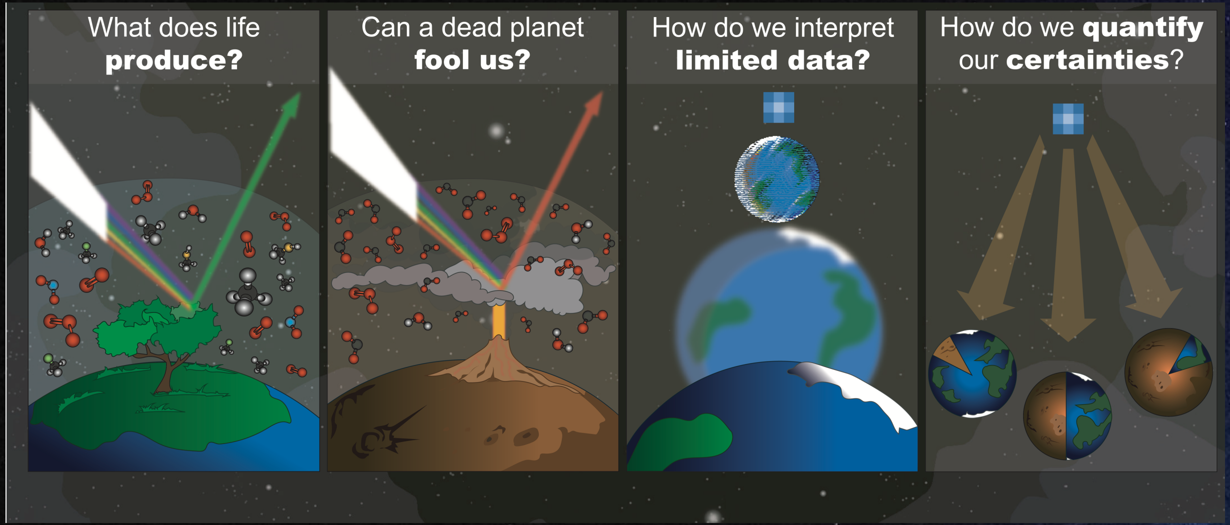
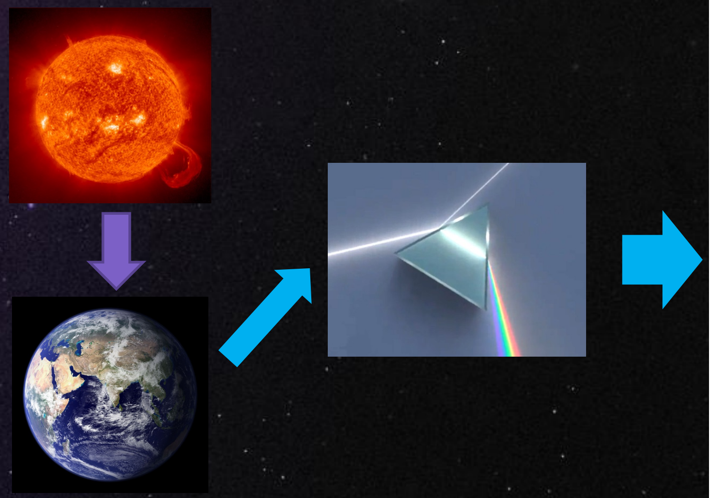
See Biosignature Reviews and Perspectives By, e.g.,: Seager+2012,2016 (Astrobiology), Kaltenegger+2017 (ARAA. 2017. 55:433); Grenfell+2017 (Phys.Rep), Krissansen-Totton+2022 (Nature Astro); Standards of Evidence Report (2022). Astrobio Special Issue: Catling+, Fujii+, Kiang+, Meadows+, Schwieterman+, Walker+2018

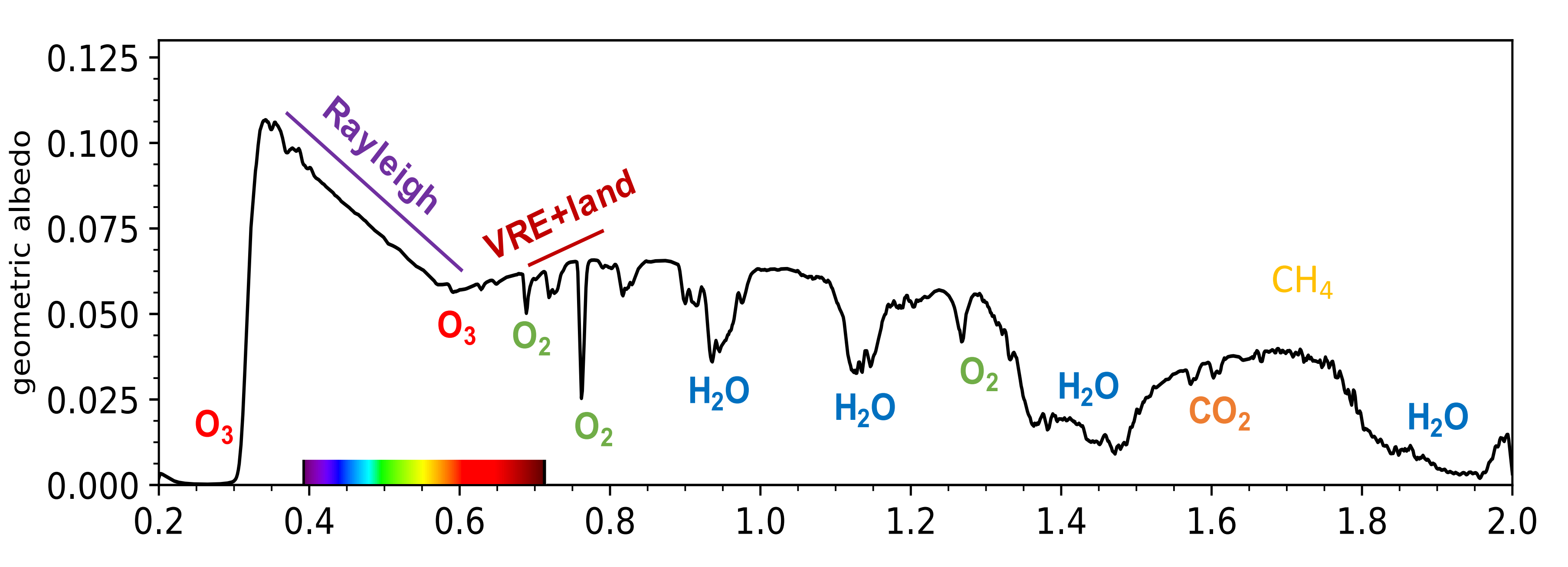


See Special Issue of *Astrobiology* on Exoplanet Biosignatures (2018): https://www.liebertpub.com/toc/ast/18/6

Earth's Reflected Light Spectrum Today and Its Features

Accessible Wavelength Regions will Depend on Observing Mode and Instrumentation



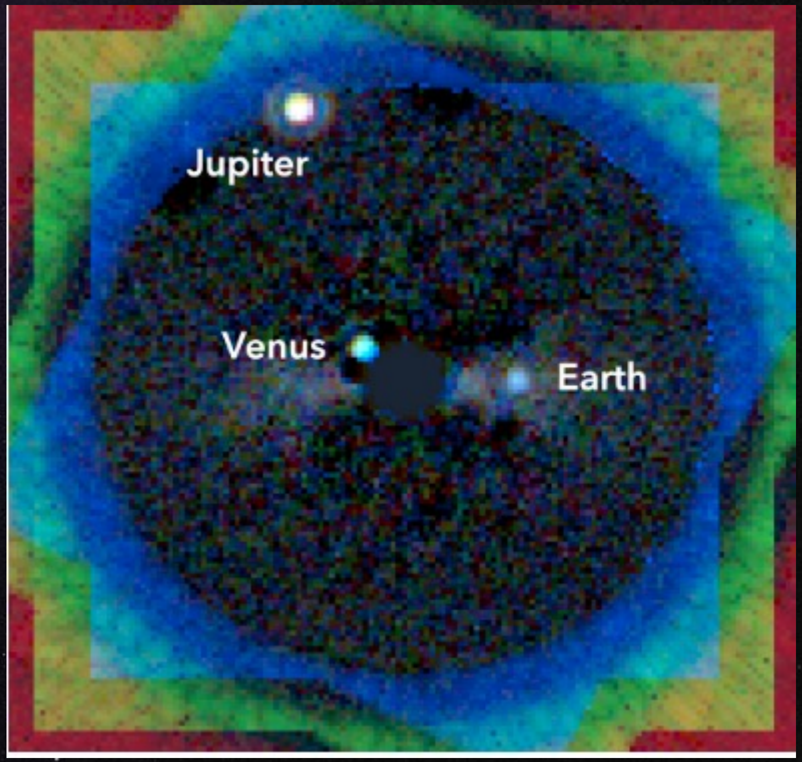


"Reflected light" – the light from the star is reflected (and/or scattered) by the planet to the distant observer.

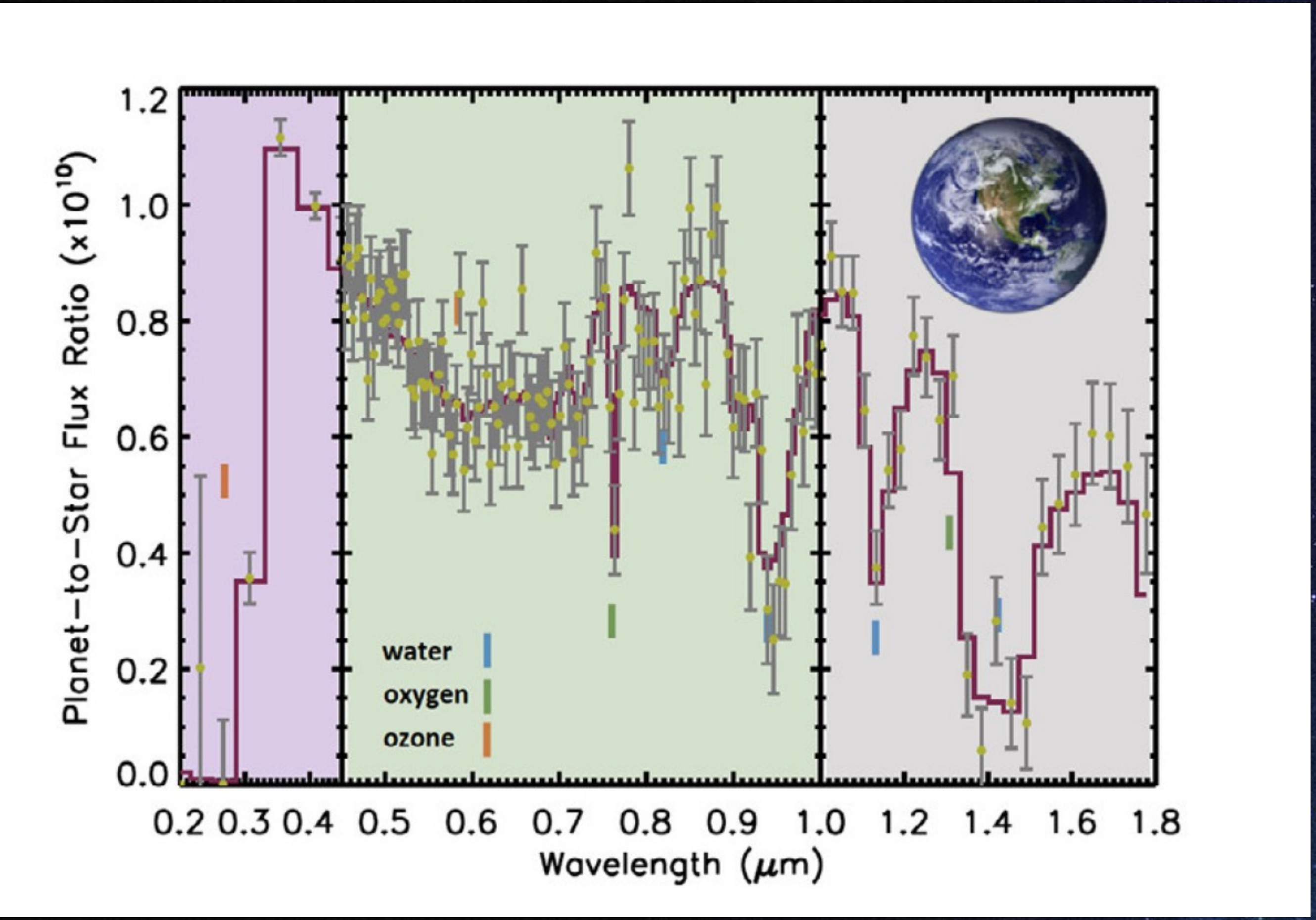
An average Earth spectrum at ultraviolet (UV), visible (VIS), and near-infrared (NIR) wavelengths shows features from oxygen (O_2), ozone (O_3), water vapor (H_2O), and carbon dioxide (CO_2). Rayleigh scattering from Earth's blue sky is shown (λ^{-4}). A small signature from Earth's vegetation red-edge (VRE) is apparent.

How An ExoEarth Would Be Observed in Reflected Light (HWO)

Star nulling by coronagraph or starshade



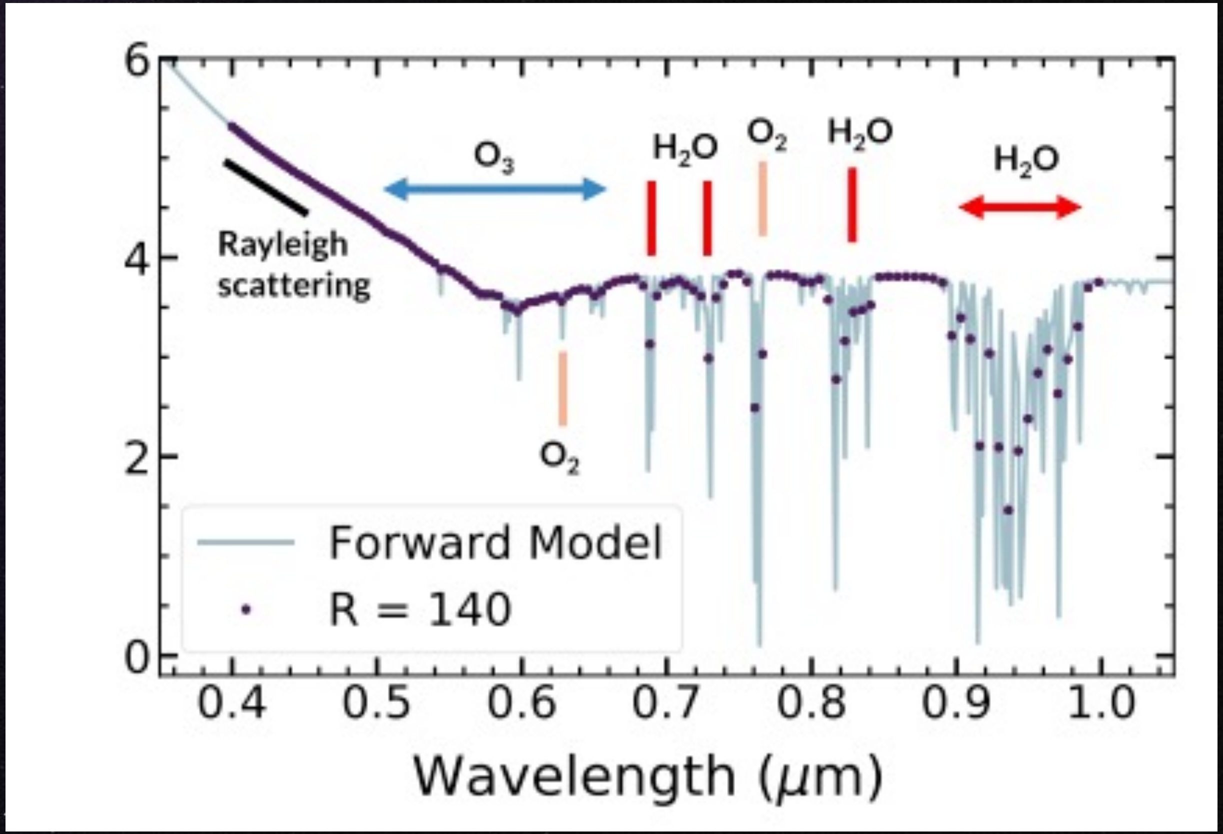
LUVOIR Report; Roberge et al. 2018



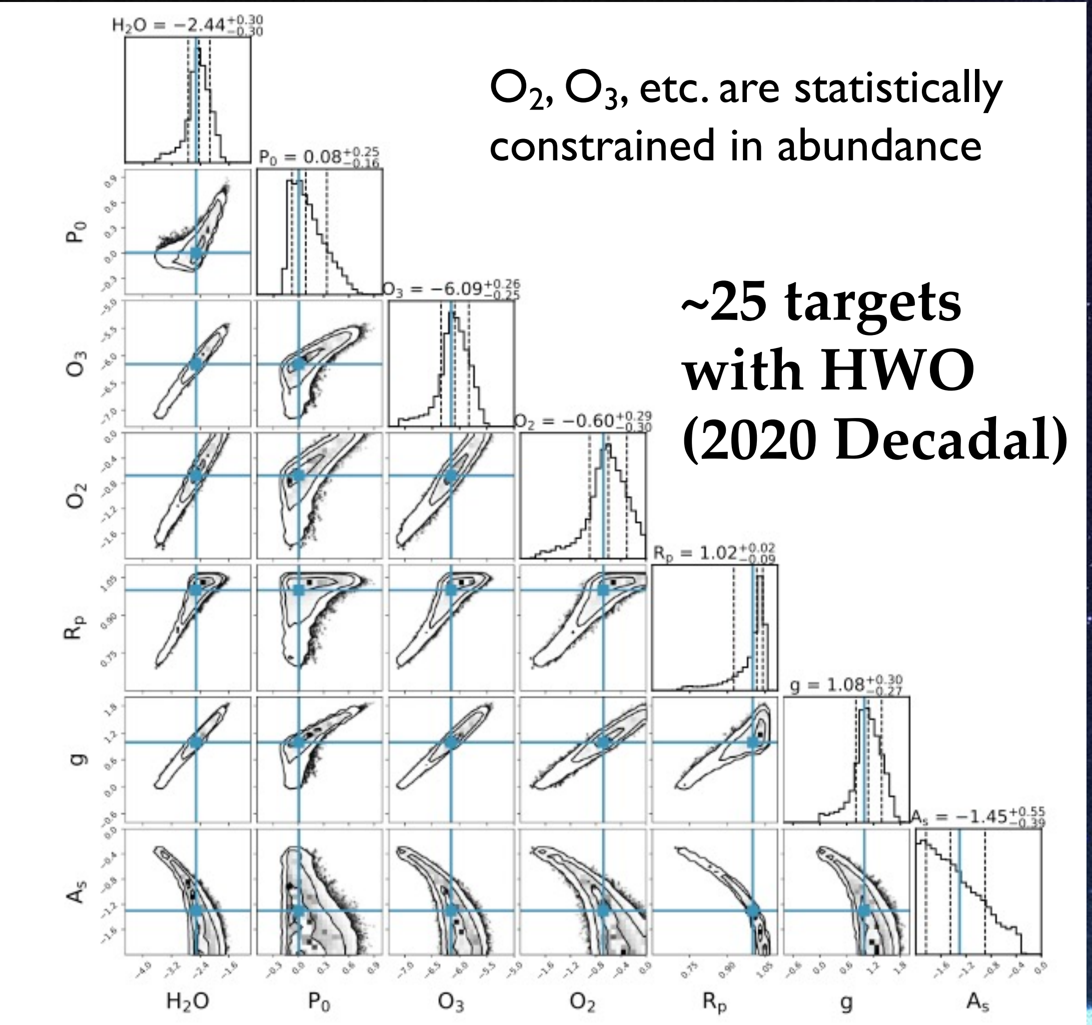
HabEx Report; Robinson et al. 2016

Atmospheric Retrievals Will Help Confirm Signatures

Employing an Inverse Model



Feng et al. 2018, AJ, 155:200



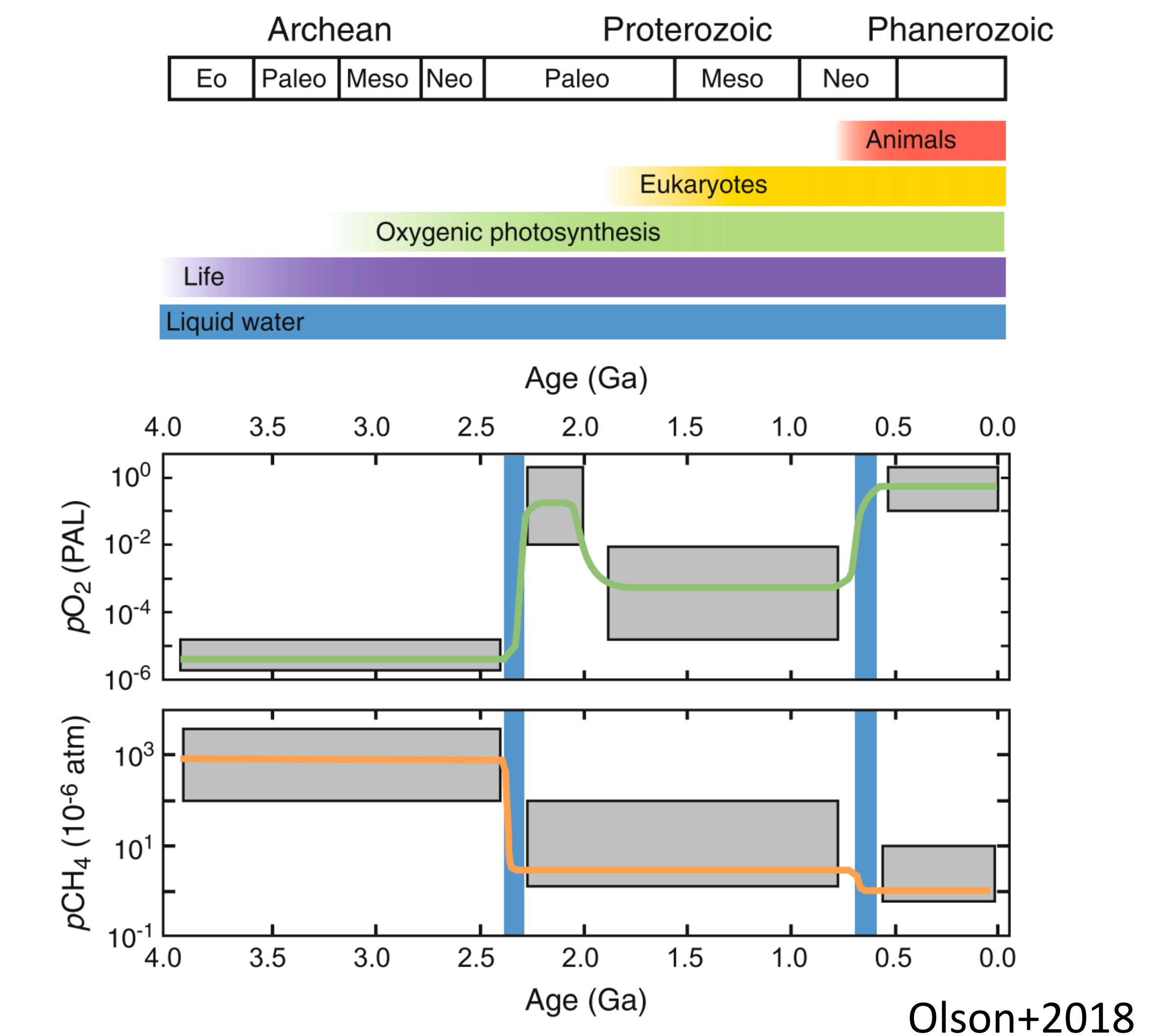
O_2, O_3, etc. are statistically constrained in abundance

~25 targets with HWO (2020 Decadal)

Using Earth and its Evolution as a "Test Case"

Earth represents not just one but a palette of possible (bio)geochemical states for rocky exoplanets with secondary atmospheres.

Using Earth and its Evolution as a "Test Case"



Olson+2018

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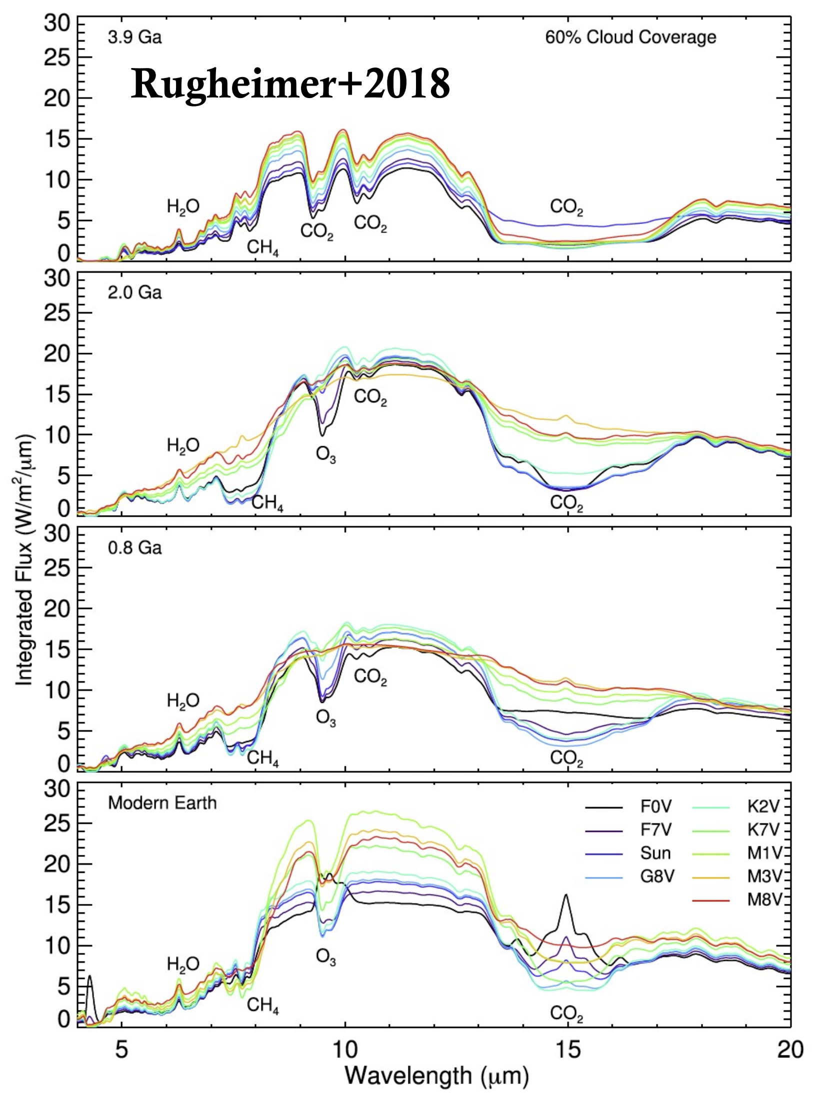
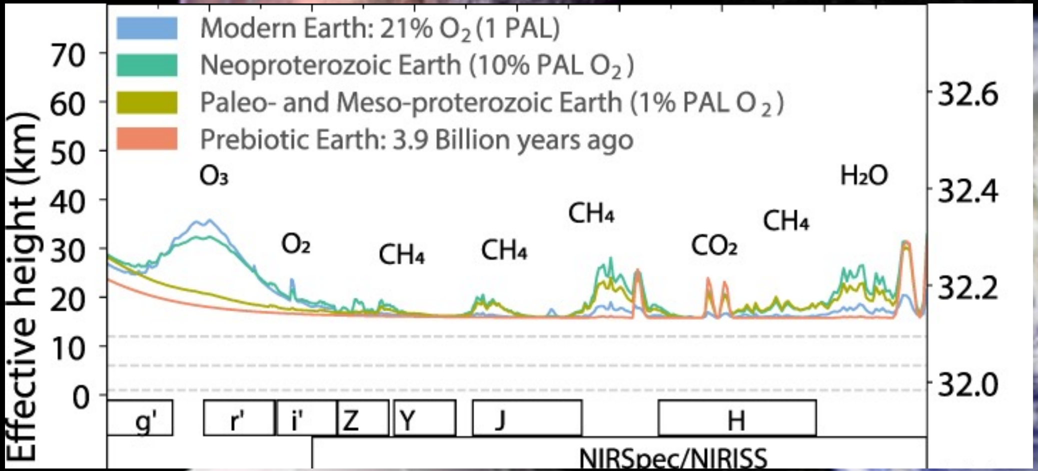
Using Earth and its Evolution as a "Test Case"





Kaltenegger+2020

See, e.g., Kaltenegger+2007, Arney+2016,2017, Reinhard+2017, Meadows+2018, Rugheimer & Kaltenegger (2018), Robinson & Reinhard (2018), Kaltenegger+2020, Alei+2022, Young+2023, and more!

Earth Through Time: Biosignature Combinations (Reflected Light)

Anoxic, no haze: CH_4 + H_2O + λ^{-4} + CO_2

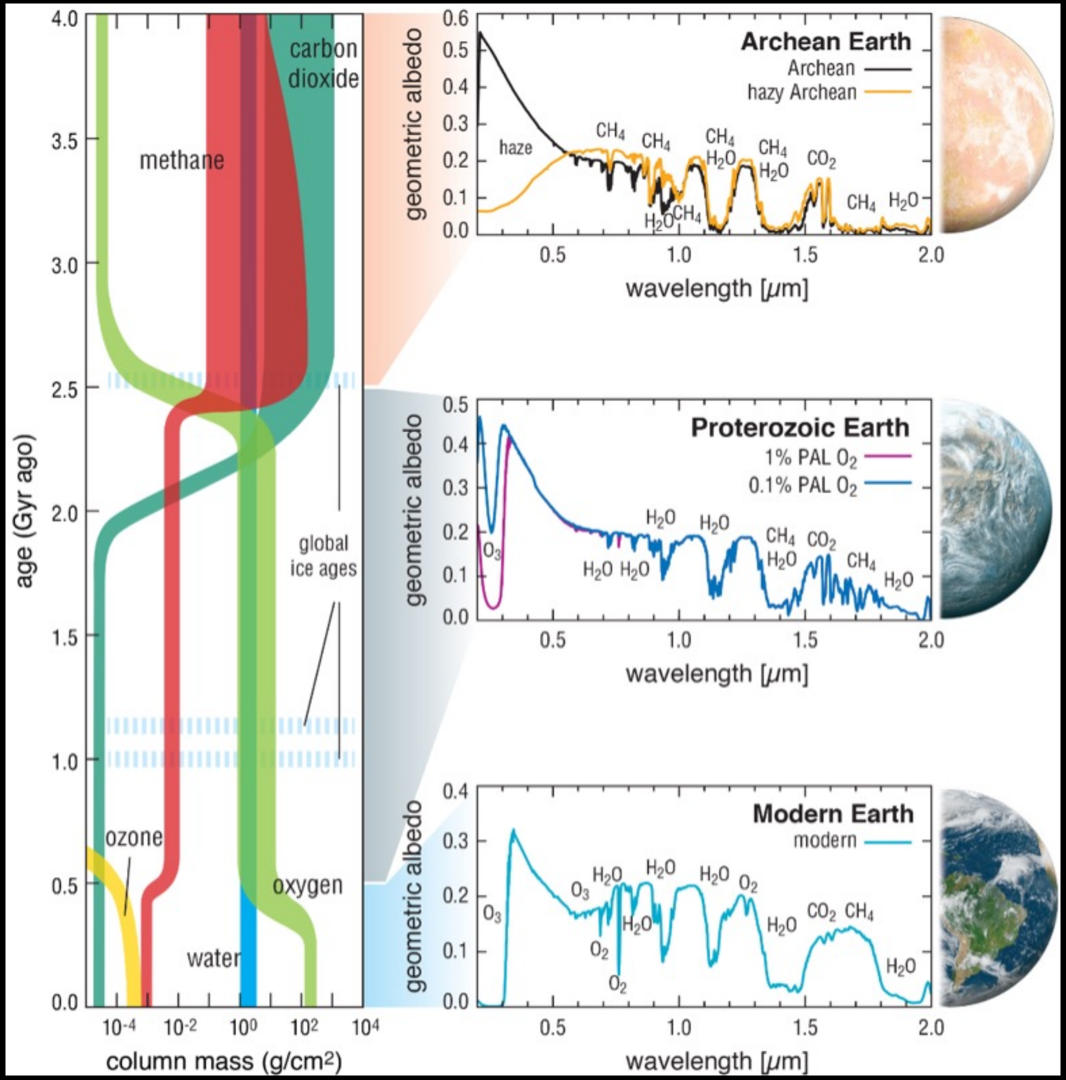
Strongest Anoxic: haze + H_2O + CH_4 + CO_2

Weakly Oxygenated: O_3 + λ^{-4} + H_2O [+ CH_4]

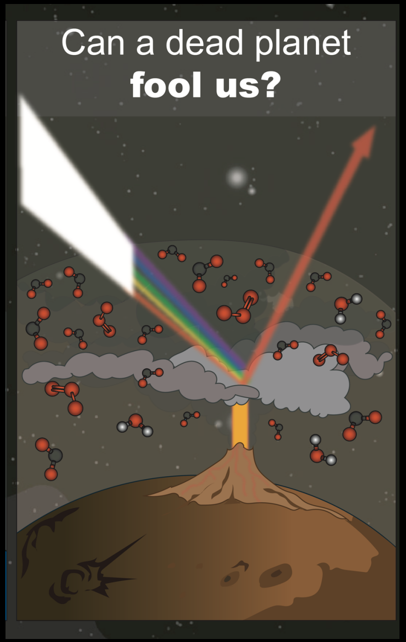
Strong Oxygen-rich: O_3 + λ^{-4} + H_2O + O_2

Strongest Oxygen-rich: O_3 + λ^{-4} + H_2O + O_2 + CH_4

Biosignatures and false positive evaluators are ordered by their relative detectability in atmospheric spectra



LUVOIR Final Report



Context can help rule out "false positives"

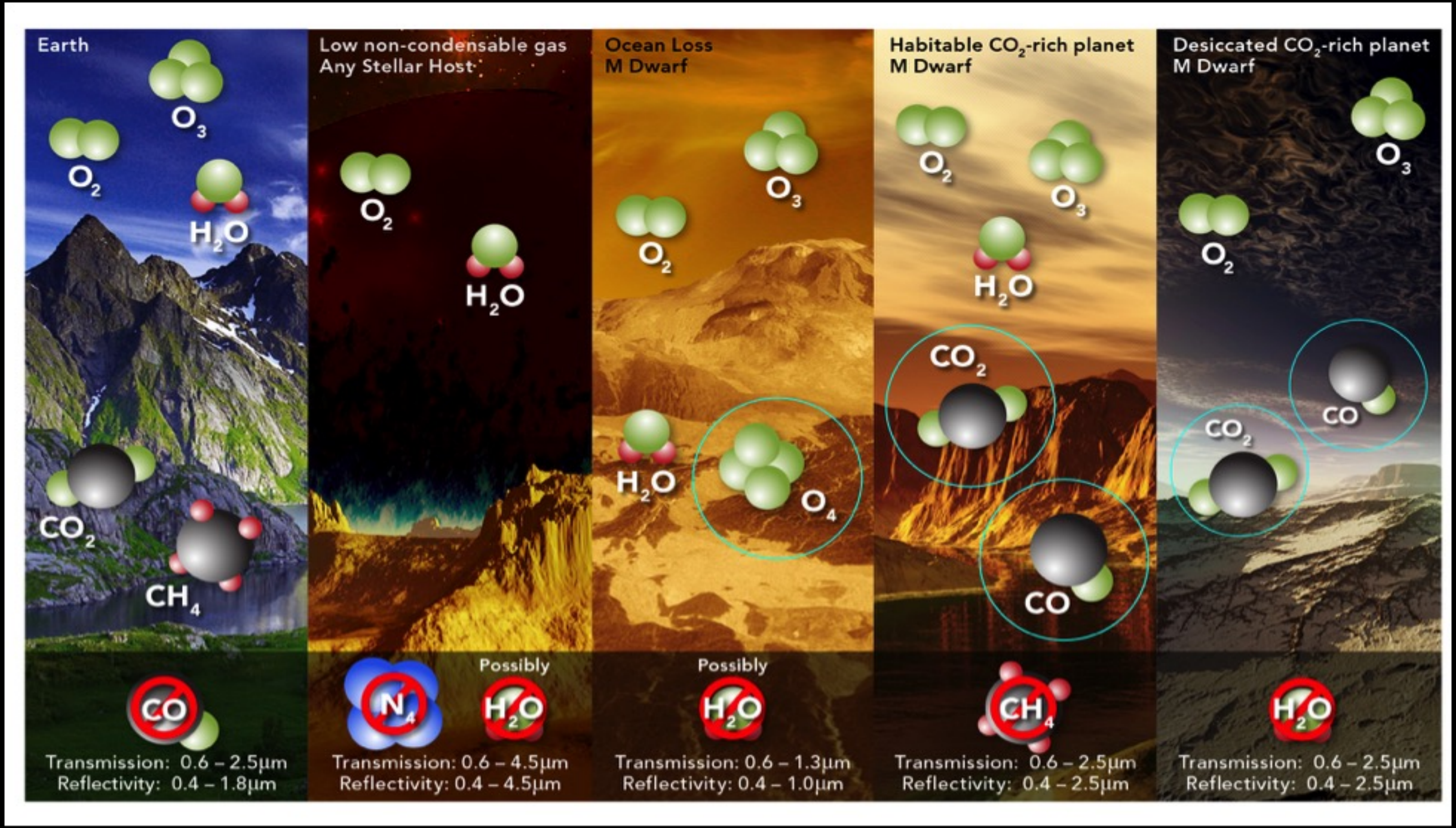


Image Credit R. Hasler

Detecting H_2O, CH_4, and/or the Rayleigh slope ($\propto \lambda^{-4}$) can confirm biological nature of O_2/O_3.

Certain features (O_2-O_2 CIA) would confirm a "**false positive.**"

e.g., Domagal-Goldman+14,Hu+2020; Meadows+2017,2018a,b; Schwieterman+2015/6

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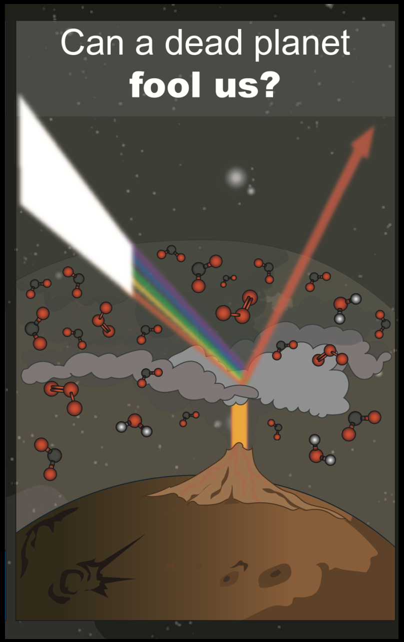
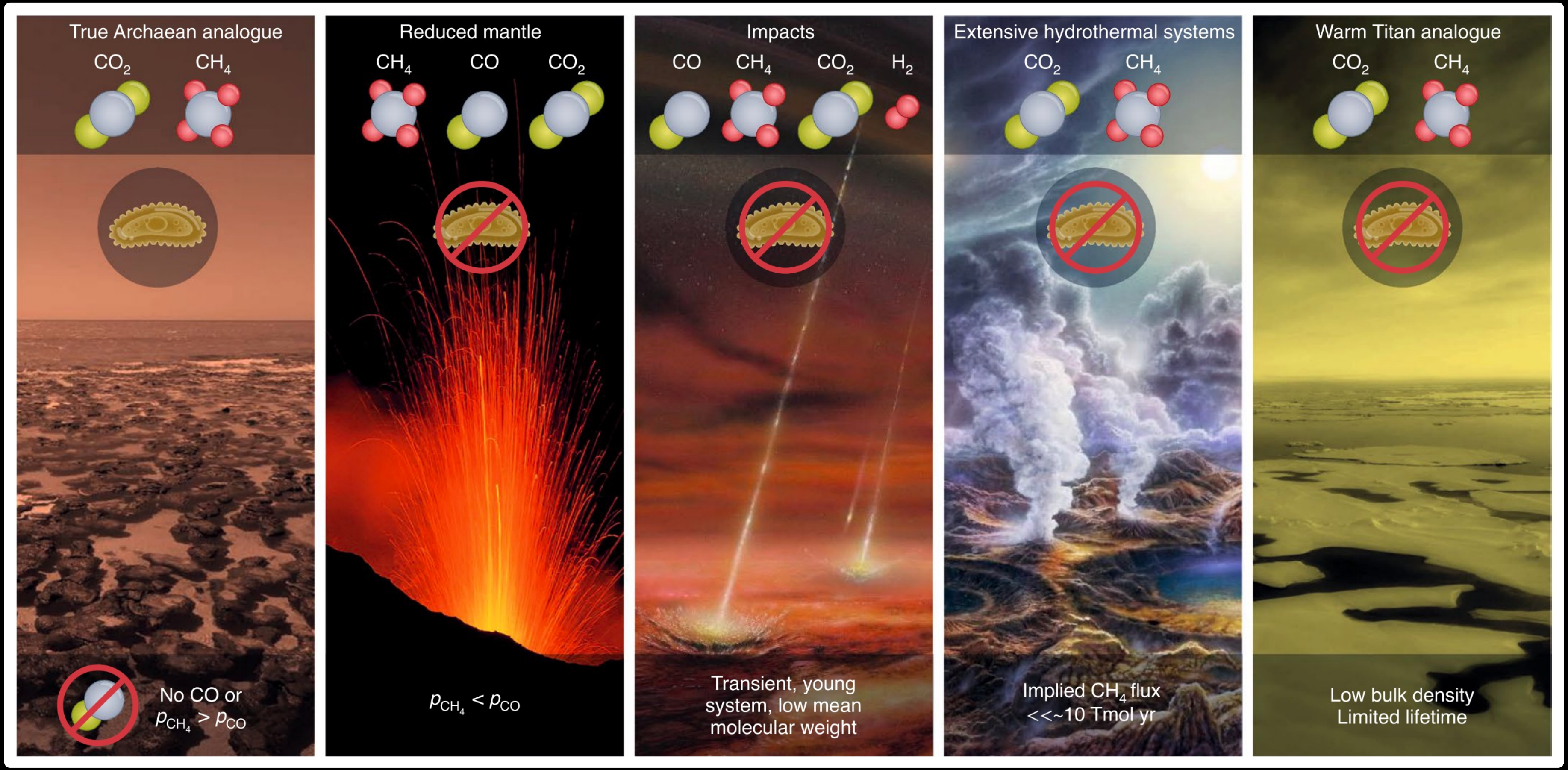




Detecting the CH_4+CO_2 couple together with low CO may imply biological CH_4 production. Though some CO is a natural outcome of CH_4 photooxidation.

e.g., Krissansen-Totton+2018,2022, Thompson+2022

Short Photochemical Lifetime: $CH_4 + OH \rightarrow CH_3 + H_2O$ & $CH_4 + h\nu \rightarrow CH_3 + H$

Searching for Life via Thermodynamic Disequilibria

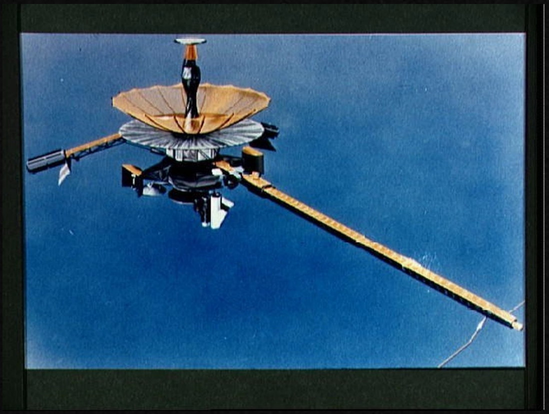
A search for life on Earth from the Galileo spacecraft

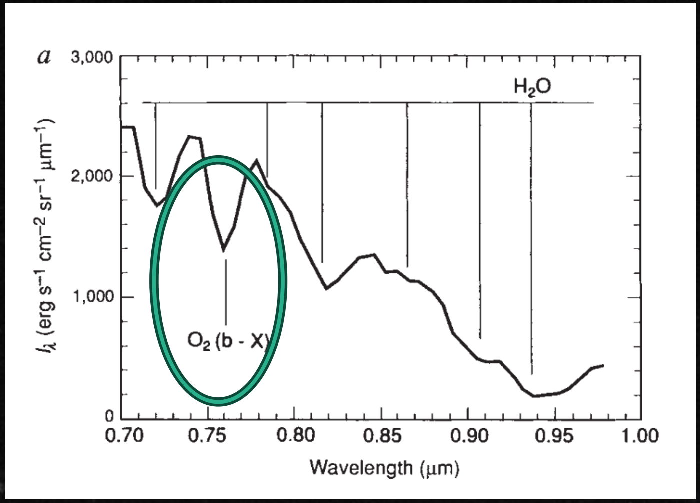
Carl Sagan*, W. Reid Thompson*, Robert Carlson†, Donald Gurnett‡ & Charles Hord§

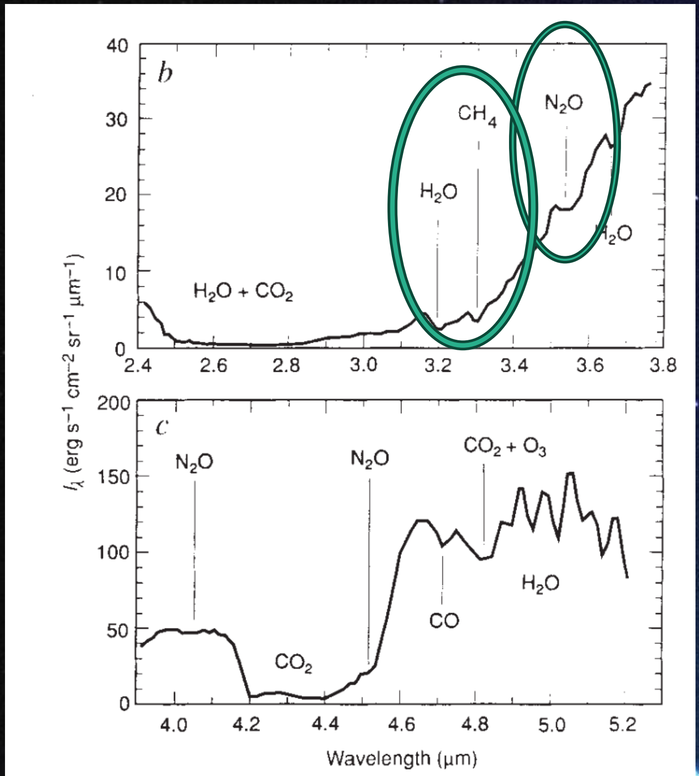
TABLE 1 Constituents of the Earth's atmosphere (volume mixing ratios)

Molecule	Standard abundance (ground-truth Earth)	Galileo value*	Thermodynamic equilibrium value Estimate 1†	Estimate 2‡
N_2	0.78		0.78	
O_2	0.21	0.19 ± 0.05	0.21§	
H_2O	0.03–0.001	0.01–0.001	0.03–0.001	
Ar	9×10^{-3}		$9 \times 10^{\ 3}$	
CO_2	3.5×10^{-4}	$5 \pm 2.5 \times 10^{-4}$	$3.5 \times 10^{\ 4}$	
CH_4	1.6×10^{-6}	$3 \pm 1.5 \times 10^{-6}$	$< 10^{-35}$	$10^{\ 145}$
N_2O	3×10^{-7}	$\sim 10^{-6}$	2×10^{-20}	2×10^{-19}
O_3	10^{-7}–10^{-8}	$> 10^{-8}$	6×10^{-32}	3×10^{-30}

* Galileo values for O_2, CH_4 and N_2O from NIMS data; O_3 estimate from UVS data.
† From ref. 16 (P, 1 bar; T, 280 K).
‡ From ref. 17 (P, 1 bar; T, 298 K).
§ The observed value; it is in thermodynamic equilibrium only if the under-oxidized state of the Earth's crust is neglected.

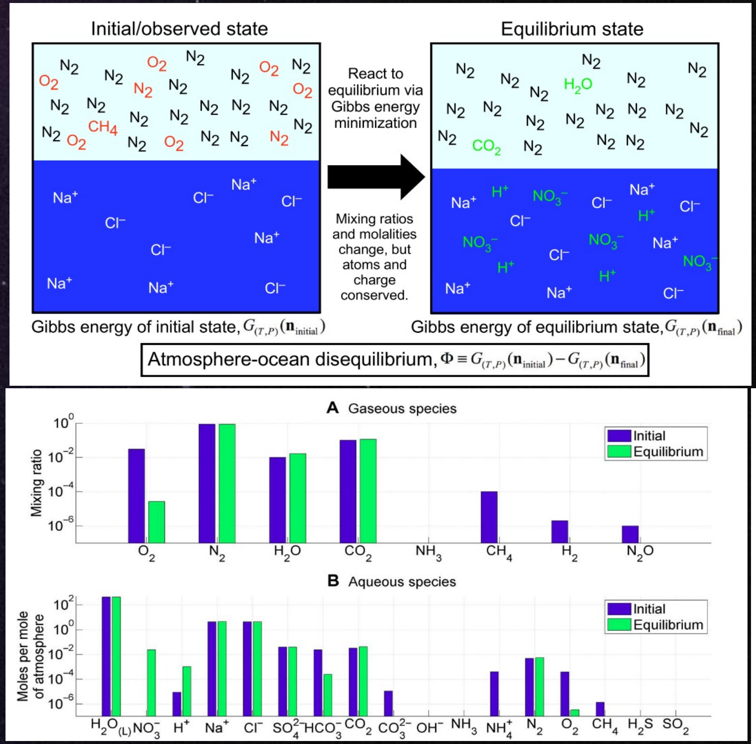




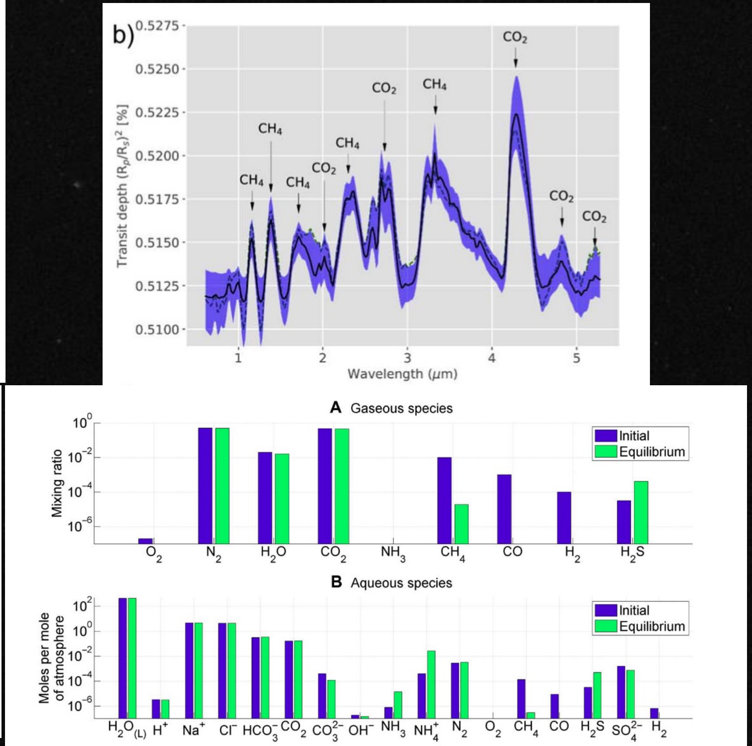


Searching for Life via Thermodynamic Disequilibria

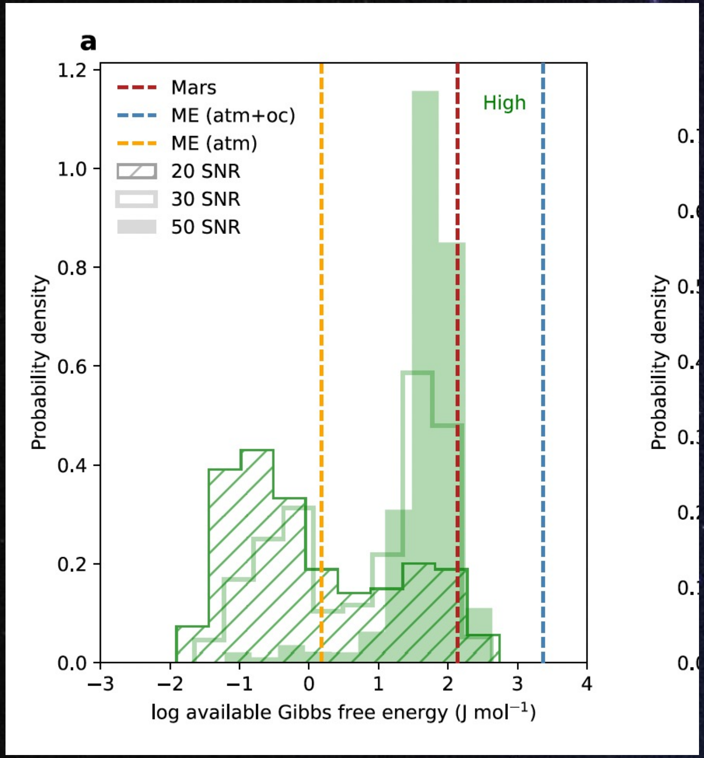
Modern Earth



Archean Earth



Proterozoic Earth (Young+2023)



Retrievals of atmospheric thermodynamic disequilibria ($\sum\Delta G$) have been demonstrated for Modern and Archean Earth (Krissansen-Totton+2016,2018a,b) and Proterozoic Earth (Young+2023,NatAstro,accepted)

Kinetic vs. Thermodynamic Disequilibria

$$CH_4 + 2O_2 \rightleftharpoons CO_2 + 2H_2O$$

$$\Delta G^0_{\mathrm{reaction}} = \sum G^0_{\mathrm{products}} - \sum G^0_{\mathrm{reactants}}$$

$$= \Delta G^0_{\mathrm{reaction}}/5.708 = (-(-817.9)/5.708) = +143.3$$

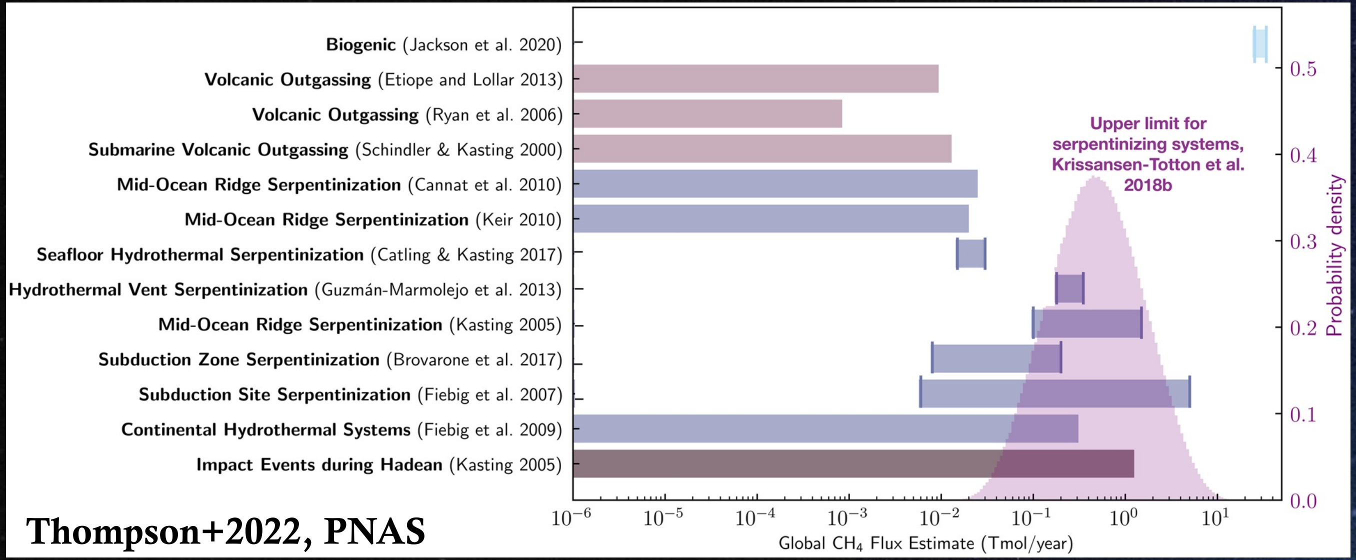
$$K_{eq} \approx \frac{p_{CO2}\, p_{H2O}}{p_{CH4}\, p_{O2}^2}$$

$$p_{\mathrm{CH4}} \sim \frac{(p_{\mathrm{CO2}})(a_{\mathrm{H2O}})}{(p_{\mathrm{O2}})^2 K_{eq}} = \frac{380 \times 10^{-6} \times 1}{(0.21)^2 \times 10^{143.29}} = 10^{-145}\ \mathrm{bar}$$

$$CH_4 + 2O_2 \rightleftharpoons CO_2 + 2H_2O$$

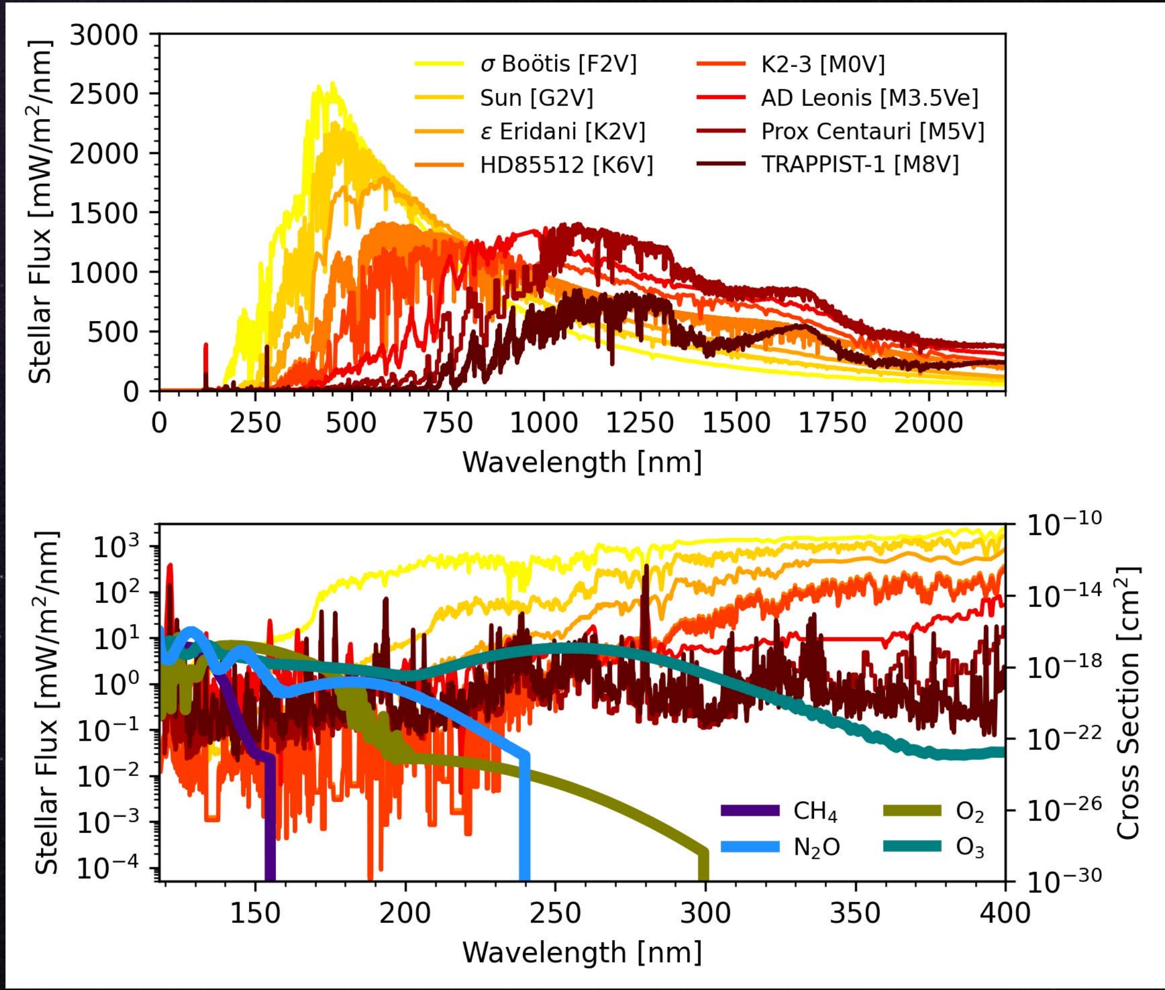
$$OH + CH_4 \rightarrow CH_3 + H_2O$$

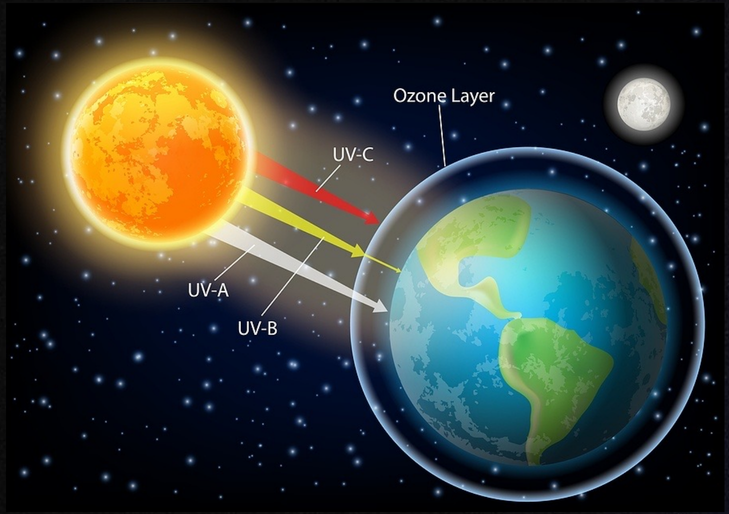
$$\tau_{\mathrm{CH4}} = \frac{n_{\mathrm{CH4}}}{\mathrm{destruction\ rate}} = \frac{\cancel{n}_{\mathrm{CH4}}}{k_{r\mathrm{CH4}}\, n_{\mathrm{OH}}\, \cancel{n}_{\mathrm{CH4}}} = \frac{1}{(3.6 \times 10^{-15}\mathrm{cm}^{-3}\ \mathrm{molec\ s}^{-1})(8 \times 10^5 \mathrm{cm}^{-3})} \sim 12\ \mathrm{years}$$

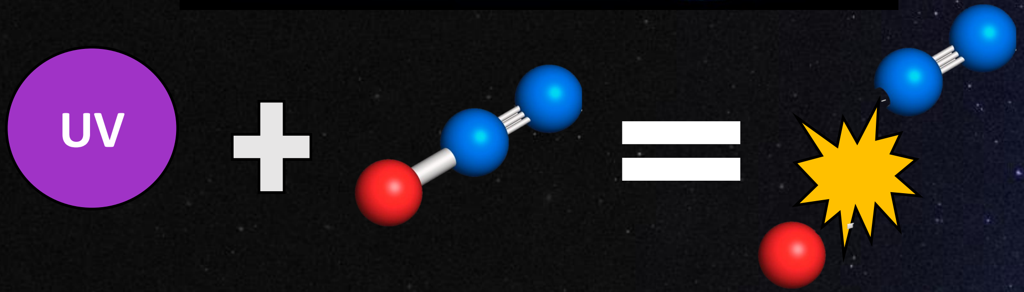


Thompson+2022, PNAS

Biosignature Flux-Abundance Relationship Vary Greatly by Star





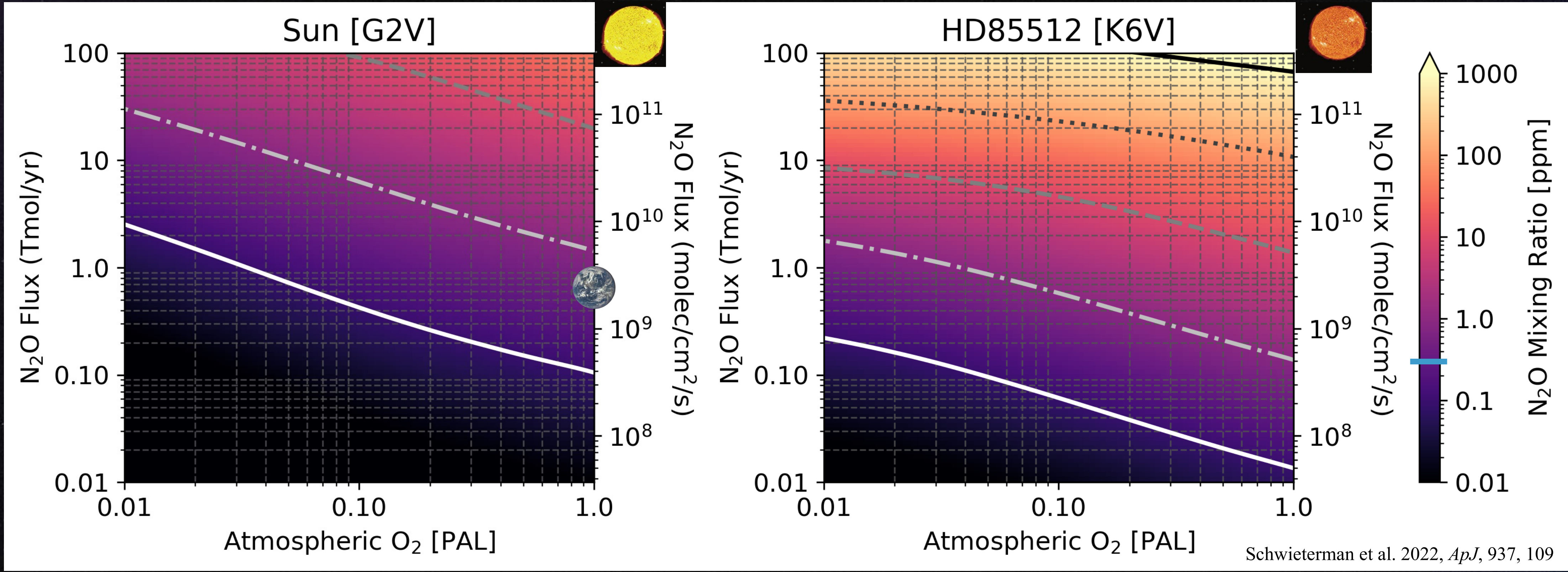


N_2O is destroyed by photochemical reactions

That rate will be different for other stars

How Much N_2O Can Accumulate in an Atmosphere? $f(pO_2, \phi_{N2O},$)

N$_2$O Produced



Schwieterman et al. 2022, *ApJ*, 937, 109

Oxygen in Atmosphere

Oxygen and Ozone can shield N_2O from photolysis (destructive UV photons)

The accumulation of N_2O is also controlled by the host star

“Equilibrium” vs. “Non-Equilibrium” Gases

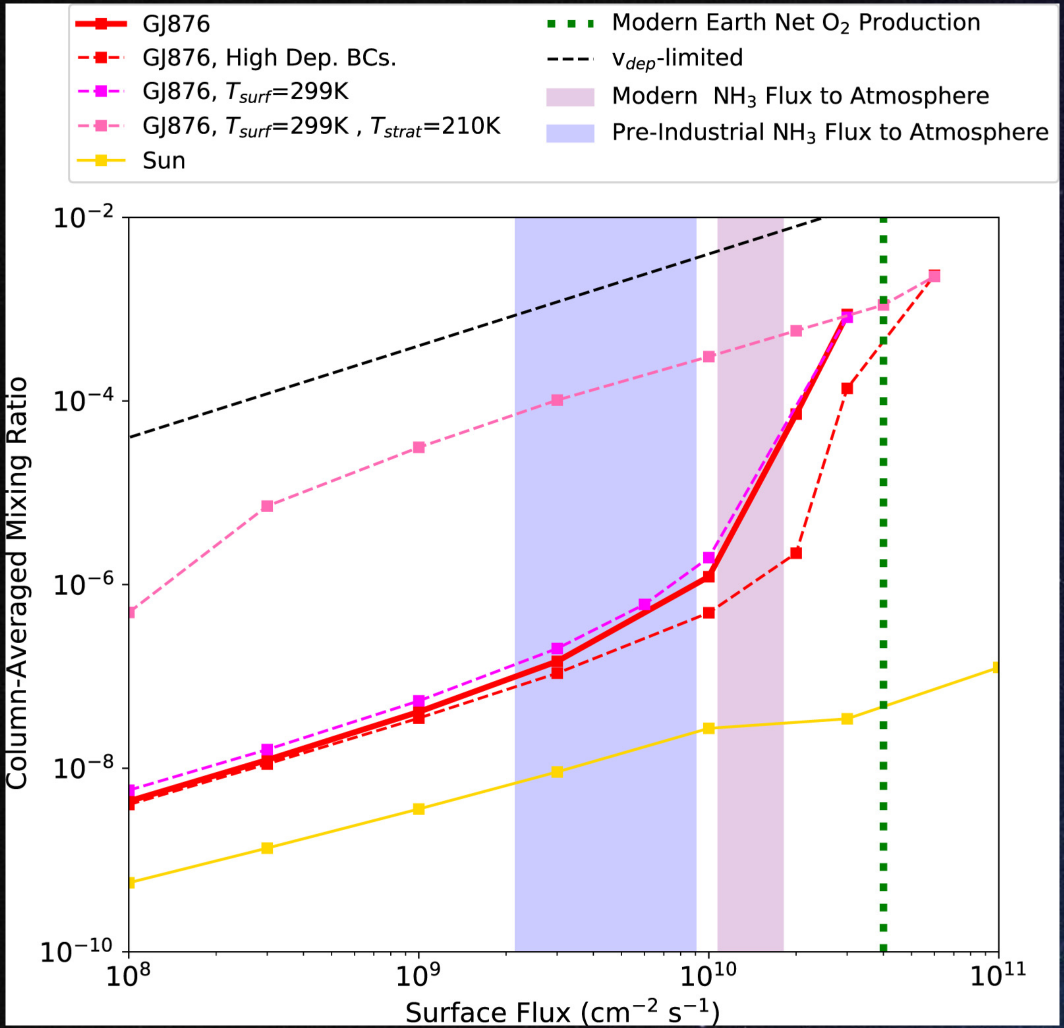
Gases formed at equilibrium in gas giant atmospheres (or via volcanism), but with strong kinetic disequilibrium in N_2-CO_2-[-O_2] or temperate H_2 Atmospheres, e.g., CH_4 (Thompson+2022), NH_3 (Philips+2021, Huang+2022), PH_3 (Sousa-Silva+2020).

Gases not formed via equilibrium (albeit with other abiotic sources), e.g., DMS/DMDS (Domagal-Goldman+2011), isoprene—C_5H_8 (Zhan+2021), halomethanes (Leung+2022; **see poster!**), N_2O (Schwieterman+2022).

In either case, can sometimes go into “runaway” upon depletion of sinks (and self-shielding).

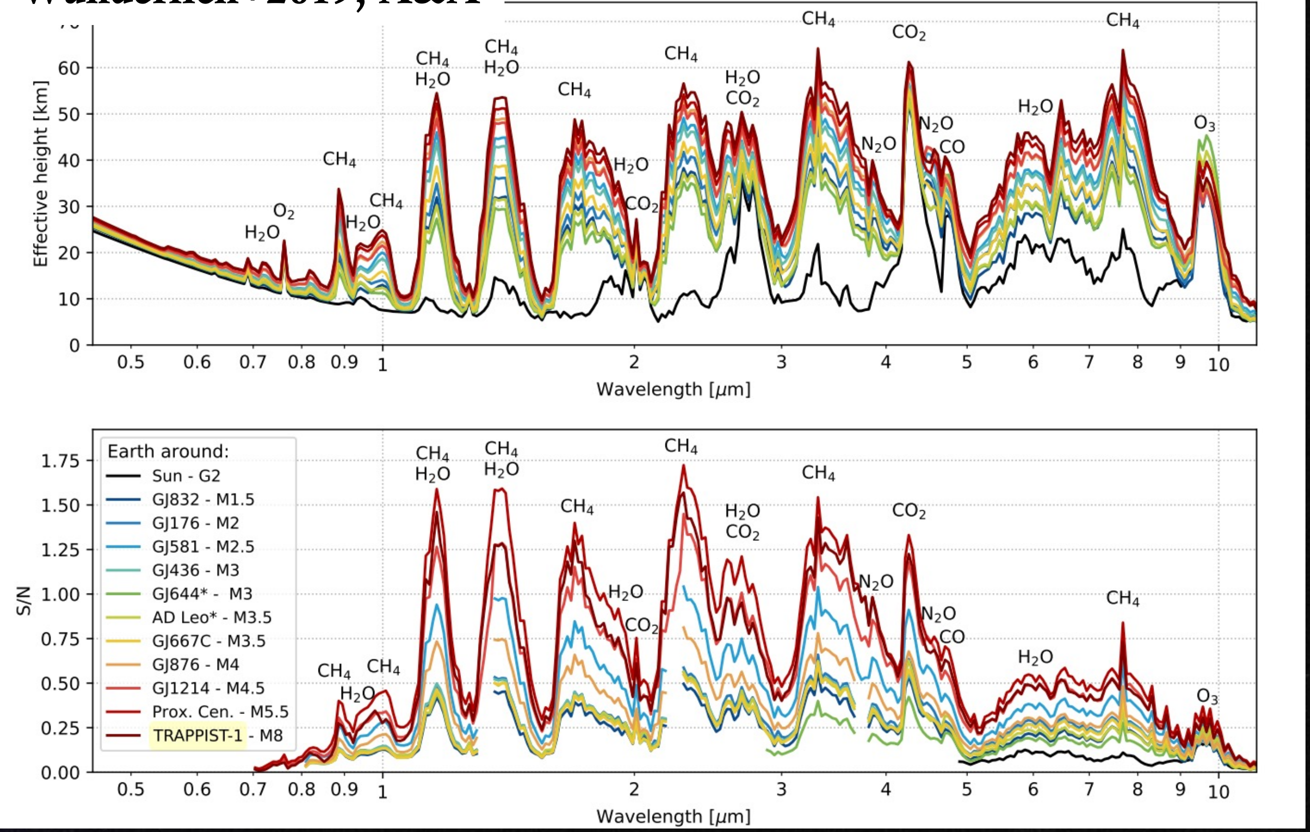
“Photochemical Runaway”

(Ranjan+2022, AJ, 930:131)

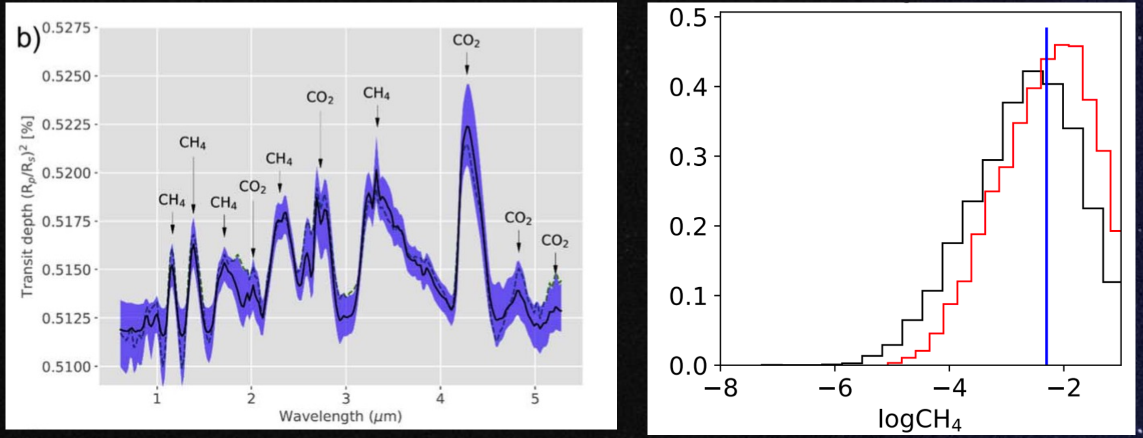


The TRAPPIST-1 System as the Best Immediate Future (JWST) Target*

Wunderlich+2019, A&A



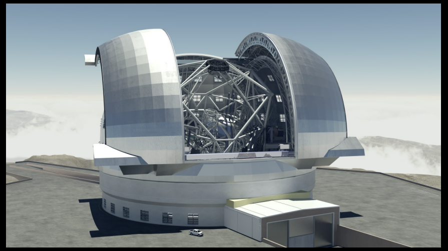
Also see Pidhorodetska+2020; Linkcowski+2018; Lustig-Yaeger+2019 *Caveats about having an atm!

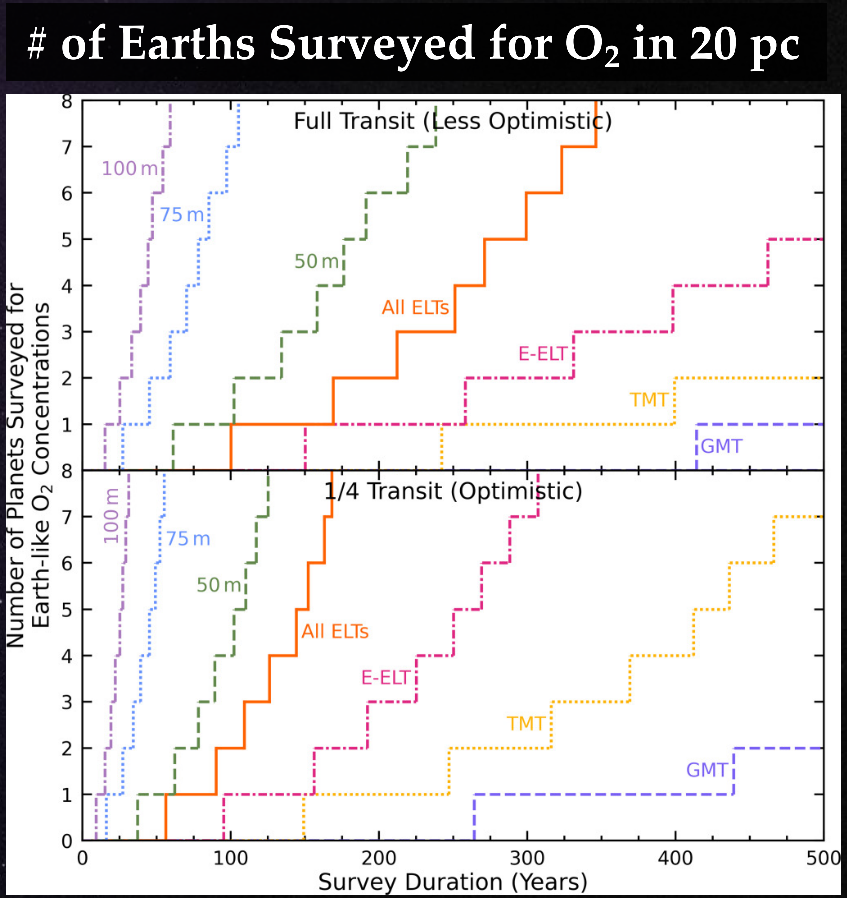


Krissansen-Totton+2018, AJ

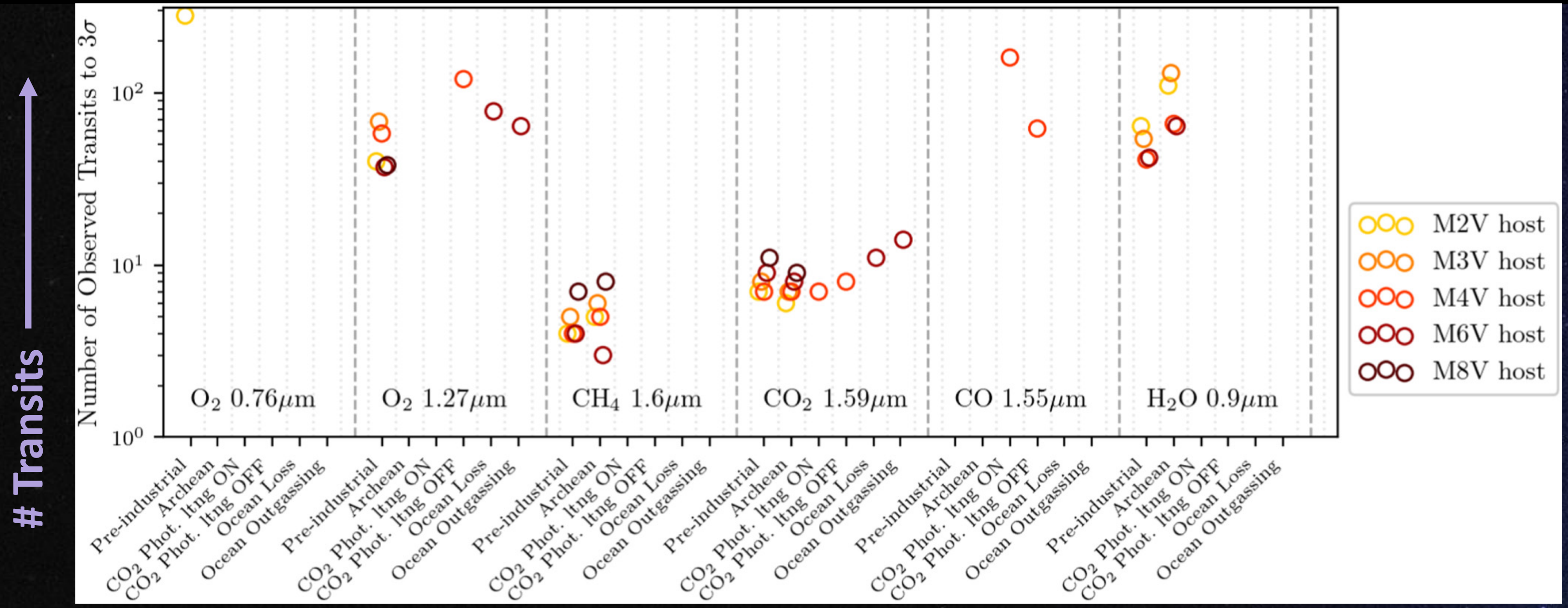
O_2 and O_3 are not likely detectable on TRAPPIST-1e for biotic (non-post-runaway) scenarios. However, CH_4+CO_2 disequilibrium could be detected due in part to longer CH_4 photochemical lifetimes (left). For some plausible biogeochemical scenarios, N_2O may also be detectable (Schwieterman+2022).

Ground-Based Search: Challenges and Opportunities





Hardegree-Ullman+2023, AJ, 165:267



Currie+2023, PSJ, 4:83

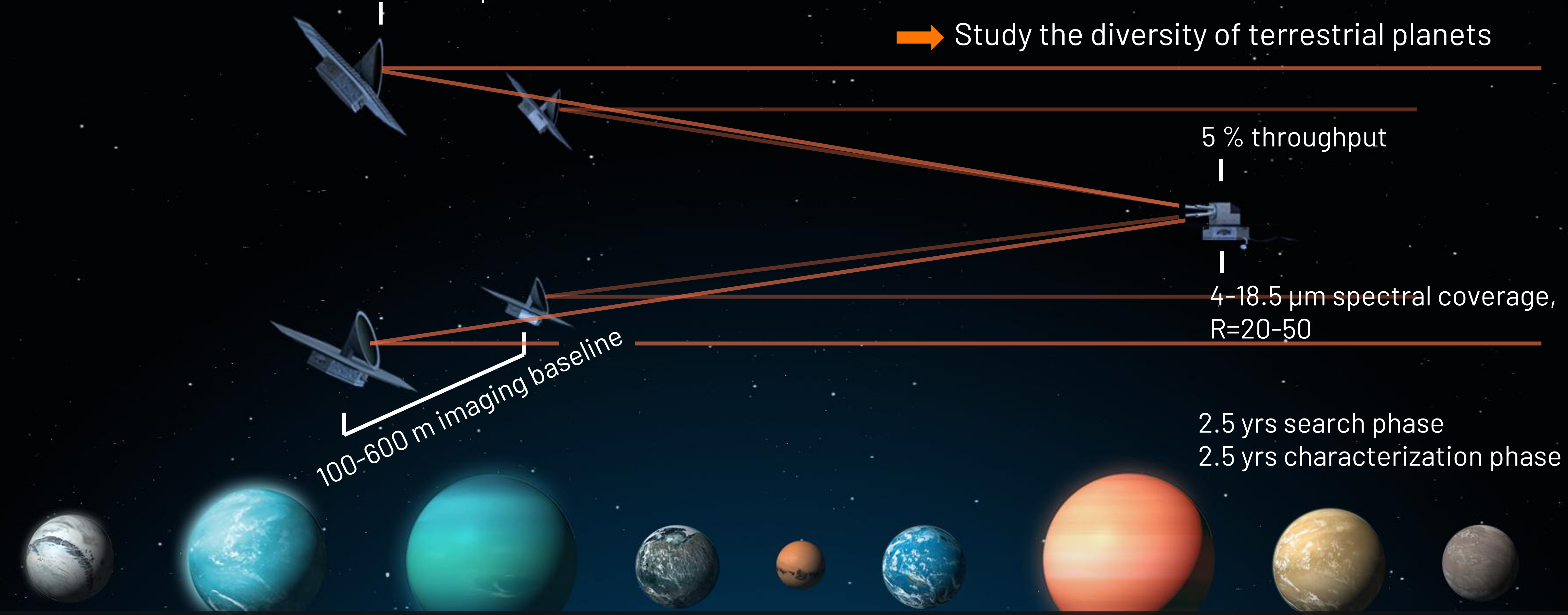
O_2 (0.76, 1.27 μm) is probably very difficult to detect via transit from the ground (even for TRAPPIST-1). However, CH_4 (1.6 μm) and CO_2 (1.59 μm) are far more detectable, and ground-based observations could be synergistic with future space-based surveys. Such efforts should start well before launch.

LIFE

LARGE INTERFEROMETER FOR EXOPLANETS

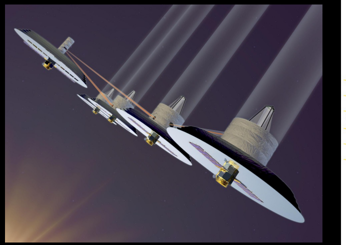
Goals:

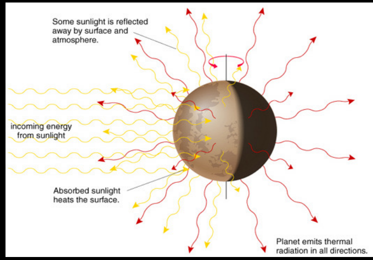
- Assess habitability
- Search for biosignatures
- Study the diversity of terrestrial planets

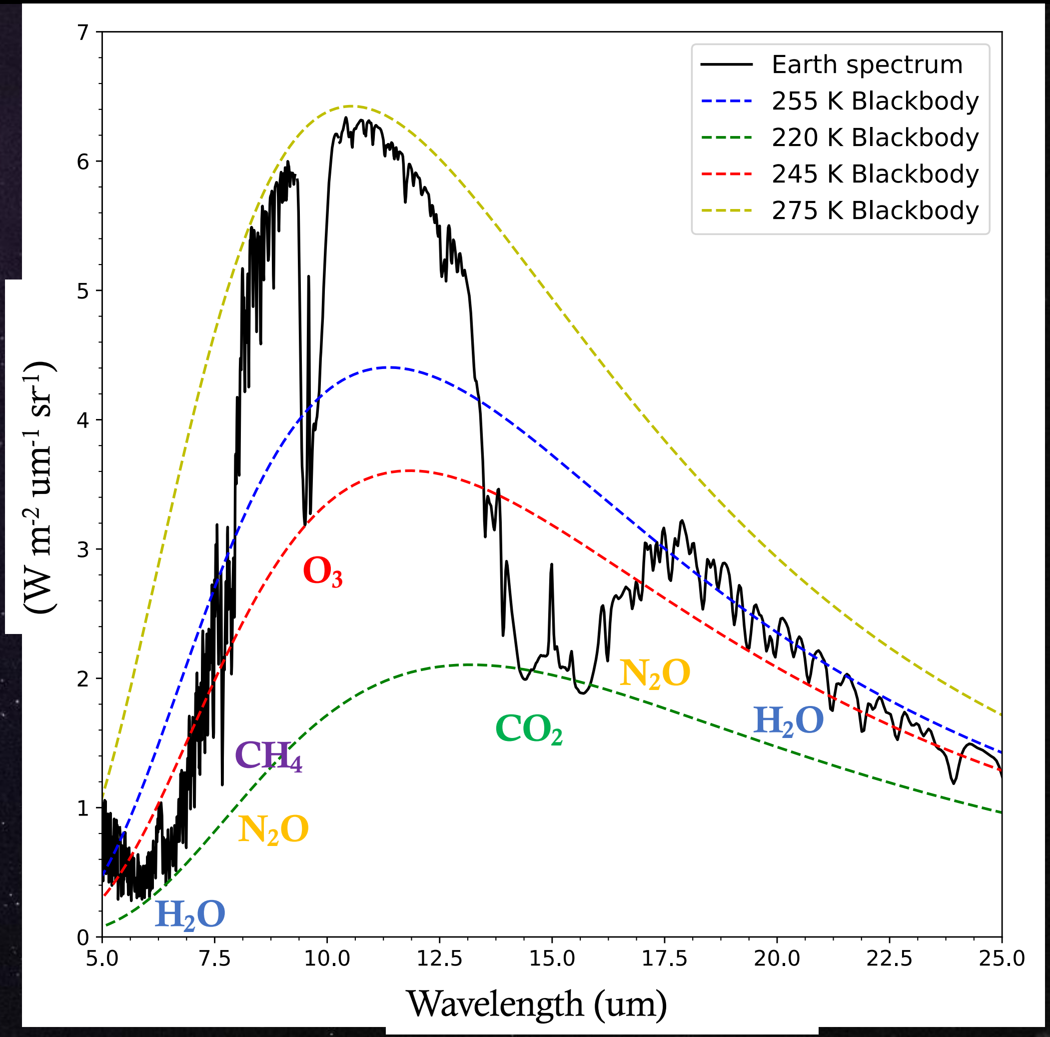


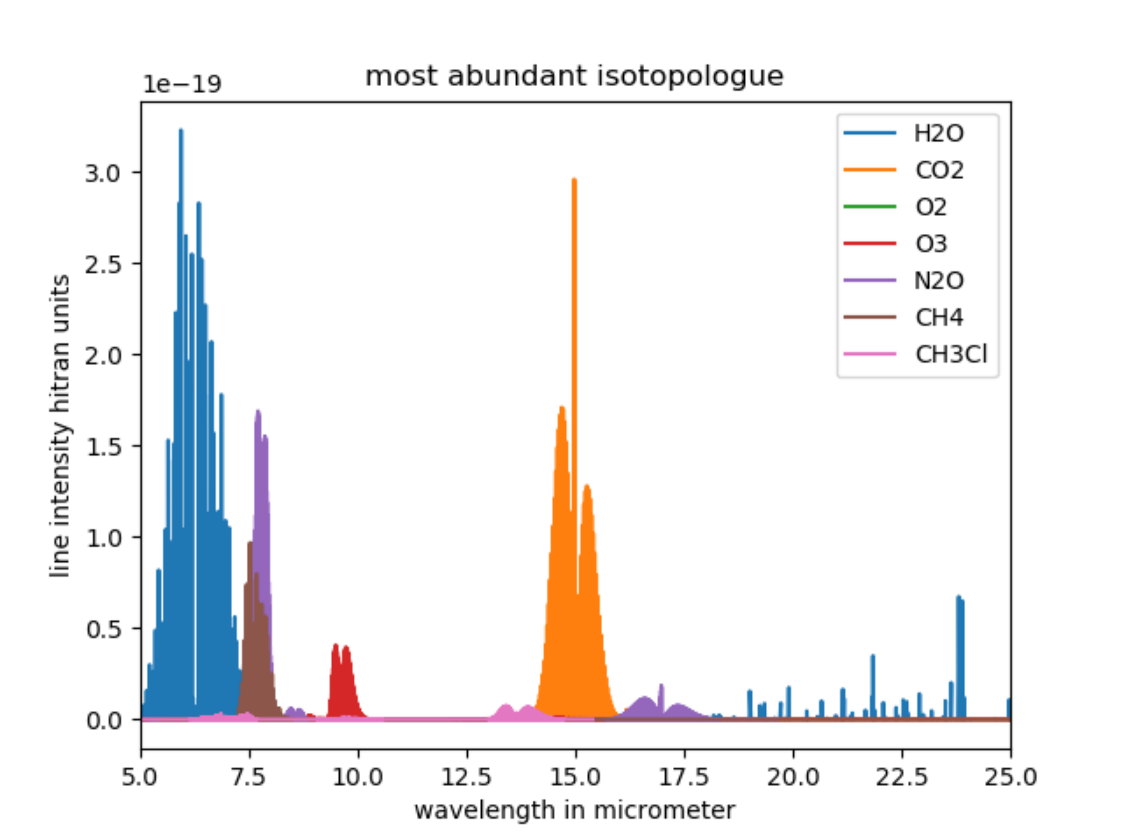
See LIFE paper series (e.g., Quanz+2022, Alei+2022): https://life-space-mission.com/

Mid-IR Earth Emission Spectra | Revealed by LIFE?



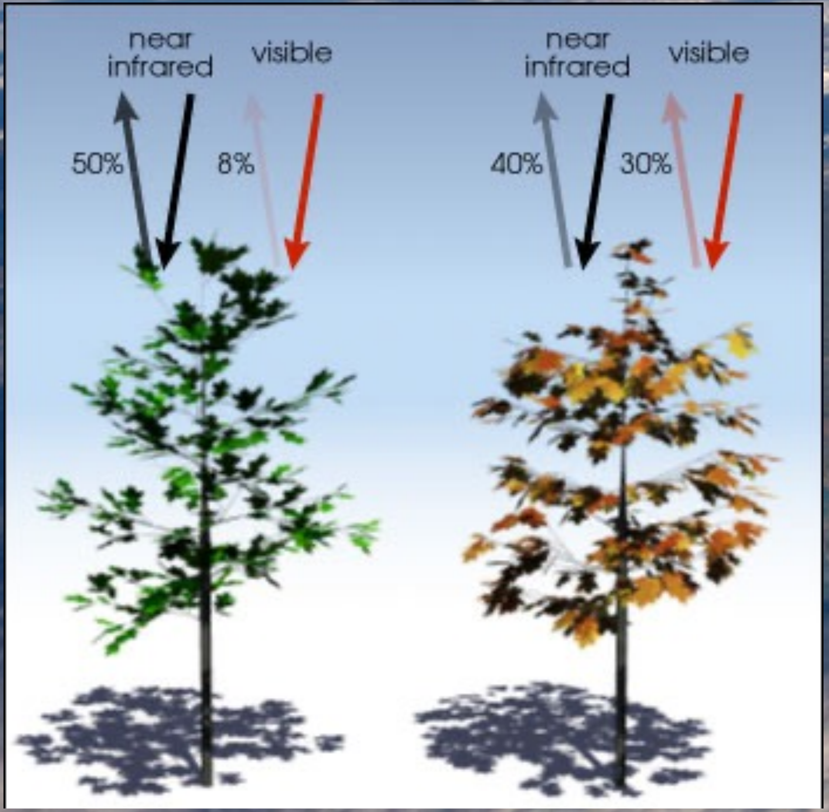




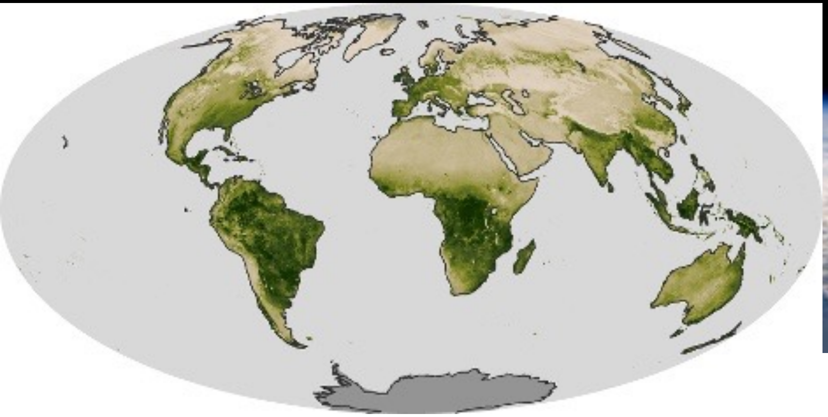


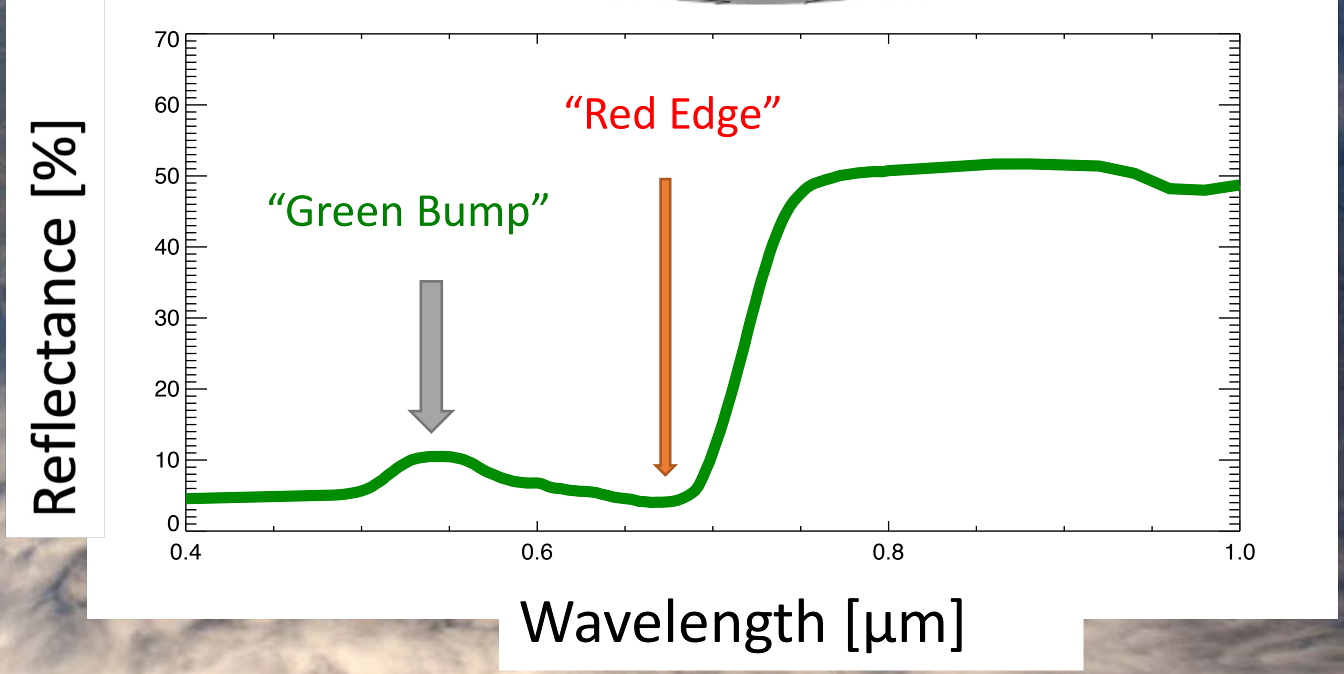
Mid-IR spectra reveal gases and planetary parameters "invisible" in reflected light.

Surface Biosignature: Vegetation "Red Edge"

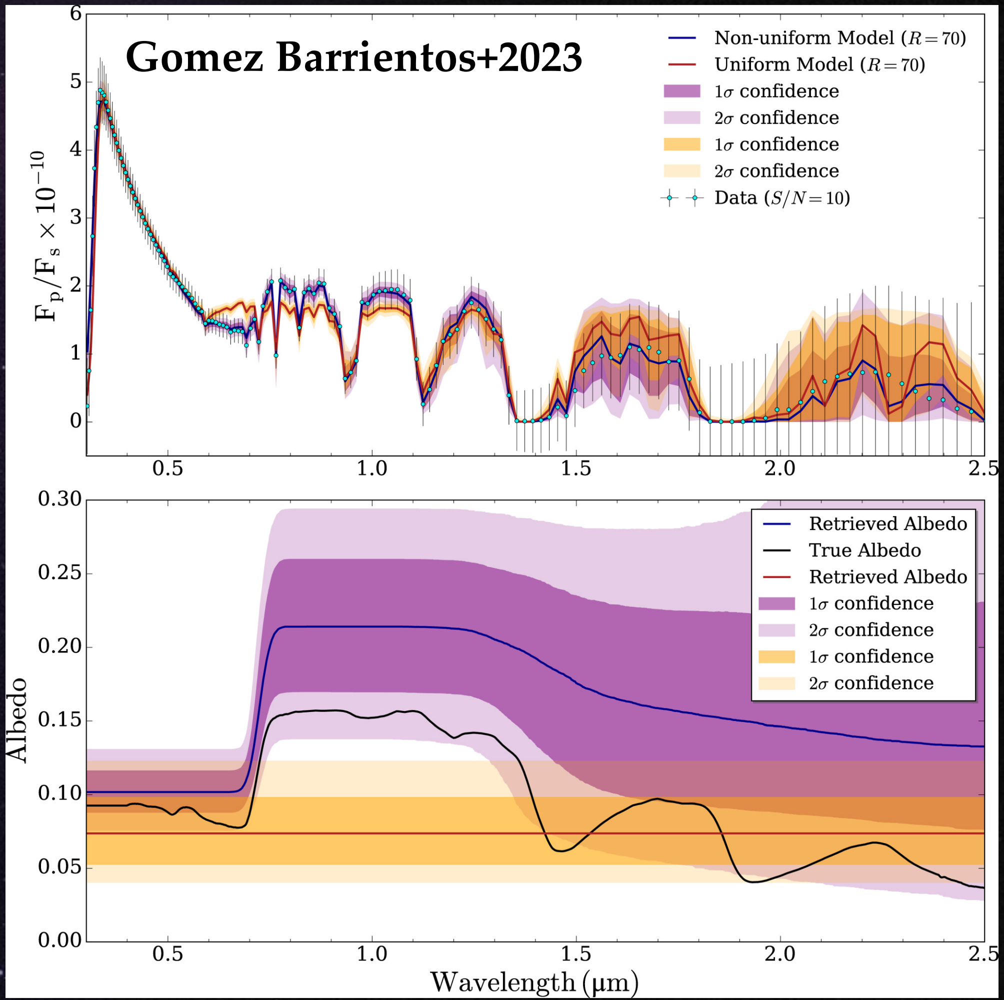


NASA Earth Observatory

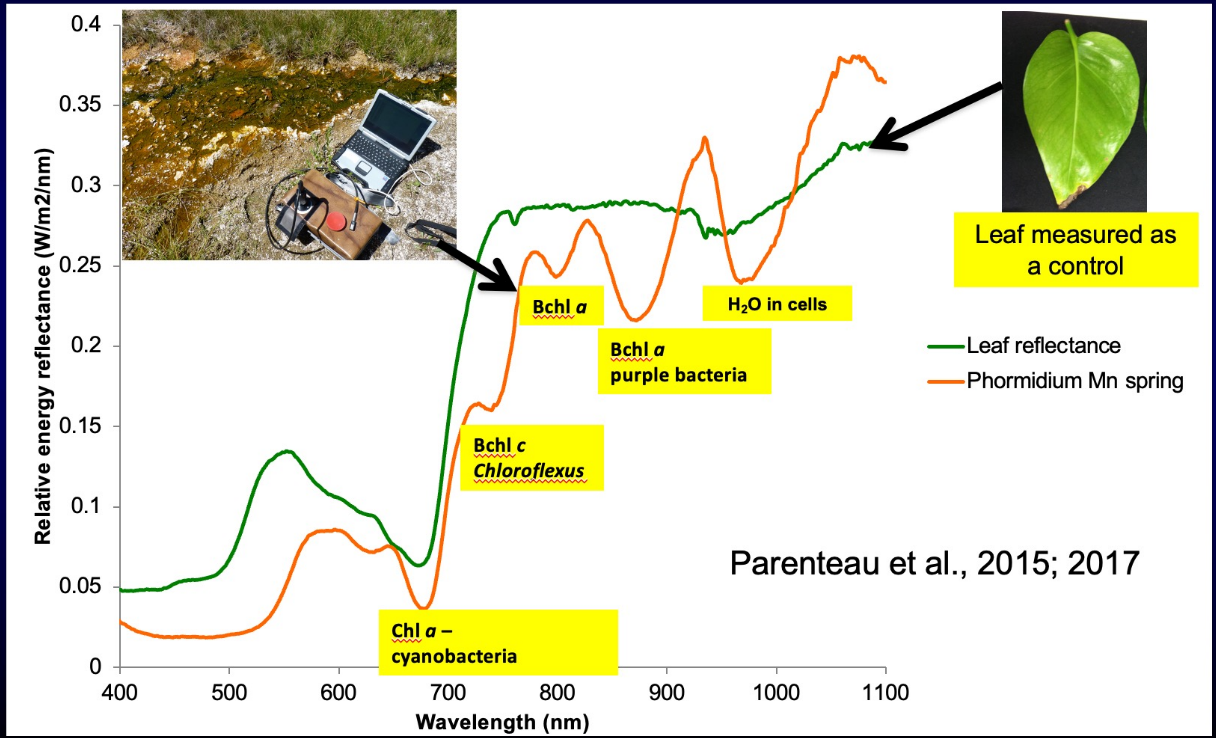




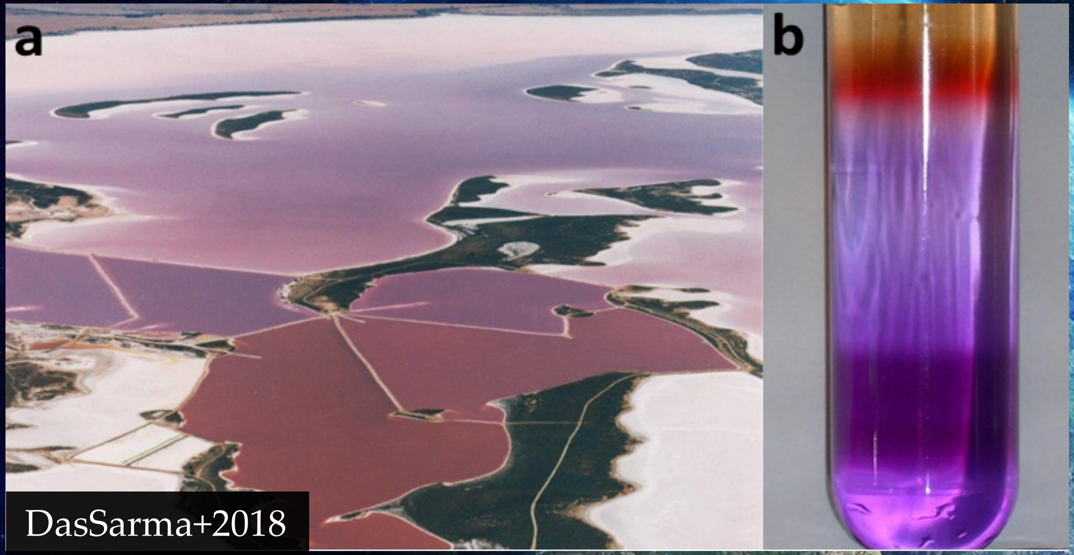
Surface Biosignatures in Reflected Light—Spectral "Edges"



- The reflectance features of bacteriochlorophyll pigments in anoxygenic phototrophs and microbial mats yield "NIR edges"
- The pigments in all underlayers of the mat are visible
- These "NIR edges" are as strong as the "vegetation red edge"

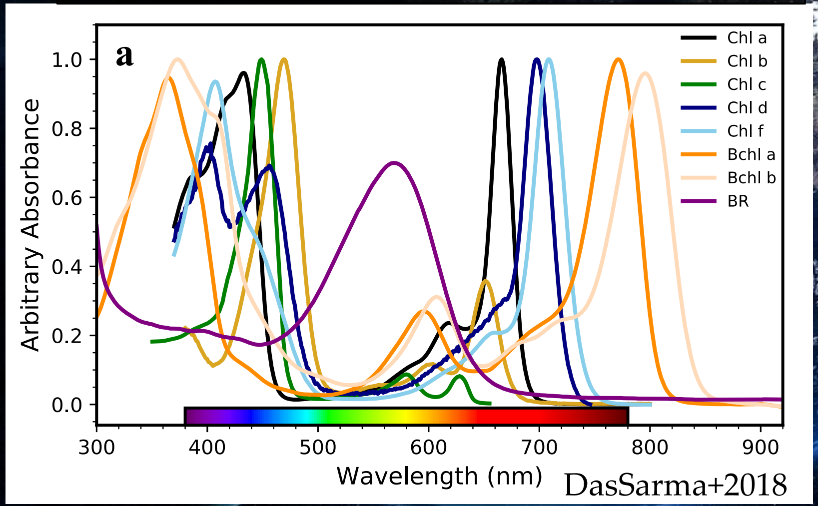


Halophiles: Rhodopsin & Carotenoids



Bacteriochlorophylls and Carotenoids

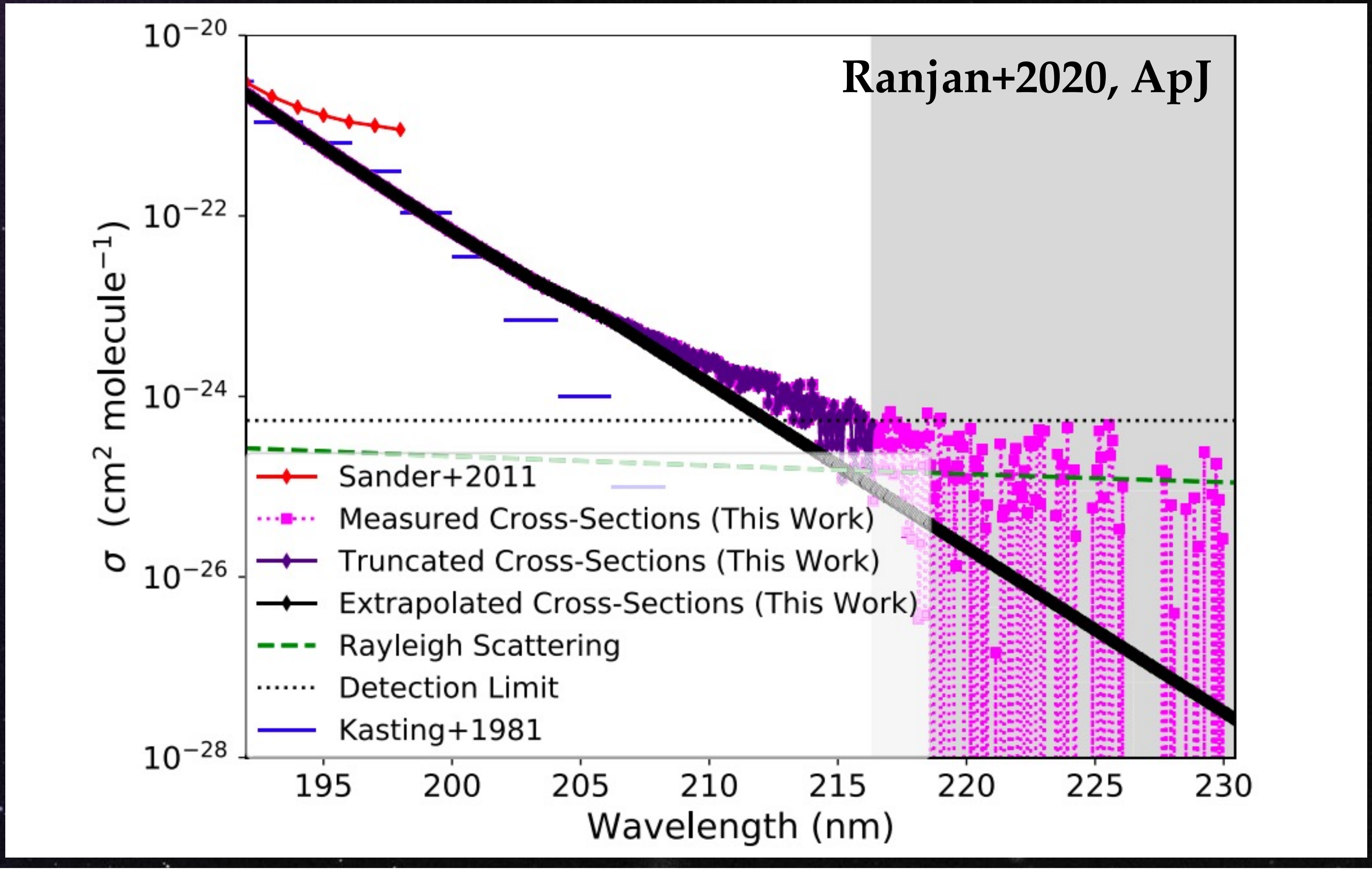
Complementary Absorption



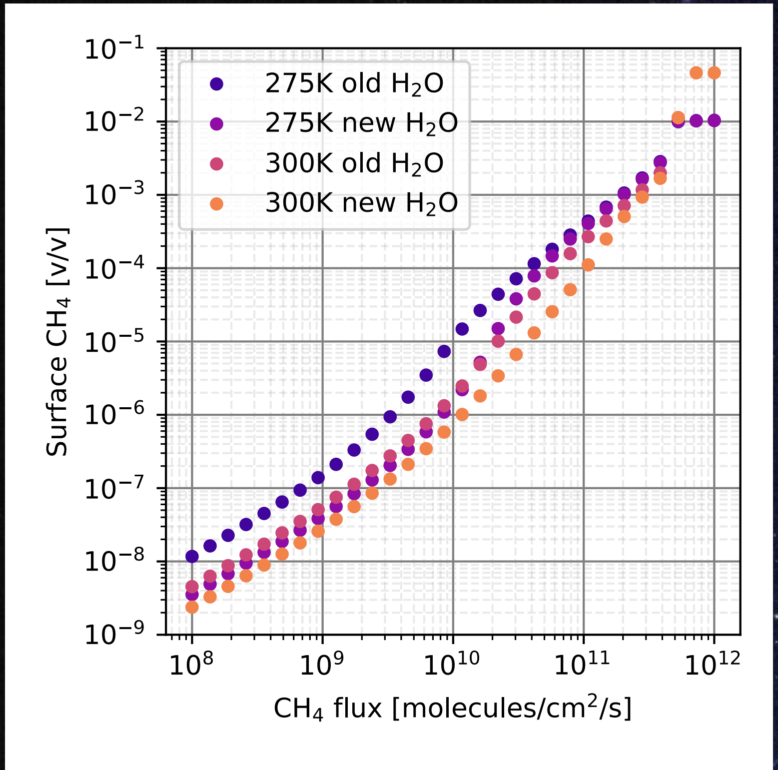
San Francisco Salt Ponds

Basic Model Inputs Still Need to Be Refined—Lab Data Needed!

Importance of updated H_2O cross-sections for analyzing O_2-False Positives



Important for CH_4 flux-abundance!



Broussard et al. in prep.—Impacts of H_2O & CO_2 NUV cutoffs.

Methylation as a Generalized Exoplanet Biosignature?

"Capstone Biosignatures" [Lab Measurements Needed!]

See, e.g., Leung+2022(ApJ)

Methylated Halogens

- CH_3Cl
- CH_2Cl_2
- $CHCl_3$
- CCl_4
- CH_3Br
- $CHBr_3$
- CBr_4
- CH_2BrCl
- $CHBr_2Cl$
- CH_3I
- CH_2I_2
- CHI_3
- $(CH_3)_2CHI$
- CH_2IBr
- $CHIBr_2$

Methylated Chalcogens

- $(CH_3)_2S$
- $(CH_3)_2S_2$
- CH_3SH
- $(CH_3)_2Se$
- $(CH_3)_2Se_2$
- CH_3SeS
- $(CH_3)_2SeS$
- CH_3SeH
- $(CH_3)_2Te$
- $(CH_3)_2Te_2$

Methylated Metal(loids)

- $(CH_3)_3As$
- $(CH_3)_2AsOH$
- $(CH_3)_3Sb$
- $(CH_3)_3Bi$
- $(CH_3)_2Hg$

Widely distributed in nature: Produced by algae, bacteria, archaea, plants, fungi, etc.

Most of these organisms are *not* making methane!

Opacity data is incomplete for most of these gases—*especially* near-IR (1-2 μm) opacities.

Can Planetary Chemical Network Topologies Suggest Life?

Toward Network-Based Planetary Biosignatures: Atmospheric Chemistry as Unipartite, Unweighted, Undirected Networks

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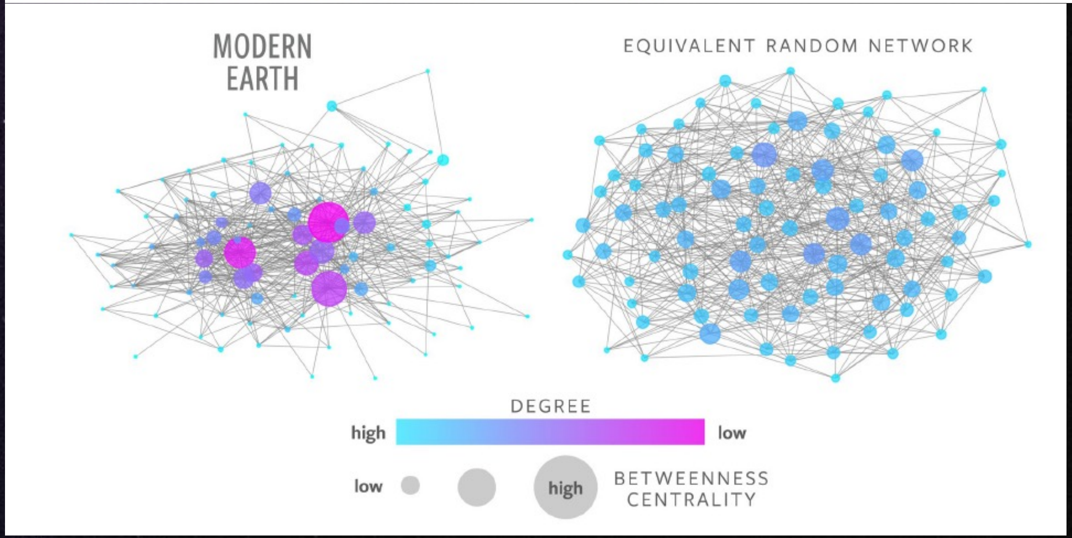
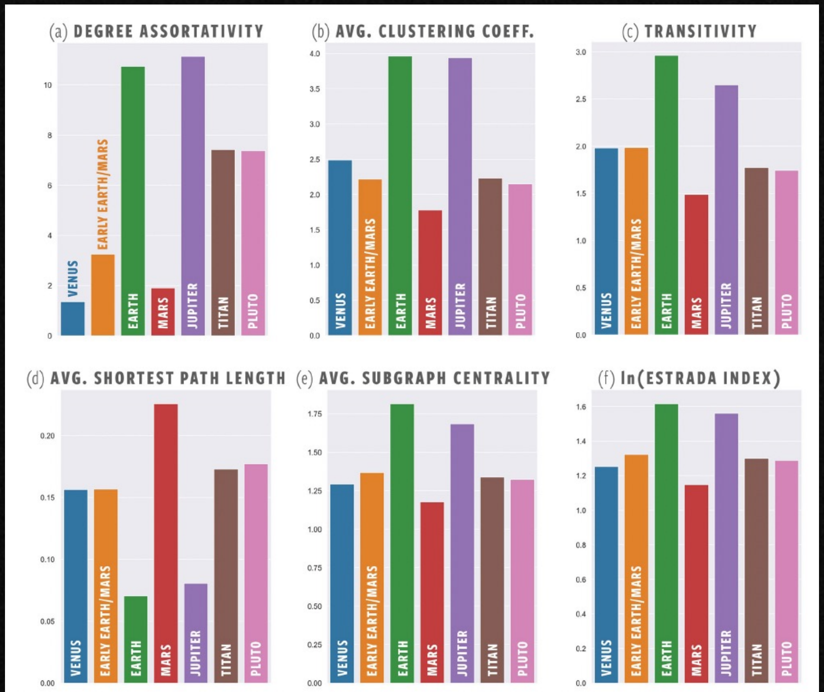
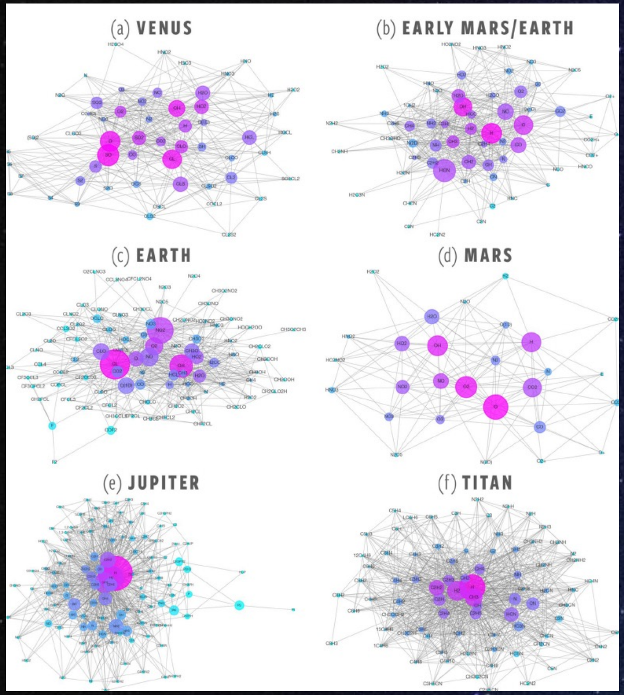
[1]Earth & Planets Laboratory, Carnegie Institution for Science, Washington, DC, USA, [2]NHFP Sagan Fellow, NASA Hubble Fellowship Program, Space Telescope Science Institute, Baltimore, MD, USA





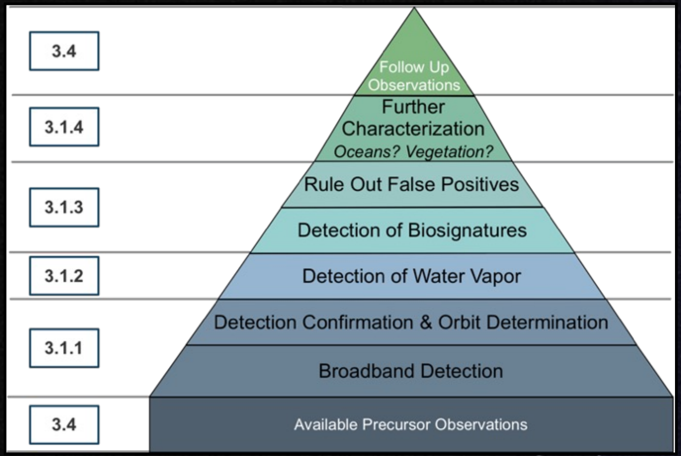


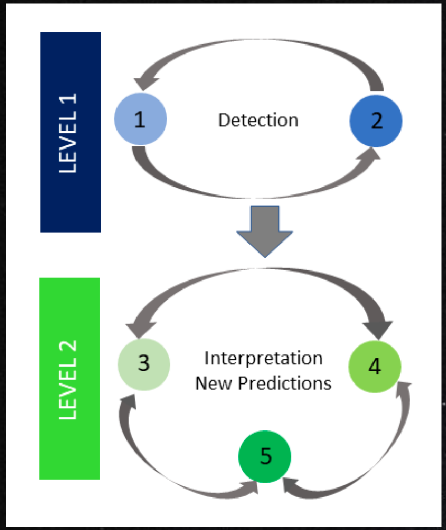
See Mike's Poster!

Earth's reaction network topology can be distinguished from solar system atmospheres via a variety of metrics (Wong+2023, JGRP). Conceivably, with rich observational information, such metrics may be developed to support biosignature interpretations on exoplanets. See also Fisher+2022 (AJ,164:53)—demonstrating this method for hot Jupiters.

Summary & Final Thoughts

- Biosignature detectability will depend on many factors including observing mode, wavelength range, resolving power, S/N, etc.
- Best chance for (tentative) biosignature in term term is via transit, e.g., TRAPPIST-1 system (if we're very lucky…)
- Habitable Worlds Observatory opens first chance for real "biosignature survey"—can find O_2!
- Context is critical—maximal wavelength range and multiple observing modes are key. Something like "standards of evidence" needed.
- Confirming life will likely require in-depth characterization—A series of discoveries (but we could get lucky).
- Still a lot to do in lab & with modeling!





Above: HabEx Report; **Left:** Biosignature Standards of Evidence Community Workshop Report.

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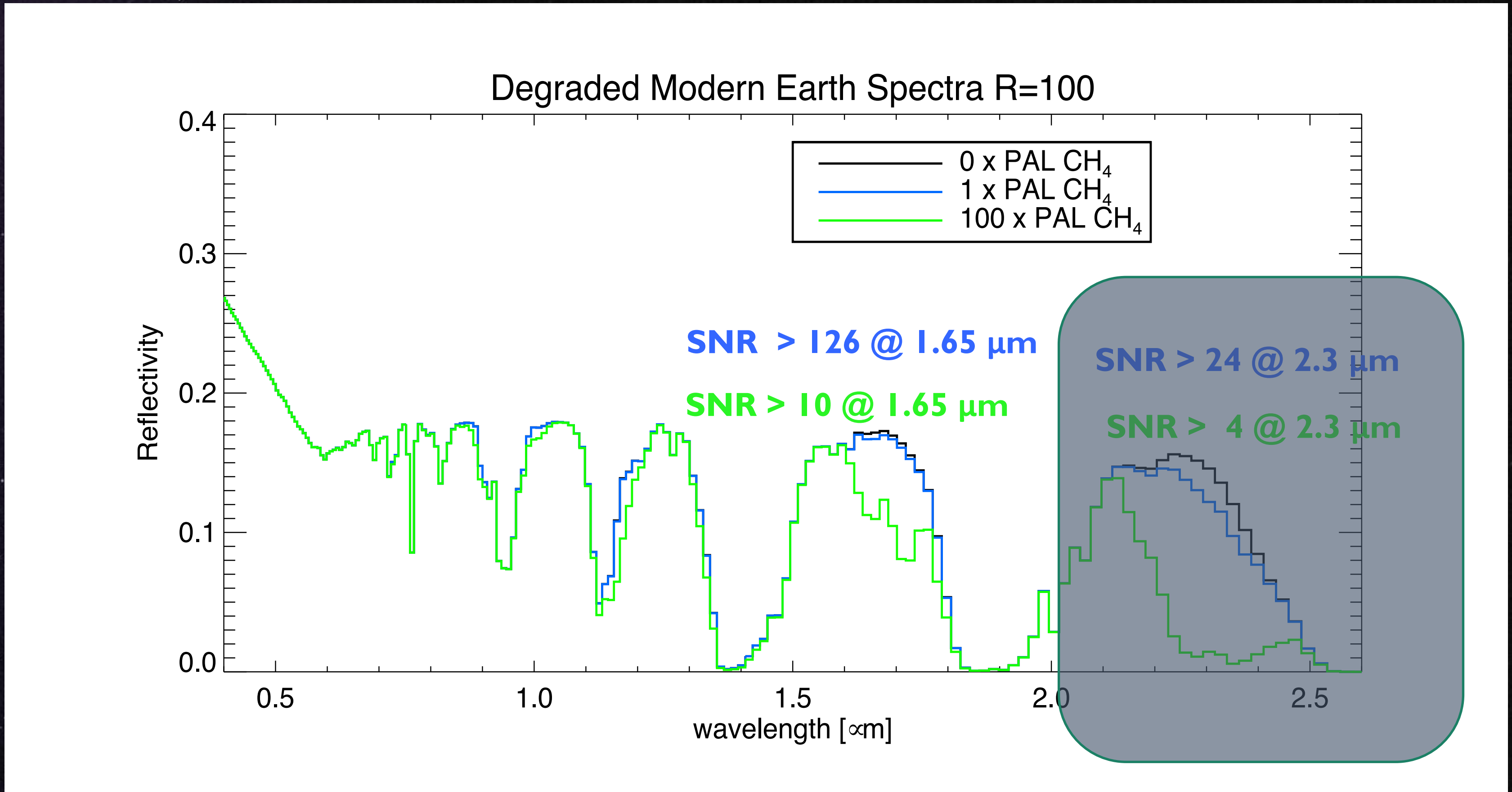
Backup Slides

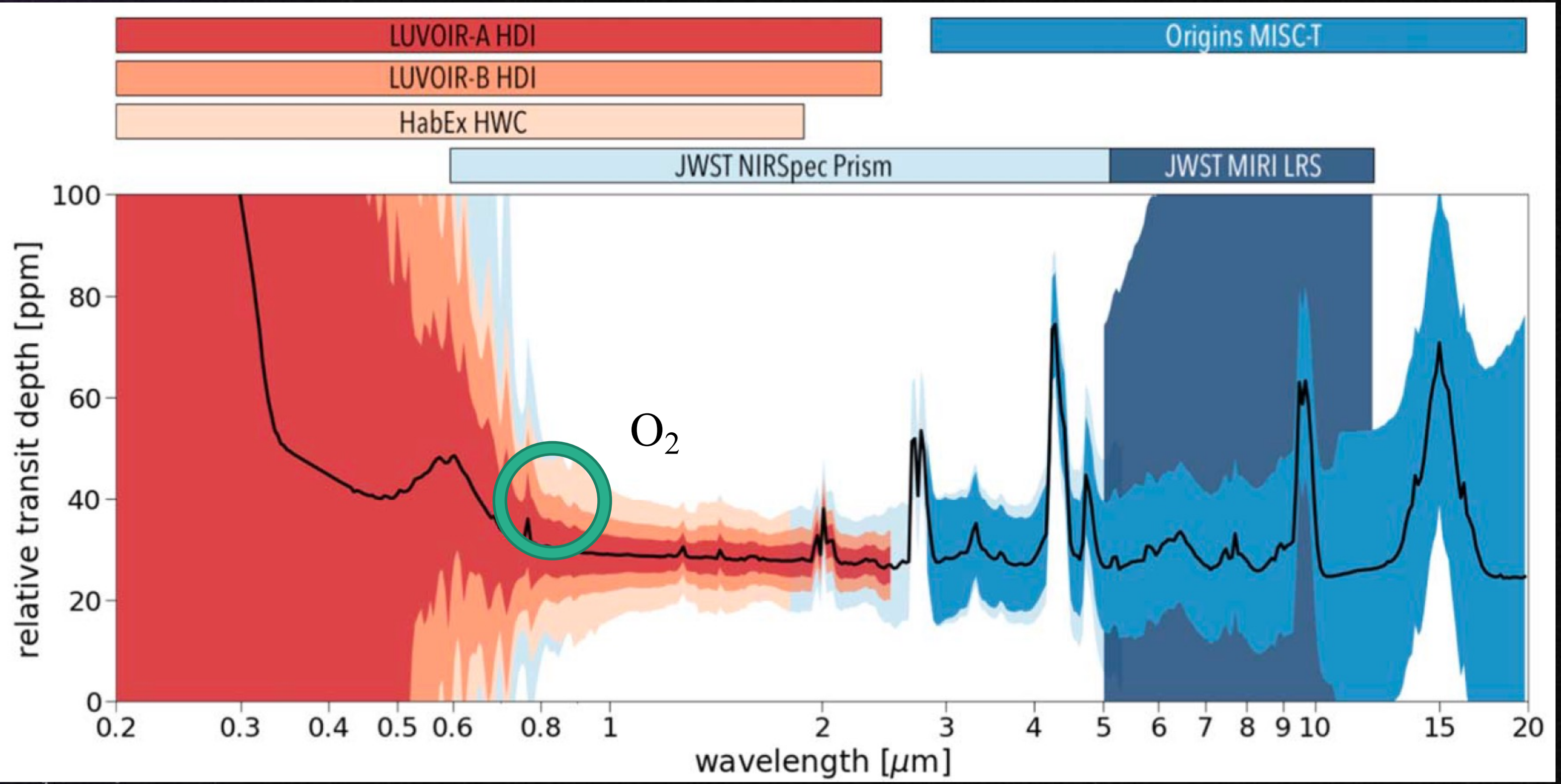
Methane Would Be Hard to Find on a Modern Earth Twin



Modern levels of CH_4 (PAL; 1.8 ppmv) are too low to produce observable features at the 1.69 µm band, likely the strongest band available to HWO. However, higher levels of CH_4 would be detectable, as have existed early in Earth history.

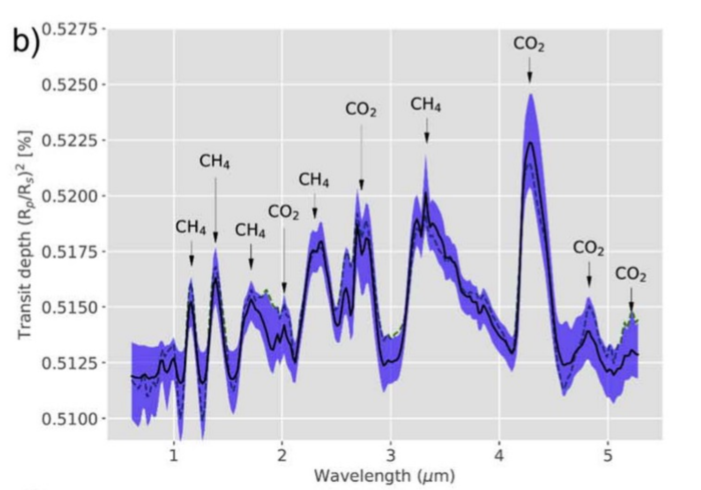
Earth-like O_2 Difficult to see in Transmission

TRAPPIST-1e Simulation



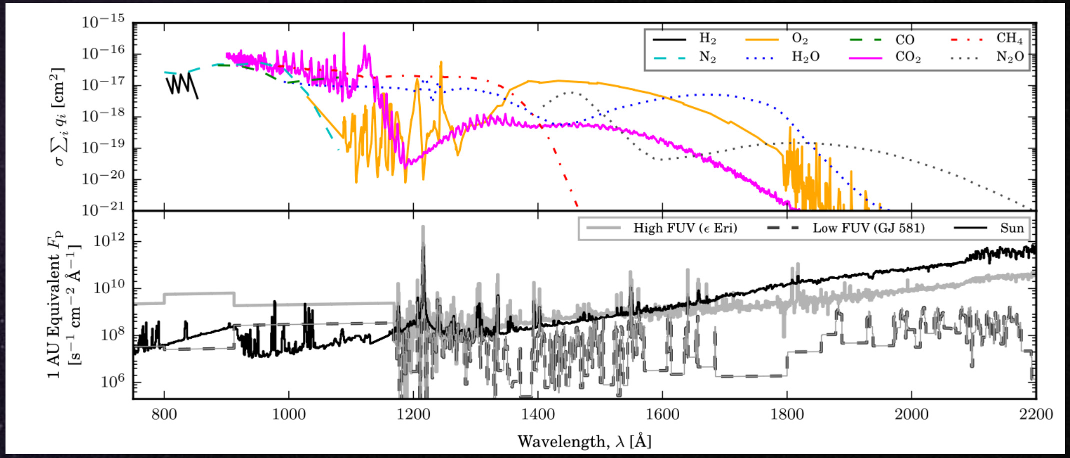
Pidhorodetska, Fauchez+2020, ApJL, 898:L33

Due to the narrowness of the band and relatively small transit depth, the O_2 molecule would not be detectable with JWST or OST. However, CH_4 is within reach for Earth-like production rates.



Krissansen-Totton+2018, AJ

Importance of Stellar Context: Impact on Flux/Abundance



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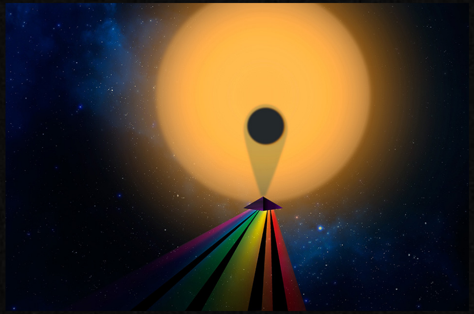
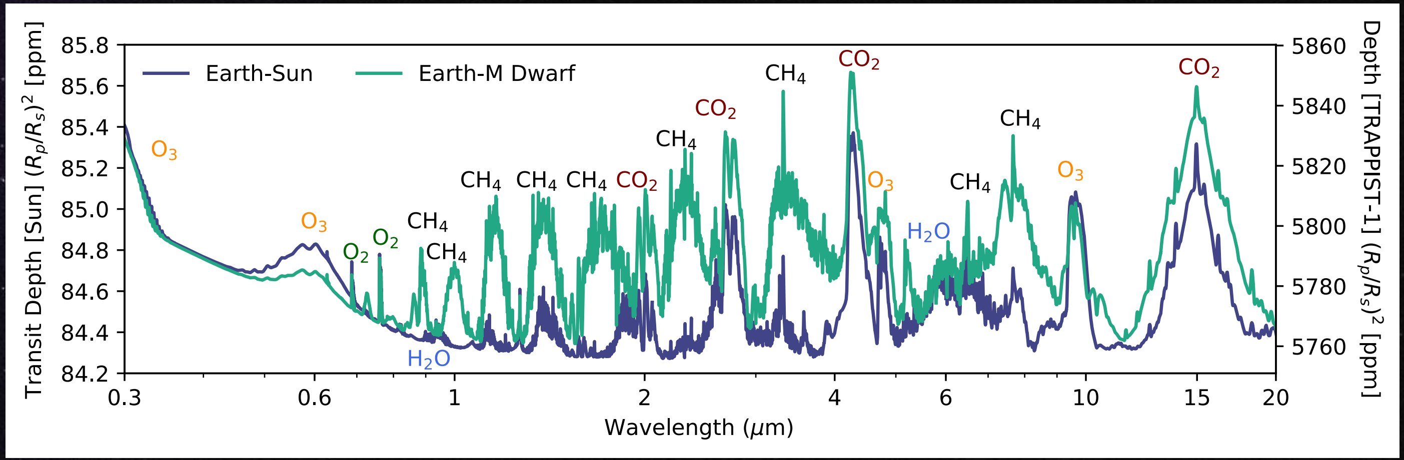


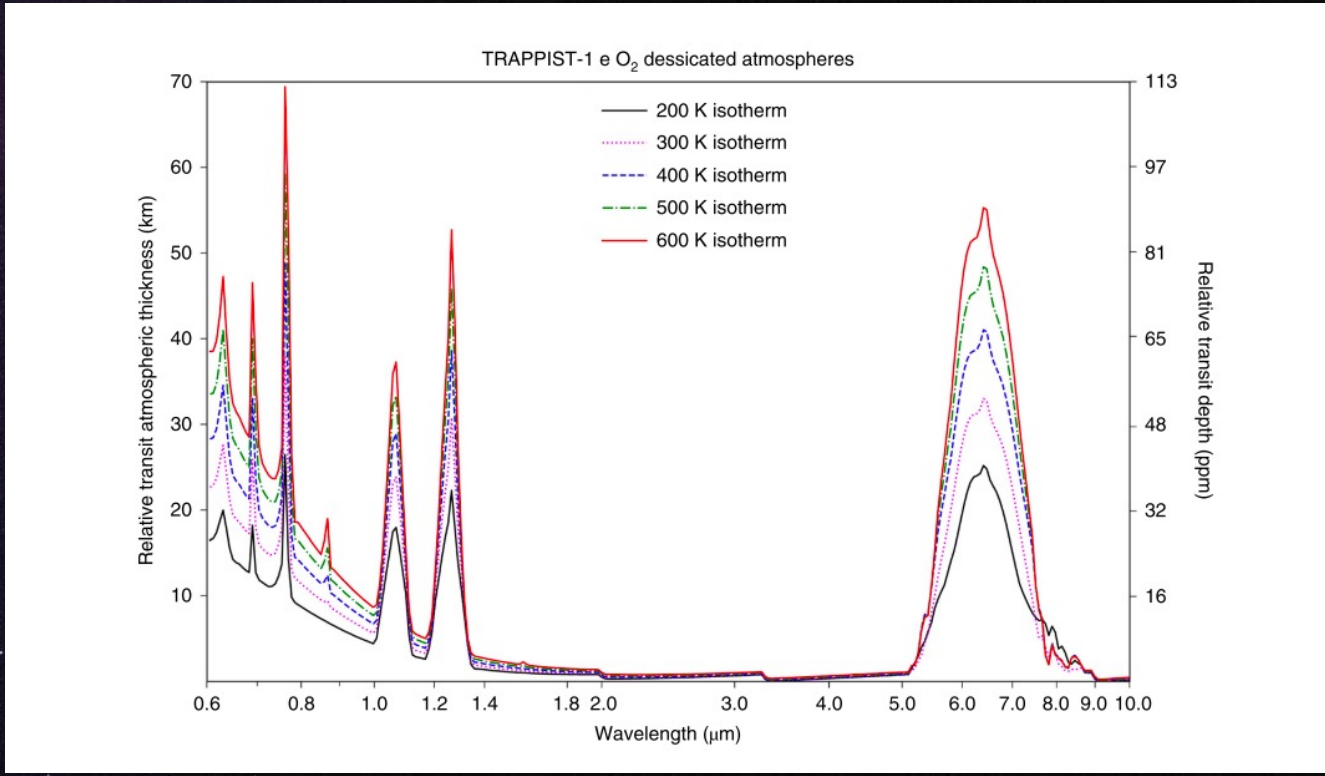


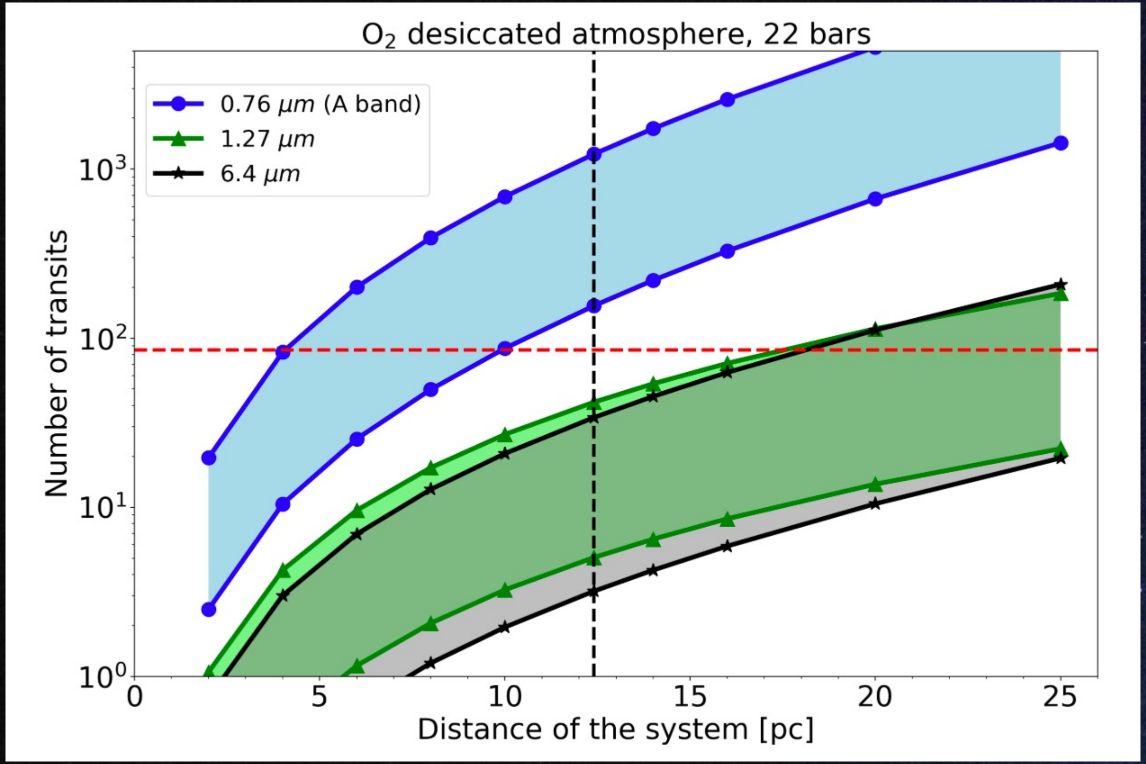
Meadows, et al., 2018, Astrobiology, Also see Lustig-Yeager+2019

Differences in stellar UV spectra can enhance or reduce the atmospheric lifetime of biosignature gases given the same surface flux (production rate).

This plot demonstrates the drastic increase in CH_4 detectability on an M dwarf planet for the same production rate as on Earth

The Mid-IR O_2-O_2 Band is Most Observable for Desiccated Cases

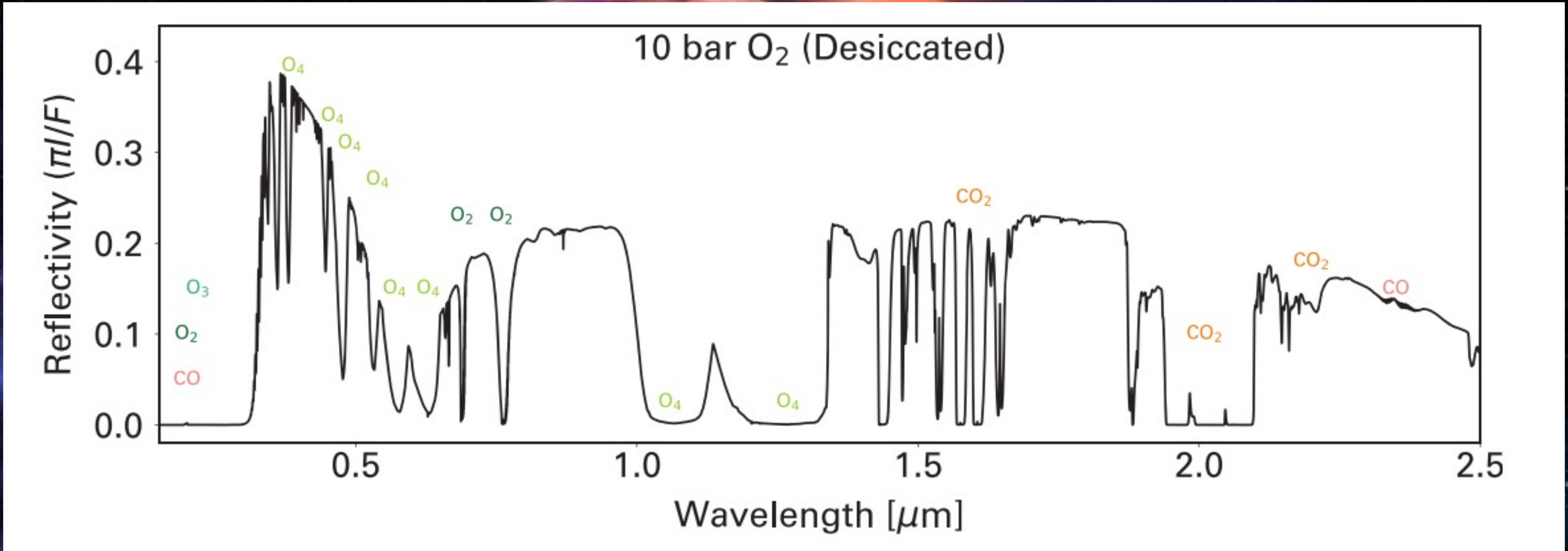




Fauchez+2020, Nat Astro

The MIR O_2-O_2 band adds to our potential toolbox of "false positive" identifiers. Will help us determine whether these abiotic O_2 atmospheres are indeed common (or rare, which would be good for biosignatures).

An O_2-Rich Planet Around Proxima Centauri b



Meadows+2018

Biosignature Anisotropy Modeled on Temperate Tidally Locked M-dwarf Planets

Howard Chen[1], Eric T. Wolf[2,3], Ravi Kopparapu[3,4], Shawn Domagal-Goldman[3,4], and Daniel E. Horton[1]
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[2] Laboratory for Atmospheric and Space Physics, Department of Atmospheric and Oceanic Sciences, University of Colorado Boulder, Boulder, CO 80309, USA
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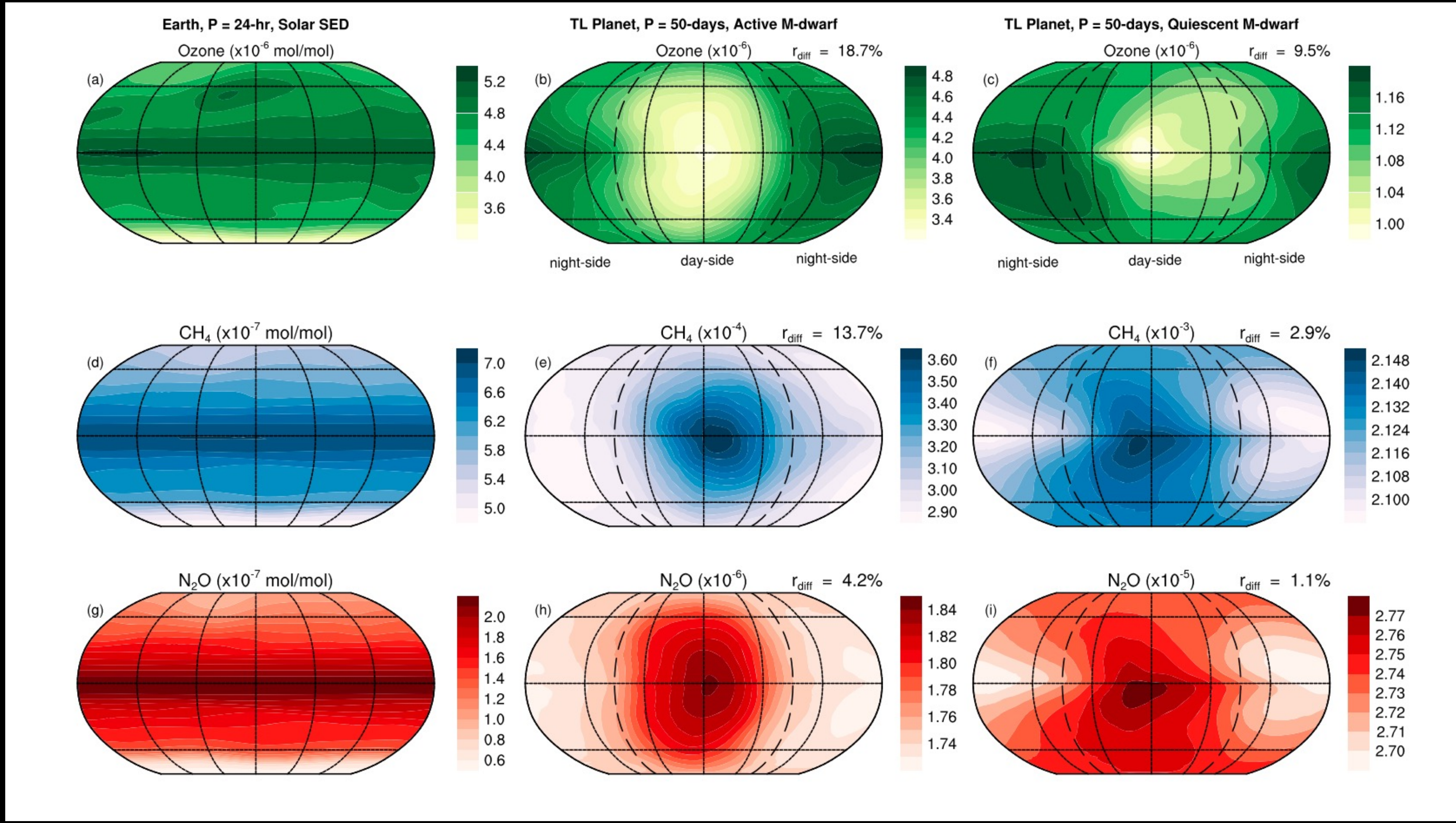
[4] NASA Goddard Spaceflight Center, Greenbelt, MD 20771, USA

Received 2018 September 10; revised 2018 October 23; accepted 2018 October 29; published 2018 November 15



5. Conclusions

This Letter reports numerical simulations using a coupled 3D CCM to explore global distribution of biosignature gases on Earth-like and tidally locked planets as a function of stellar spectral type, stellar activity, and planetary rotation period. Qualitatively similar to 1D models, we find increased mixing ratios of biogenic compounds (e.g., O_3, CH_4, and N_2O) for both active and inactive M-dwarf SEDs. These increases are most pronounced for planets around quiet M-dwarfs. Even though the effects of tidal locking are noticeable in our simulations, they are not yet discernable with current observational techniques, i.e., the primary biosignatures simulated in this work (O_3, CH_4, N_2O) show low ($\lesssim$20%) day-to-nightside mixing ratio contrasts. Conversely, simulated day-to-nightside differences of photosynthetic compounds (e.g., DMS) are found to be nearly 70% and underscore the need for heterogeneous 3D realism in modeling biosignatures and their photochemical derivatives. Overall, this