Thermal dissociation and SiO in WASP-121b

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WASP-121b has been established as a benchmark ultrahot Jupiter, serving as a laboratory for the atmospheric chemistry and dynamics of strongly irradiated extrasolar gas giants. Here, we present and analyze WASP-121b's transmission spectrum observed with NIRSpec G395H on board the James Webb Space Telescope and find evidence for the thermal dissociation of H_2O and H_2 on the planet's permanent dayside. Additionally, we detect SiO at a statistical significance of 5.2σ which is compatible with chemical equilibrium in the atmosphere. Constraining the abundance of SiO and abundance ratios between silicon and volatile atoms in WASP-121b's atmosphere could help discriminate between possible migration histories of the planet. The three-dimensional nature of thermal dissociation on WASP-121b's dayside and of recombination on its nightside, however, poses a challenge to constraining molecular abundances and elemental abundance ratios from the transmission spectrum. To account for this, we implemented an atmospheric model in the NEMESIS framework that splits the planet's atmosphere into dayside and nightside. A retrieval applying our atmospheric model to WASP-121b's transmission spectrum favors a higher H_2O abundance on the nightside than on the dayside, demonstrating the impact of hemispheric heterogeneity when attempting to constrain WASP-121b's bulk H_2O inventory.

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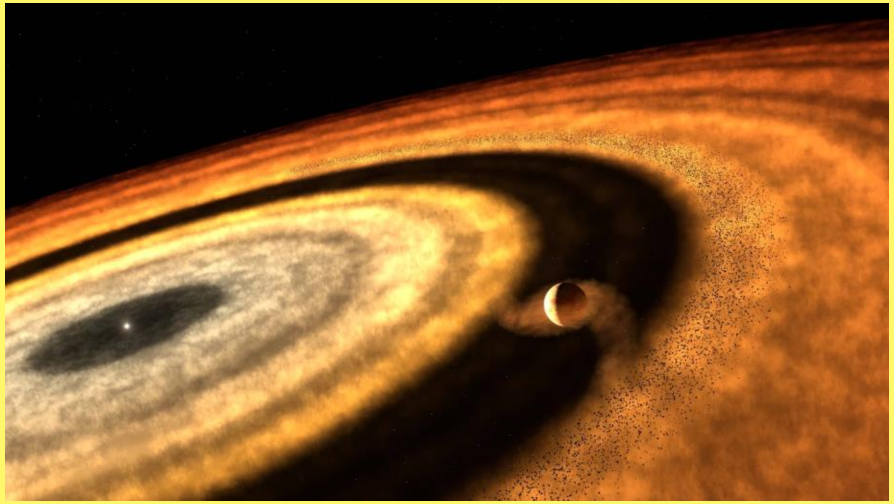
Introduction

WASP-121b is an ultrahot Jupiter orbiting an F6-type star in a distance less than two times the star's diameter, making it one of the hottest knwon exoplanets. As an exoplanet outstandingly suitable for atmospheric characterization, it has been observed regularly using both ground-based and space-based observatories, leading to a comprehensive picture of its atmospheric chemistry and dynamics. WASP-121b's dayside exhibits a temperature inversion, implying the presence of short-wavelength absorbers. Indeed, the planet's transit depth was observed to increase rapidly towards shorter wavelengths in the near-UV, however, no individual absorber creating this near-UV rise was conclusively detected. One candidate molecule that could be responsible for the observed short-wavelength absorption is SiO that also has absorption bands in the infrared.



Artist's impression of the late stage of WASP-121b's formation. Credit: T. Müller (MPIA/HdA - CC BY-SA)

Measuring WASP-121b's SiO abundance could yield crucial insight into the formation and migration of the planet to its current orbit, as the amount of rocky material accreted in the form of planetesimals would be constrainable through refractory-to-volatile ratios. These ratios are only expected to be constrainable in the ultrahot Jupiters, because in exoplanets with equilibrium temperatures below ~2000K, the refractory elements are expected to condense into clouds or to be locked into deeper atmospheric layers. This is sometimes referred to as the 'Ultrahot Jupiter Opportunity'.

Observation and Data Reductions

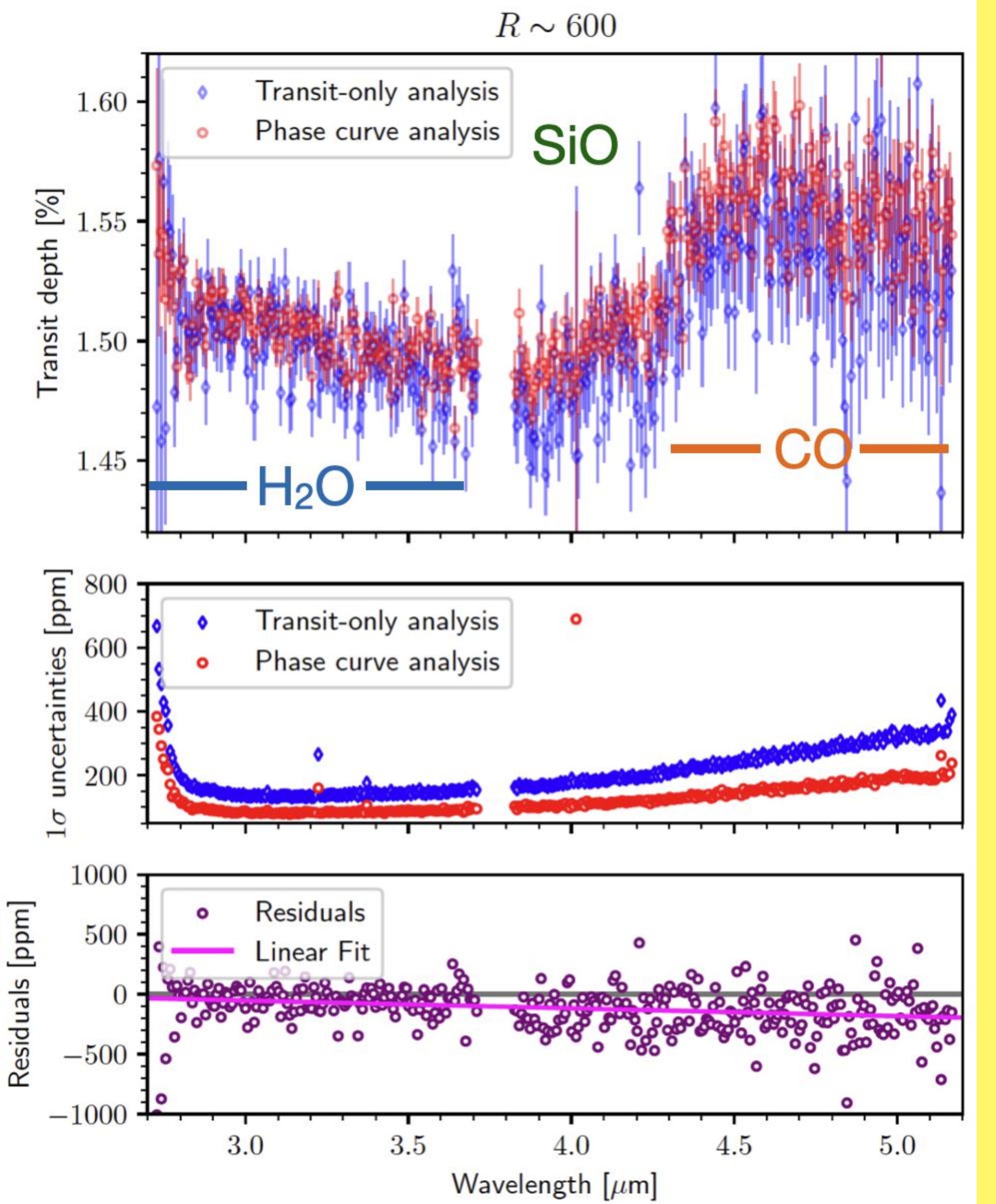
Here, we analyse WASP-121b's transit observed as part of the JWST/NIRSpec G395H phase curve (GO-1729, PI: Evans-Soma, co-PI: Kataria) that was previously reduced using the FIREFLY pipeline. For an extraction of the transmission spectrum, we only analyzed the observations from 3.5hr before to 3.5hr after the transit-midtime which we compared to the transmission spectrum derived as part of the analysis of the entire phase curve. Because of the curvature induced by the planet's phase curve around the transit, we used a quadratic polynomial for the instrumental and systematics' baseline.

Comparing the transmission spectrum from our transit-only analysis with the one obtained from the phase-curve analysis (see plot on the right), we observe:

1. The transit-only transmission spectrum returns error bars that are ~70% larger than the phase-curve transmission spectrum's. In the transit-only light curve fits, the **curvature of the baseline is correlated with the transit depth**, thus increasing the transit depth uncertainty. In the phase-curve analysis, the phase curve is better constrained from fitting all available data, resulting in a more-precise transmission spectrum.

2. The transit-only transmission spectrum gives smaller transit depths and this offset increases with wavelength. The reason for this is **contamination of the transit light curves with the planet's night side emission** that becomes larger with wavelength as the planetary-to-stellar flux ratio increases. In the phase curve analysis that also fits the planet's eclipses before and after the transit, this contamination is removed.

We conclude that for this data set, the most reliable way to derive the transmission spectrum is to analyze all available phase-curve data.

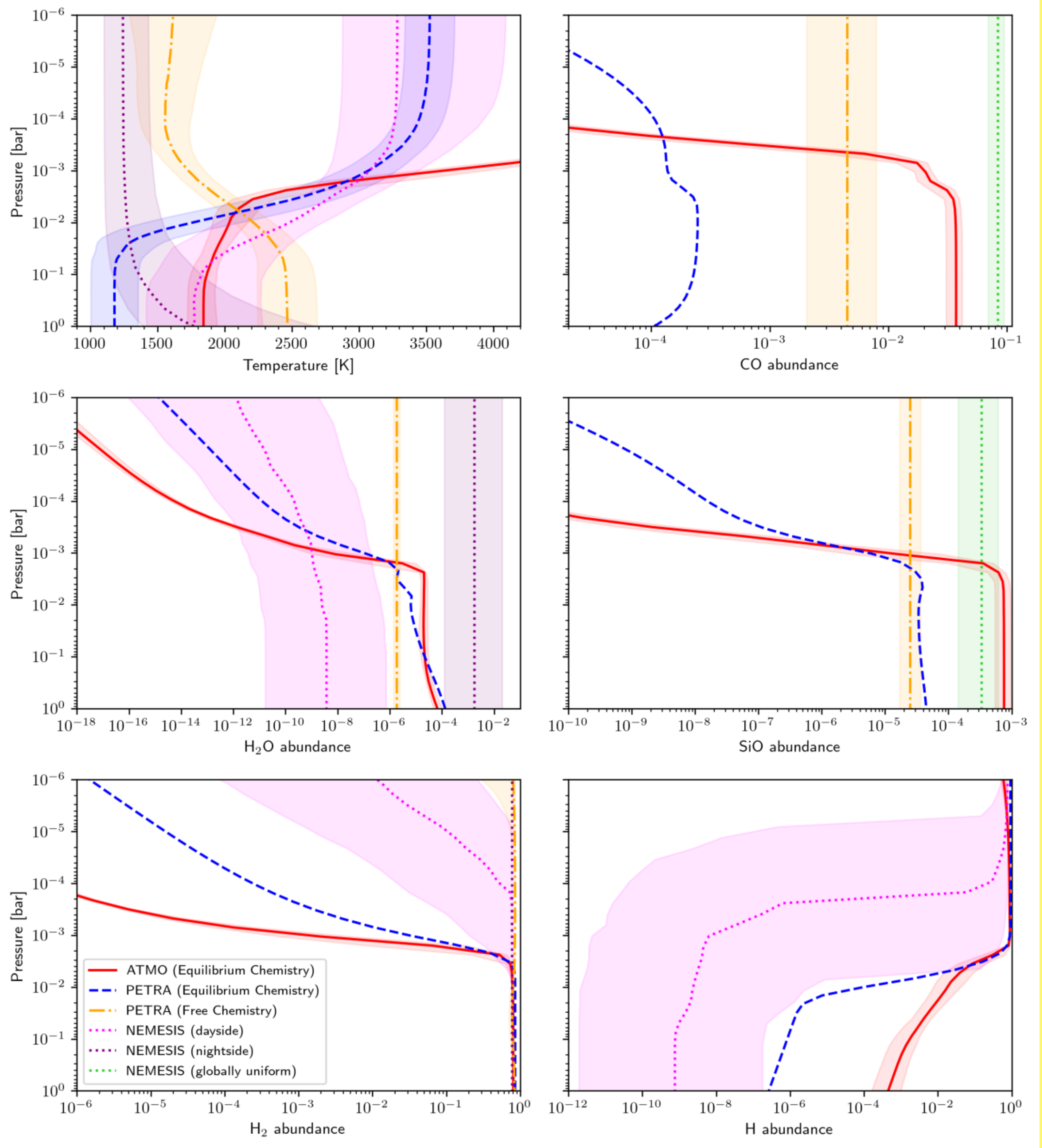


Atmospheric Retrievals

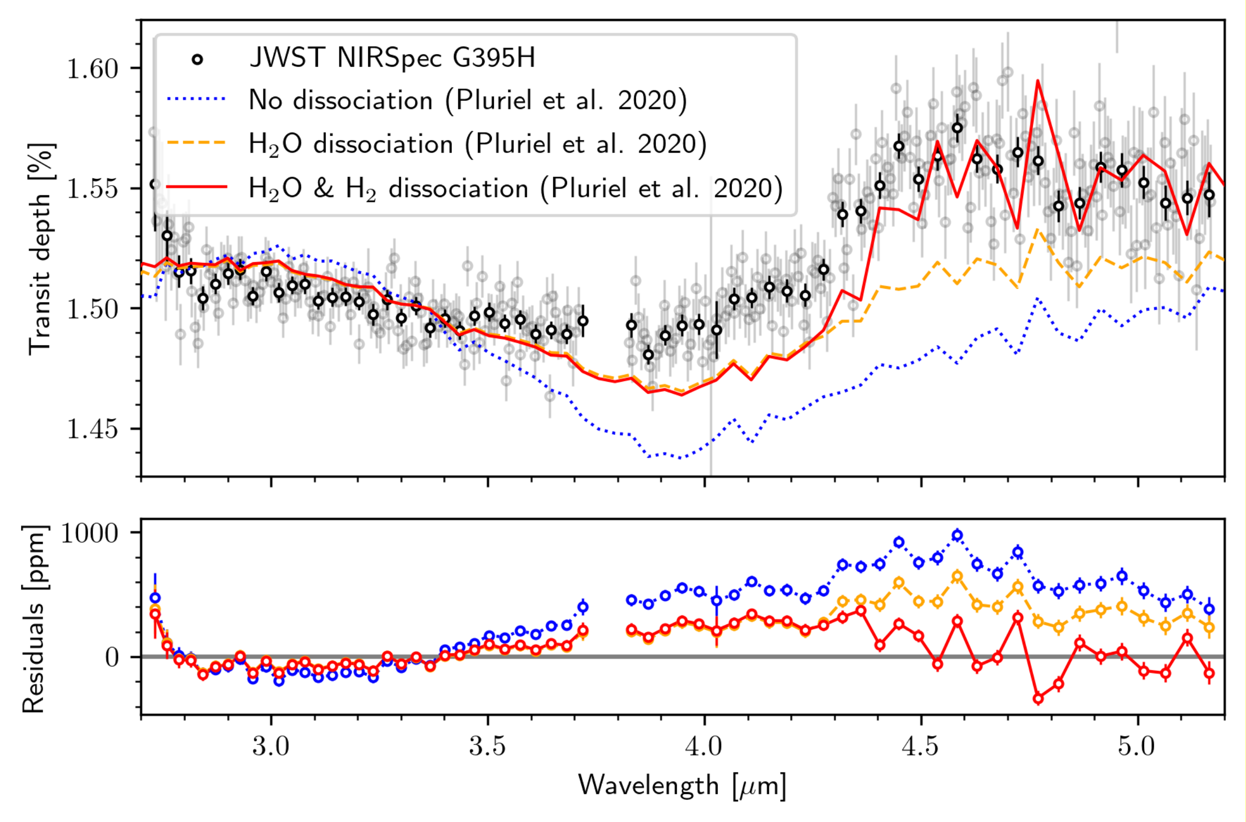
To identify atmospheric absorbers and their abundances from WASP-121b's transmission spectrum, we ran retrievals with the atmospheric models ATMO, PETRA and NEMESIS on the data. Since WASP-121b's atmosphere is highly irradiated, it's day- and nightside have vastly different temperatures. To account for this, we modified the atmospheric model in NEMESIS to split the ray through the atmosphere into dayside and nightside integrals and solved for two different temperature profiles. For H_2 and H_2O, we also allow the abundances to vary between dayside and nightside (see plot on the right).

We included H_2O, SiO and CO, which have clear absorption features in NIRSpec/G395H's wavelength range (see Observation and Data Reductions), in our models. For SiO, we derive a detection significance of 5.2σ from NEMESIS, marking SiO's first conclusive detection in any planet's atmosphere. Since the ATMO and PETRA models that prescribe chemical equilibrium in the atmosphere find similar SiO abundances as NEMESIS and PETRA employing free chemical abundances, SiO's observed absorption feature is in line with chemical equilibrium in the atmosphere.

From the ATMO and PETRA models prescribing chemical equilibrium in the atmosphere, we find C/O ratios of 0.978 +0.004/-0.006 and 0.80 +/- 0.06, respectively.



Discussion



In the results of the atmospheric retrievals, there are large discrepancies between the chemical abundances found in the different retrieval frameworks, especially for CO (see previous section). To investigate possible reasons for these differences, we also compare WASP-121b's transmission spectrum to model spectra predicted using a general circulation model (GCM, see *Pluriel et al. 2020*). The atmospheric model presented there was post-processed to include the effect of thermal dissociation of H_2O and H_2 on the atmosphere's local mean molecular weight and and latent heat.

The comparison between the GCM and observations reveals that:

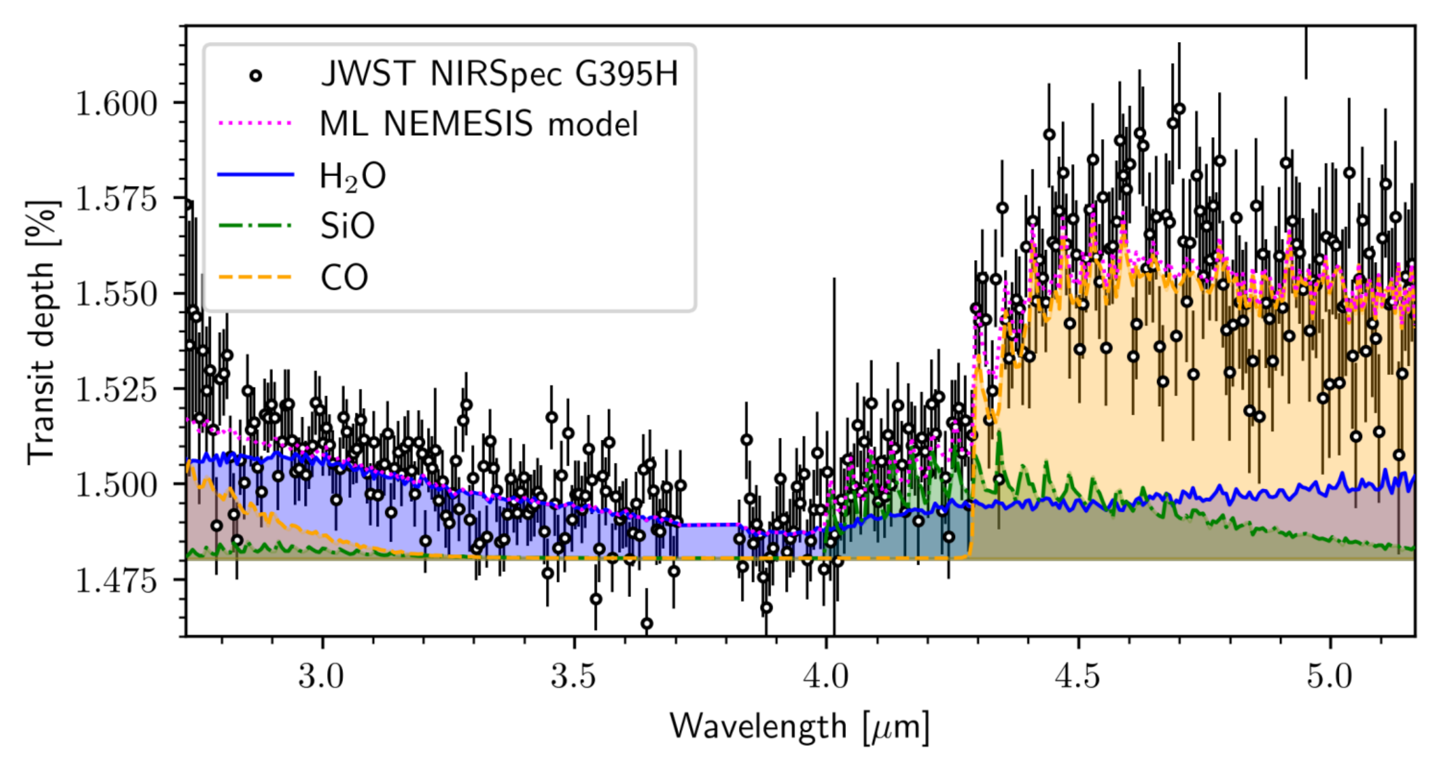
1. Neither including H_2O nor H_2 dissociation leads to a poor match between the model and data (blue dotted line).
2. Including H_2O dissociation (orange dashed line) leads to a better approximation of the fairly flat H_2O feature between 2.8 and 4.0µm.
3. Further including H_2 dissociation (red solid line) leaves the H_2O feature unchanged but inflates the CO feature in the model to the observed level.

Unlike the H_2O feature, the CO feature is sensitive to H_2 dissociation that occurs on the planet's dayside, because CO is stable against thermal dissociation. Thus, the H_2O feature probes the nightside's atmospheric conditions while the CO feature is primarily set by the much more extended dayside. So, the transmission spectrum is a composite of atmospheric opacities from the planet's day- and nightsides, constituting a major challenge to one-dimensional atmospheric retrievals.

Since the CO feature is thus set by both the planet's CO abundance and H_2 dissociation on the dayside, there might be a negative correlation between CO abundance and the amount on H_2 dissociation in our atmospheric retrievals. The discrepancies between our models' CO abundances (see previous slide) could be primarily driven by this degeneracy. As H_2O is not afflicted with the same degeneracy, the C/O ratio we derived from this transmission spectrum using one-dimensional models might be biased.

Summary and Outlook

A phase-curve observation of WASP-121b with JWST/NIRSpec G395H revealed the planet's transmission spectrum shaped by H_2O, CO and SiO. For the latter, we derive a detection significance of 5.2σ using the NEMESIS atmospheric retrieval framework.



1. Due to the high signal-to-noise ratio of WASP-121b's phase curve, the transit light curves are **contaminated with the planet's nightside emission**, leading to a biased transmission spectrum and larger uncertainties when only the transit is analyzed.
2. **SiO** is present in WASP-121b and likely in chemical equilibrium.
3. The **H_2O and CO features probe different parts of the atmosphere** due to their different susceptibilities to thermal dissociation. This probably biases the C/O ratio inferred from one-dimensional retrievals to higher values.

The detection of SiO opens up the possibility of measuring WASP-121b's refractory-to-volatile ratio, an important constraint for the planet's formation. However, the three-dimensional variability of WASP-121b's chemistry that is probed in transmission can bias inferred atomic abundance ratios. Thus, for reliably measuring the planet's refractory-to-volatile ratio from the transmission spectrum, a **careful representation of its atmospheric heterogeneity in atmospheric models** is needed.