SAG 26: Exoplanet Reflectance Spectroscopy for HWO

Jan 2025 Update

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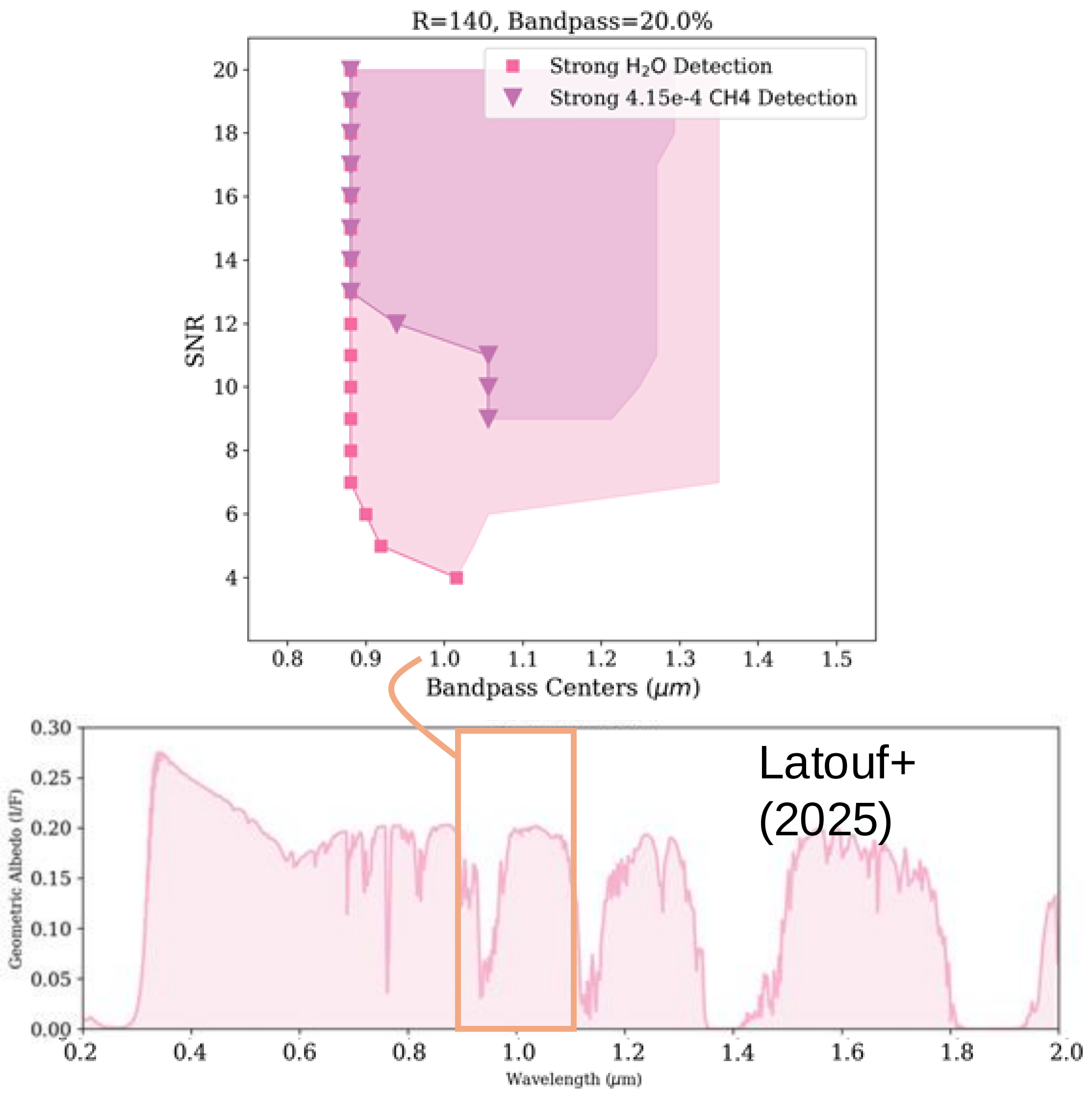
Lightning Summary

- **Motivation**: Prepare and validate the suite of tools that will help define the measurables and requirements for HWO.
- **Goals**: Execute a community-driven intercomparison of spectrum generating tools and determine a set of best practices for spectral simulation/retrieval.
- **Timeline**: Spring 2024 – Fall 2025
- **Participants**: 23, with active participation from 6+ US and international research groups.
- **Status**: Roughly 50% of intercomparison cases completed. Report in-prep.

Motivation

- HWO responds to Astro2020's challenge to pursue a "robust sample of ~25 atmospheric spectra of potentially habitable exoplanets[.]"

- Understanding of how direct imaging instrument performance connects to spectrum quality (and subsequent environmental inferences) is **strongly model-based**.



Latouf+ (2025)

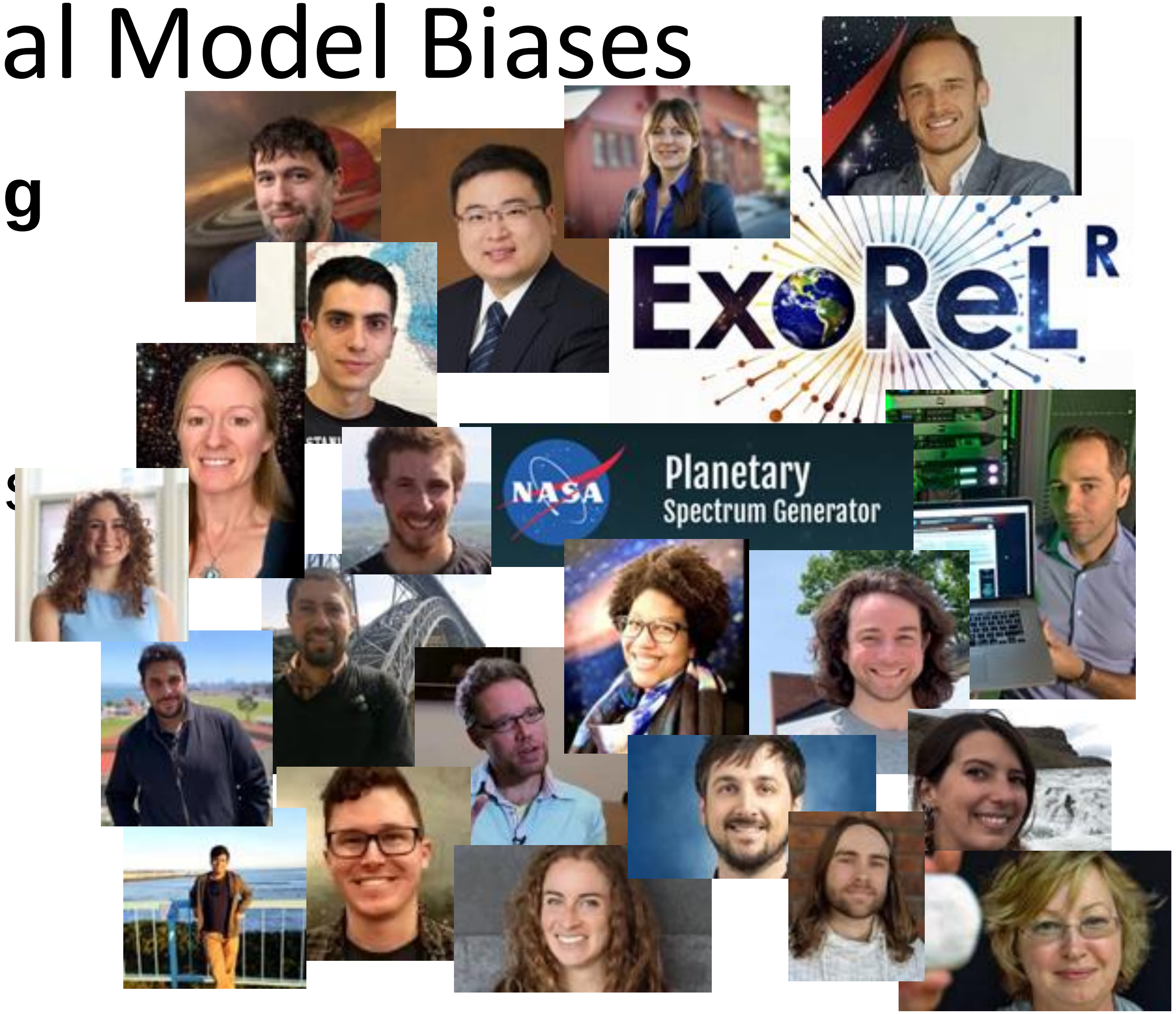
Risk

- Model-derived errors and/or biases could translate to overly stringent (or overly loose) instrument requirements for HWO.

- E.g., Model X says that SNR of 10 at 1.1 μm yields a strong H_2O detection while Model Y says that SNR of 20 is required.

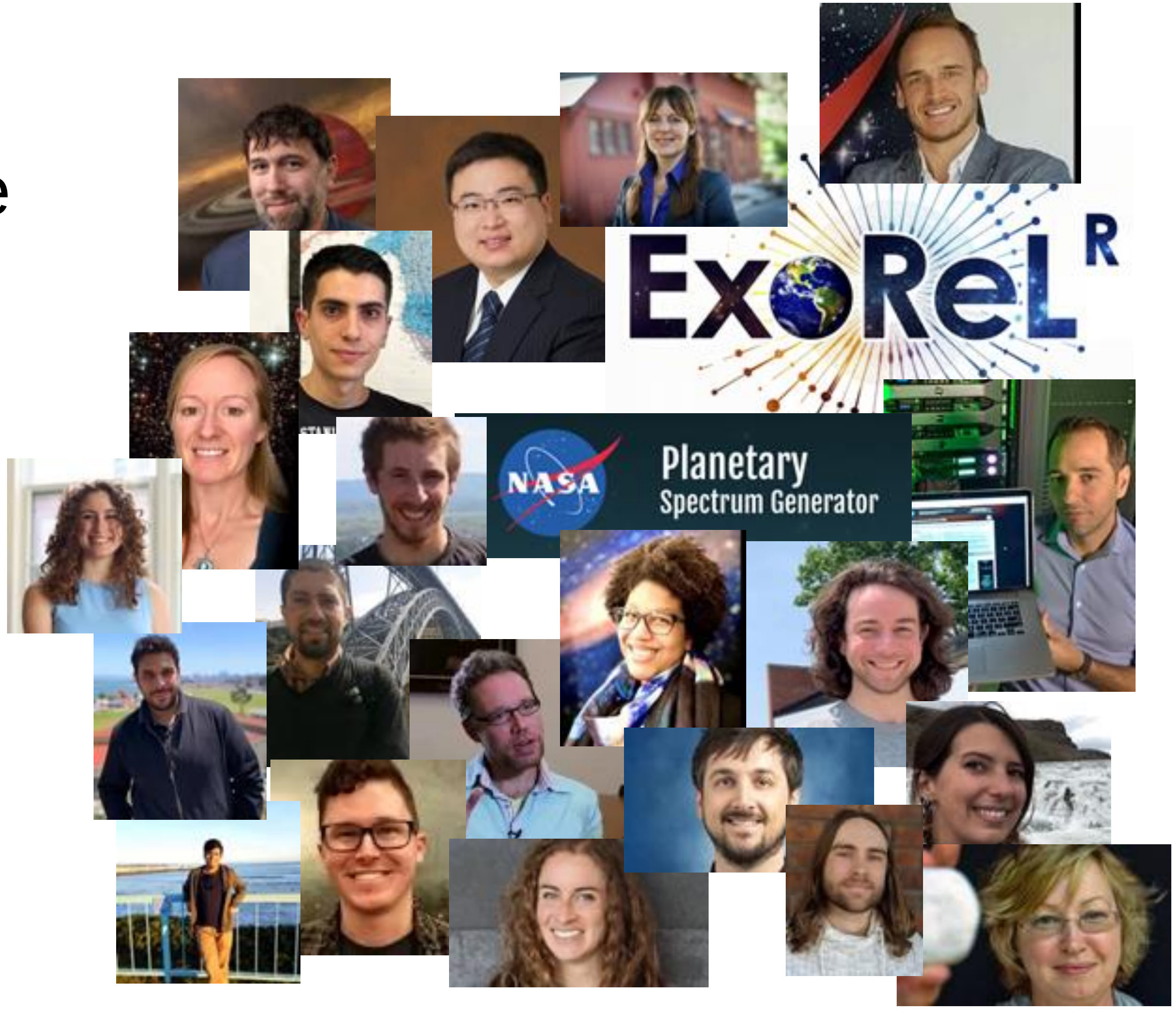
SAG 26: Addressing Spectral Model Biases

- Develop **common understanding** across all engaged research groups.
- Compare and **validate** opacities, spectral forward models, retrievals
- Understand **required model complexities.**
- Identify **best practices**.
- Find **any important areas of disagreement** that could impact HWO science and design.



Organization

- Participants assembled after wide advertising.
- Kick-off April 2024.
- Bi-weekly telecons.
  - Recorded.
  - Notes and homework circulated.
- Maintaining:
  - Shared Google Drive where all participants upload results.
  - Living SAG 26 report.



Approach

- Intercomparisons start with fundamental inputs, increase in complexity.
- Compare:
  1. Opacities
  2. Spectral Models
  3. Retrievals
- Each comparison case has a well-defined setup document.

Experimental Setup

CH4 Line Absorption

Inputs

Case: CH4 line absorption
Purpose: Comparison of high-resolution ro-vibrational opacities for CH4
Pressure(s) (Pa): {1e3,1e5}
Temperature(s) (K): {300}
Broadening: {foreign (native to model), self [optional]}
Isotopologues: (whatever is native to given model)
Wavelength Range (um): 0.2–5.0
Resolving Power: >10,000 (cross sections); >1,000 (transmission)

Outputs

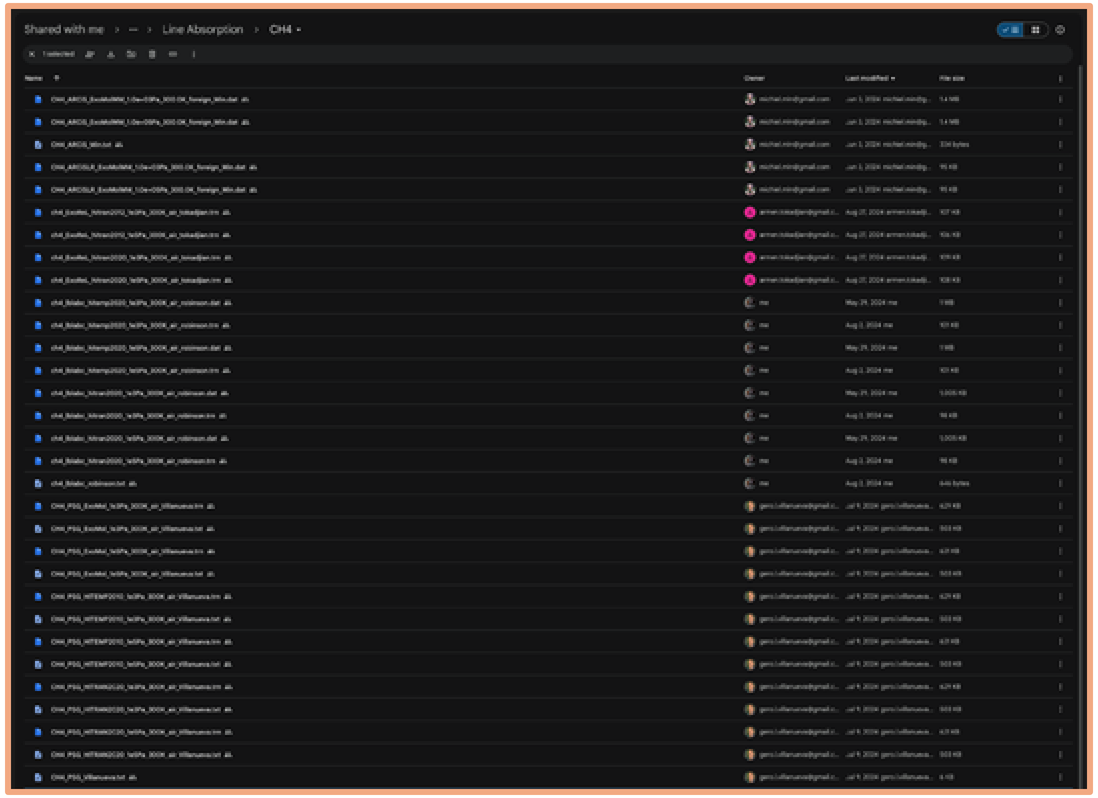
1. Cross section file
   a. ASCII-formatted
   b. Columns of wavelength (um), absorption cross section (cm^2/molecule)
2. Transmission file
   a. ASCII-formatted
   b. Columns of wavelength (um), transmission through a column:
      $$N_c = p/g/m$$
      where N_c is the number of molecules per unit area, p is the pressure for this case (e.g., 1e3 Pa or 1e5 Pa), g = 10 m s^{-2}, and m is the molecular weight for the line absorbing gas.
3. Supplementary file
   a. Model details (e.g., citation, line cutoff)
   b. Example Python script to read cross section file

Naming Conventions

1. Cross section file
   a. ch4_[model]_[linelist]_[pressure]_[temperature]_[broadener]_[submitter].dat
   b. e.g., ch4_abstool_hitran2020_1e3Pa_300K_N2_sagan.dat
2. Transmission file
   a. ch4_[model]_[linelist]_[pressure]_[temperature]_[broadener]_[submitter].trn
3. Supplementary file
   a. ch4_[model]_[linelist]_[submitter].txt

Approach

- Participants upload results to Google Drive.
- Digest plots created and circulated prior to telecons.
  - Thanks Armen!
- Discrepancies analyzed during telecons.
  - Iterate as needed.



Results: Overview of Progress To-Date

- Completed intercomparison of:
  - Line absorption (CH_4, CO_2, CO, H_2O, O_2, O_3)
  - Rayleigh scattering (CH_4, CO_2, CO, H_2, H_2O, O_2, N_2, O_3)
  - Collision-Induced Absorption (H_2-H_2, O_2-O_2, N_2-N_2)

- For all opacity cases, differences attributable to known model assumptions.

- Ongoing intercomparison of spectral models.
  - Single-component, scattering cases.

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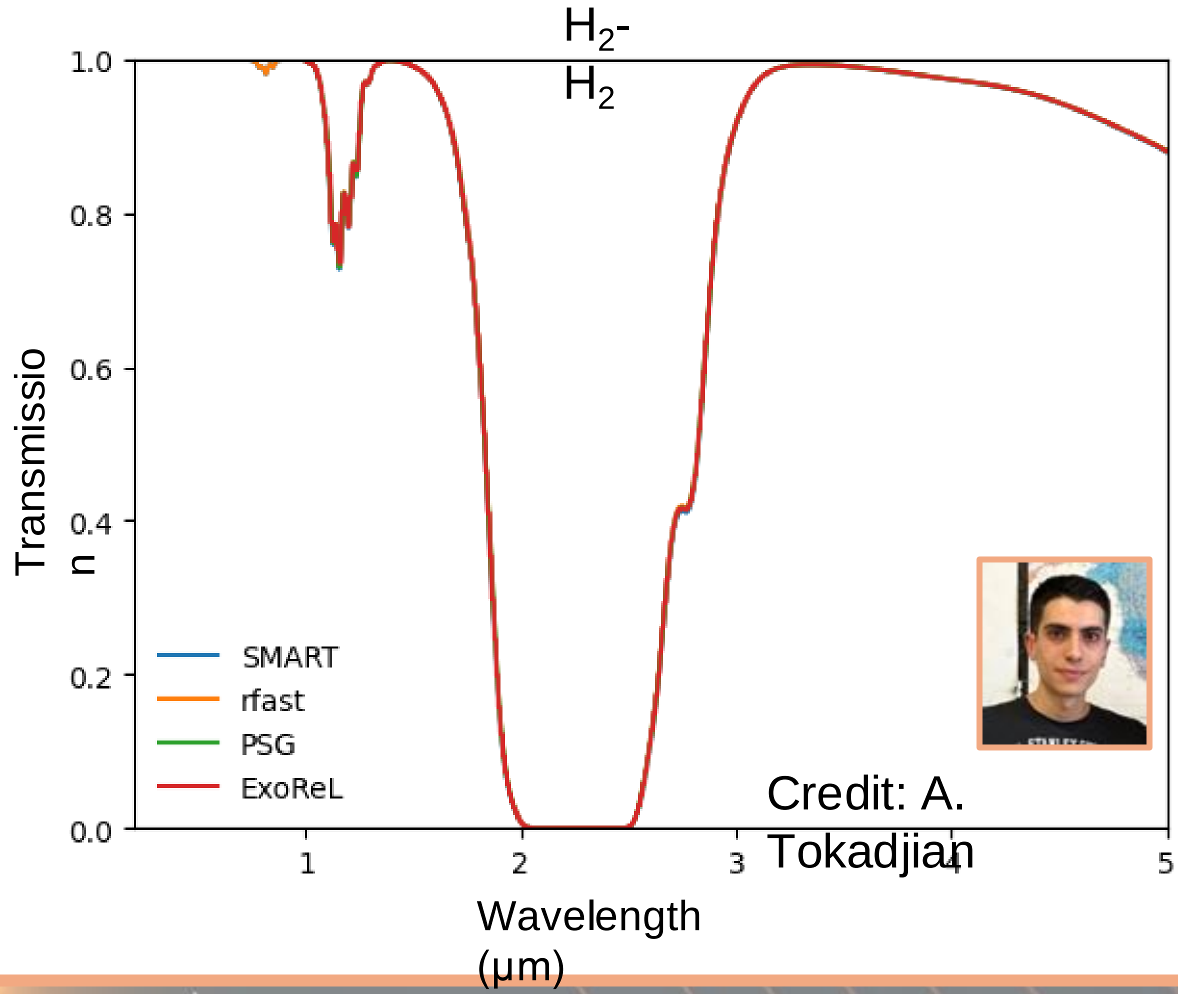
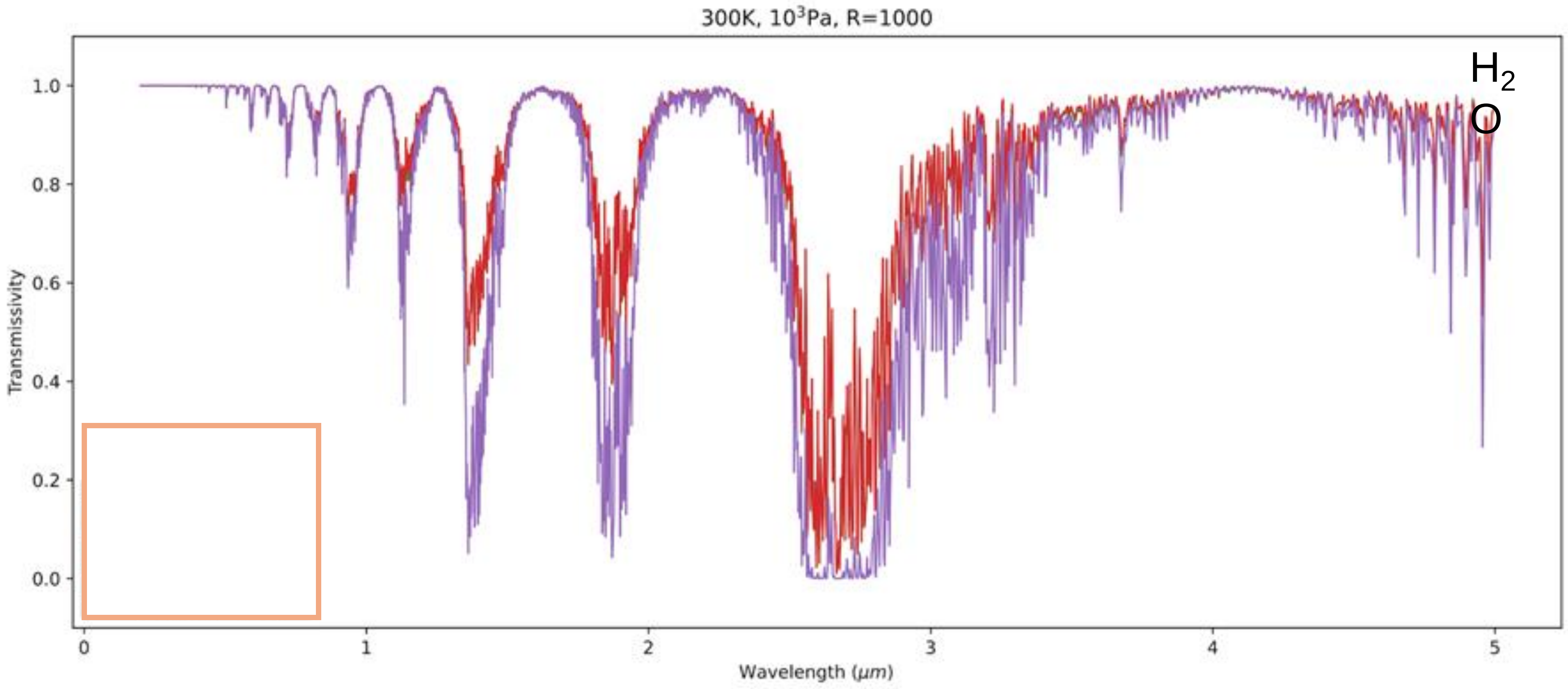


Credit: A. Tokadjian

Results: Line Absorption

Earliest comparisons revealed:

- major model differences, and
- flaws in experiment design.



H_2O

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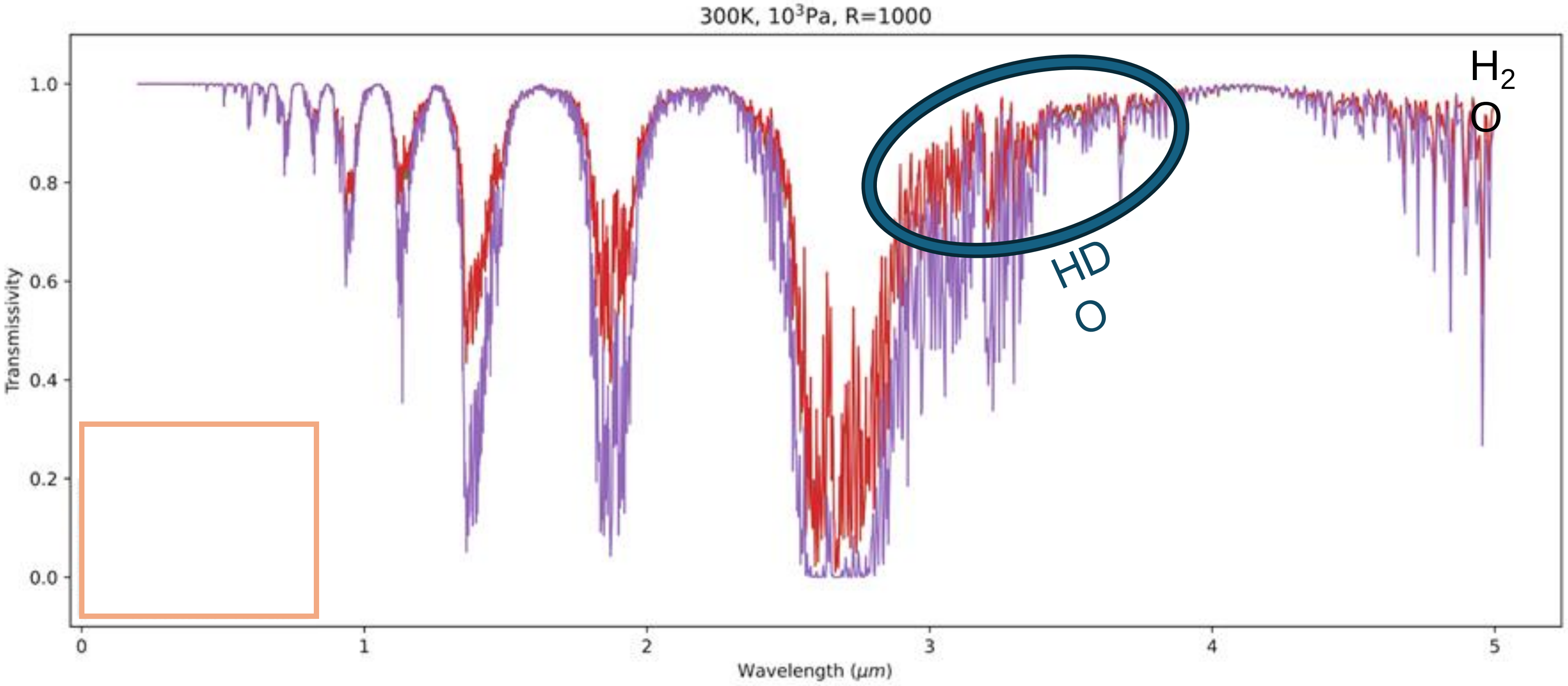

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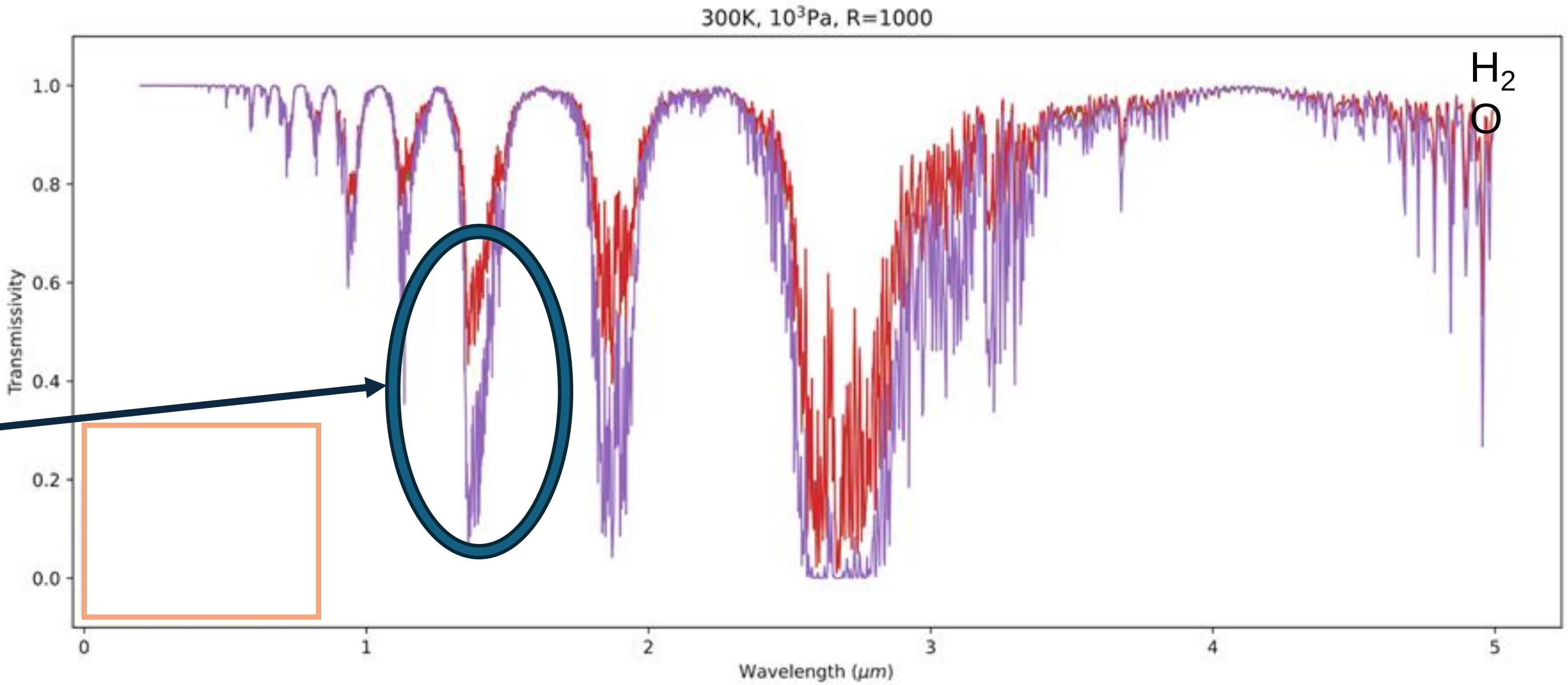
sensitive to resolution of participant-provided opacities



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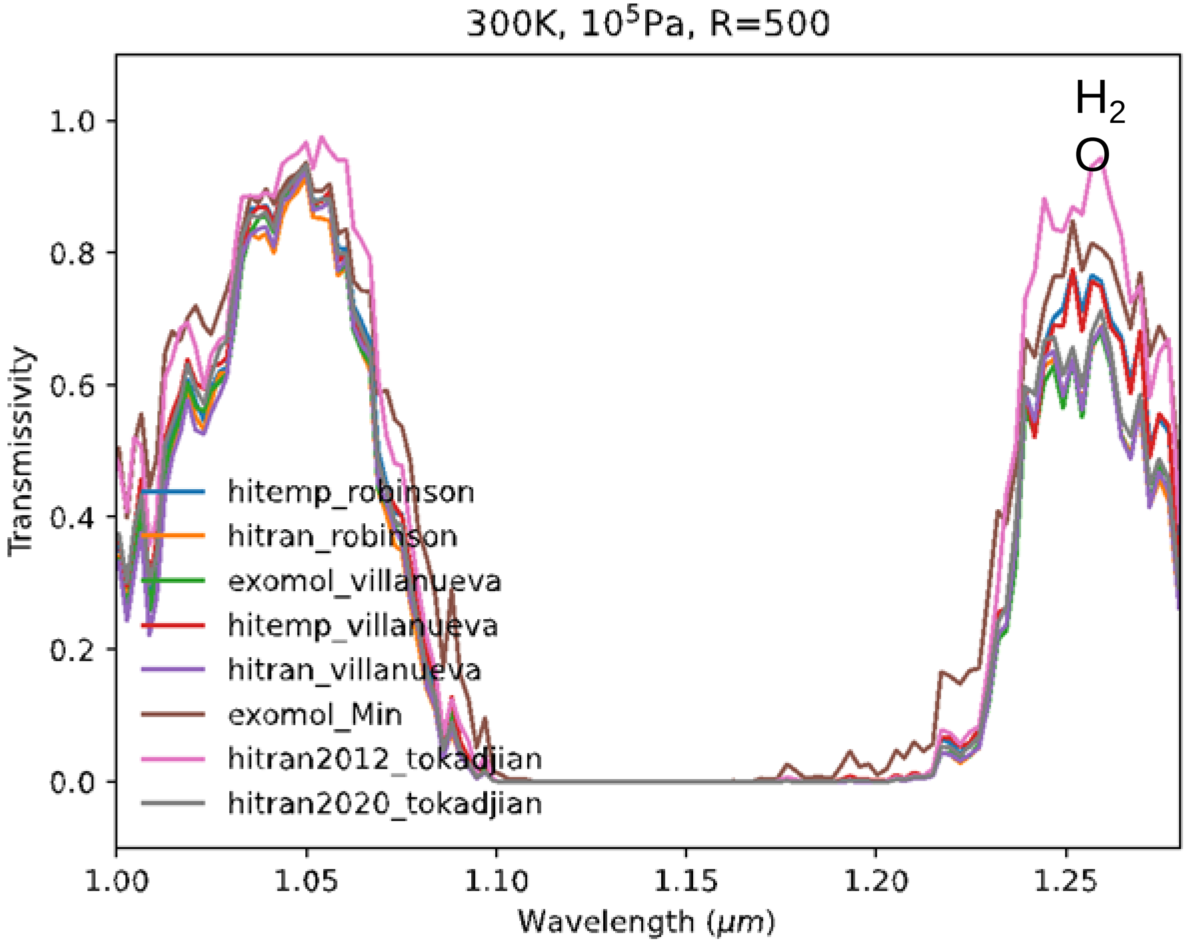
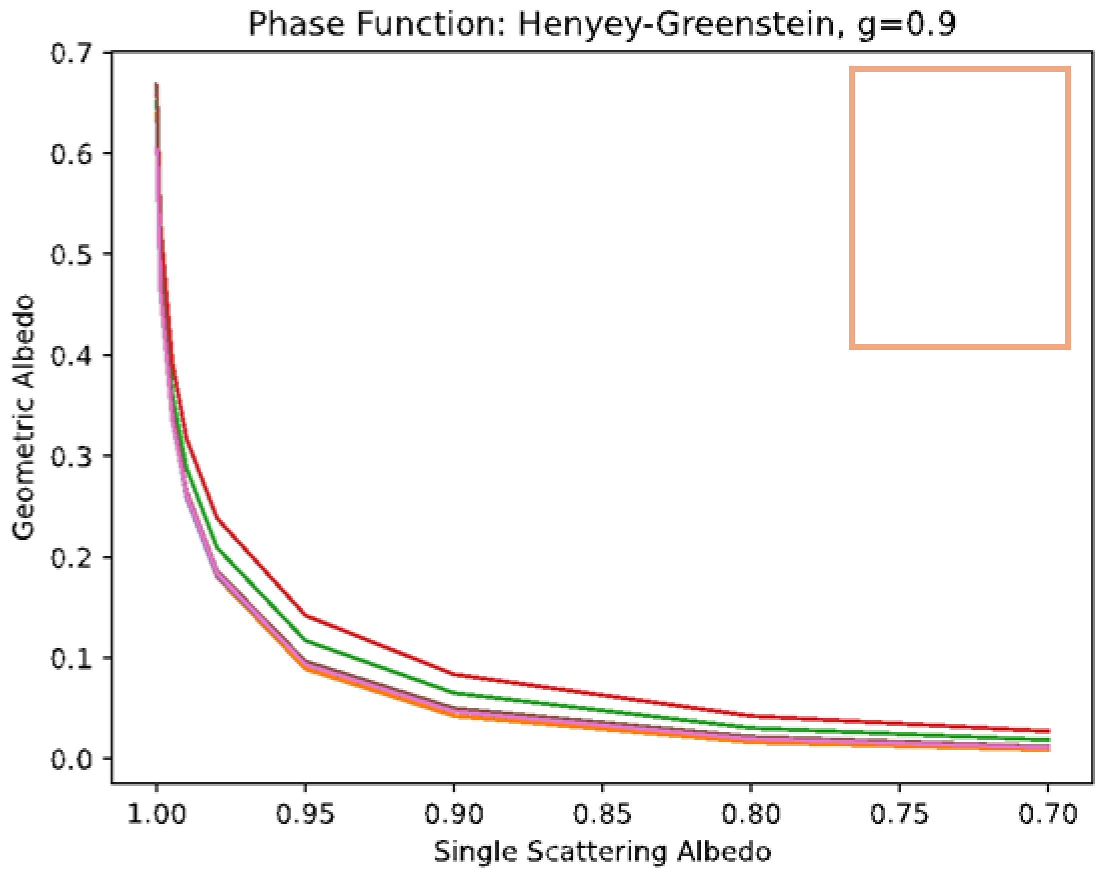
Results: Line Absorption



Credit: A. Tokadjian

Results: Spectral Models



Credit: A. Tokadjian

Lessons Learned

- Empower teamwork. Seek complementarity.
  - CUISINES MALBEC/RISOTTO and Turnbull Precursor Science

- Opacity comparisons (esp. line absorption) benefits from a nested approach.

- Results likely sensitive to adopted linelist.
  - E.g., HITRAN 2012 vs. 2024.

- Spectral models have first-order sensitivity to adopted radiative transfer approach(es).

Next Steps

- Complete ongoing comparisons of forward (spectral) models. (Sp25)
  - Propagate opacity spread through RT models.
  - Consider cases w/cloud scattering.

- Design, execute retrieval intercomparison. (Su25)
  - Work with ongoing RISOTTO intercomparison (Young/A[illegible]).

- Update and complete SAG 26 report. (Sp25-Fa25)

- Package results for long-term preservation and long-lived utility.

Summary Redux

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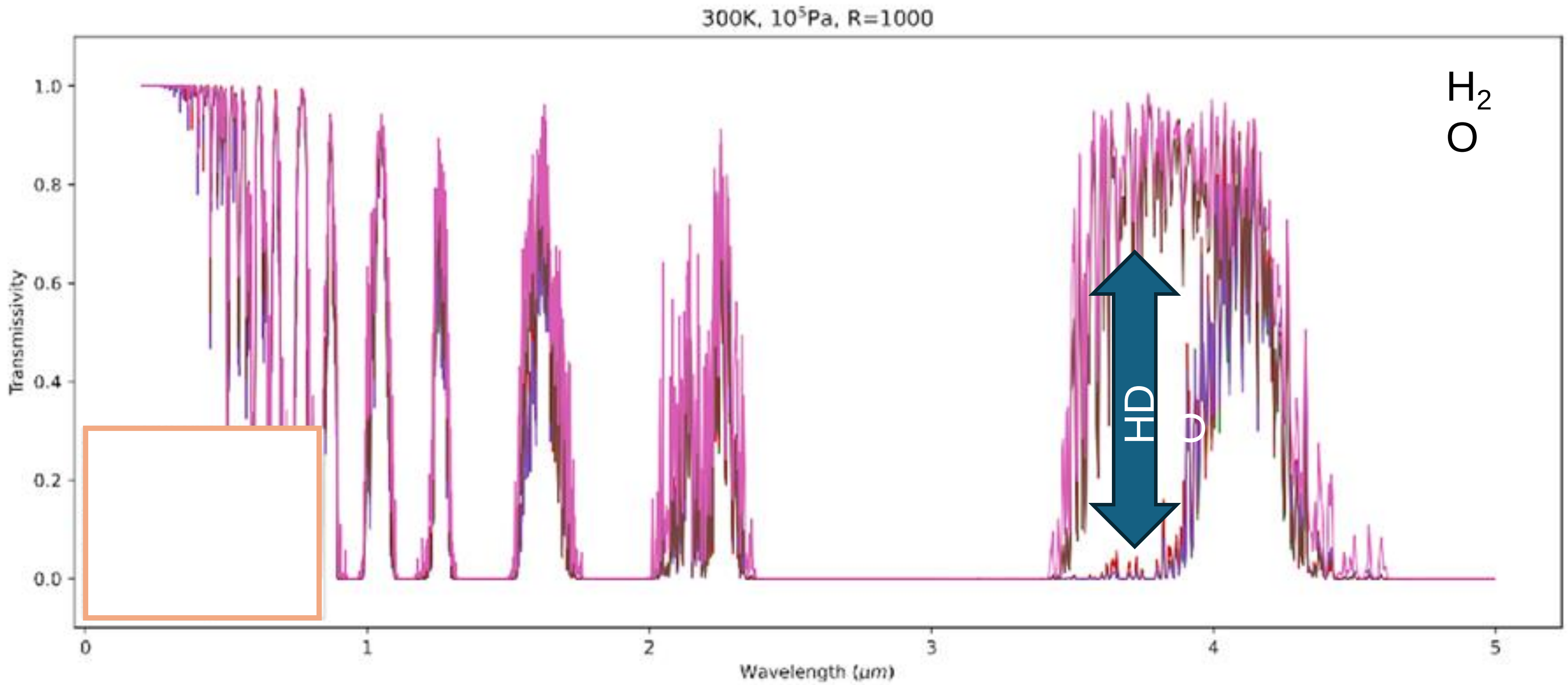
Begin Backup Slides

Results: Line Absorption

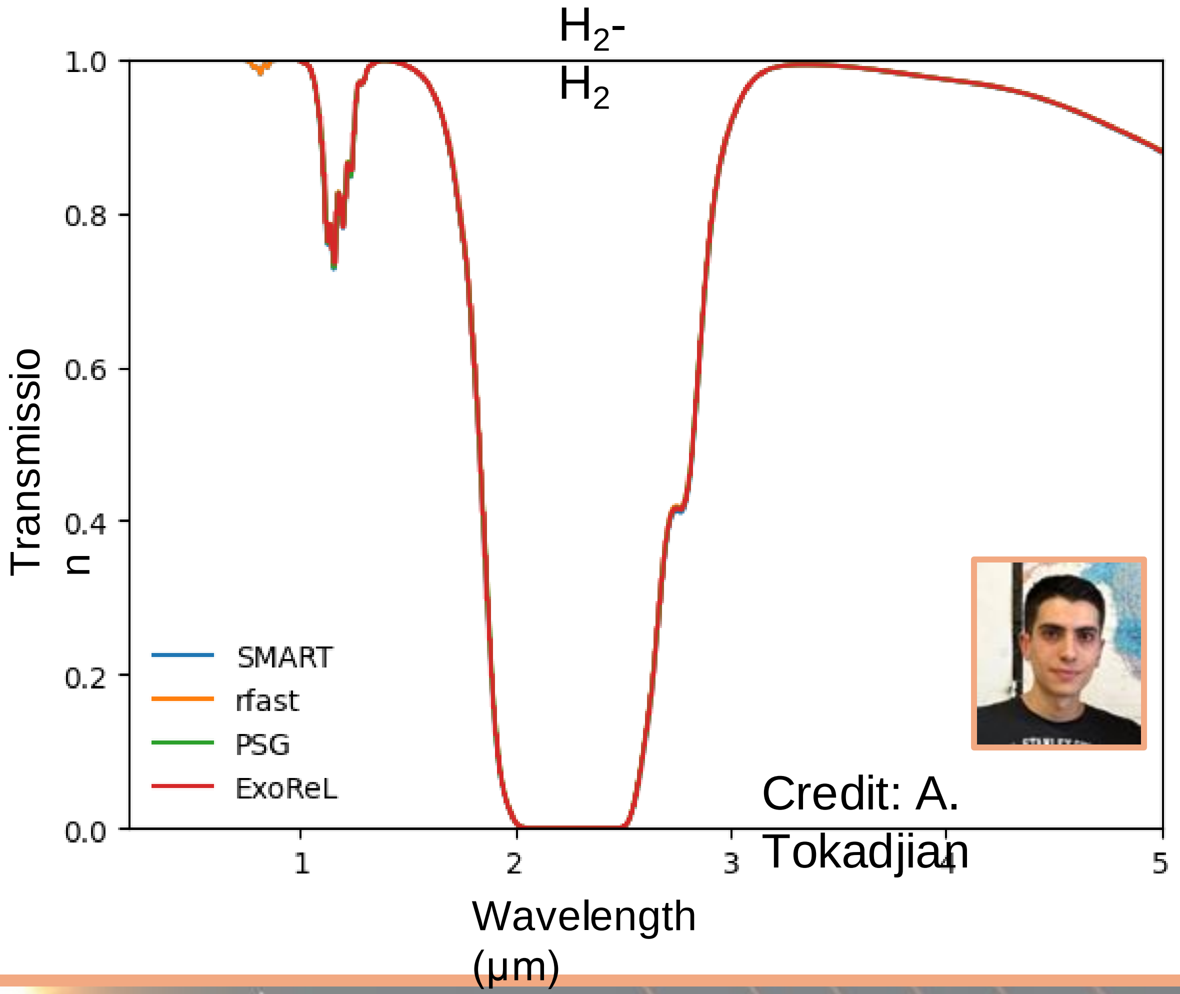


Credit: A. Tokadjian

Results: Collision-Induced Absorption

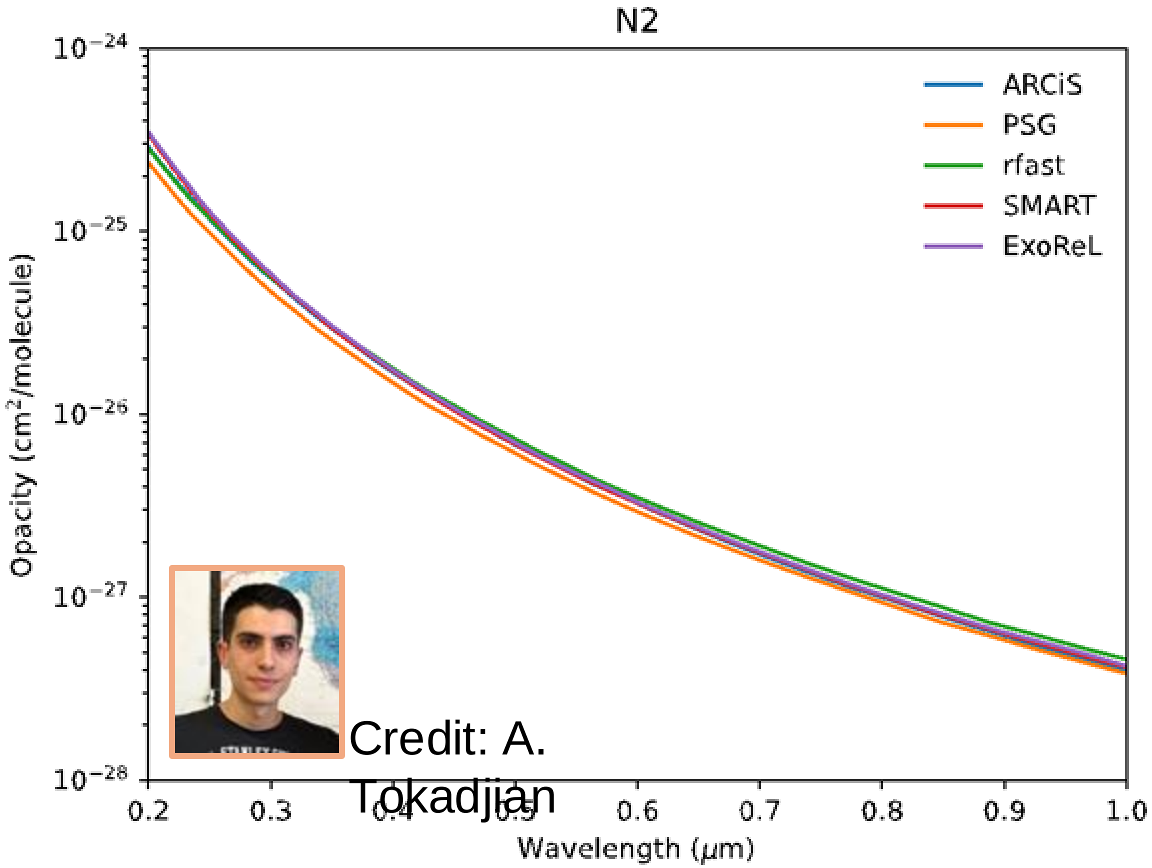
- Compared all of:
  - H_2-H_2, O_2-O_2, N_2-N_2

- Small differences attributable to data augmentations beyond HITRAN.



Credit: A. Tokadjian

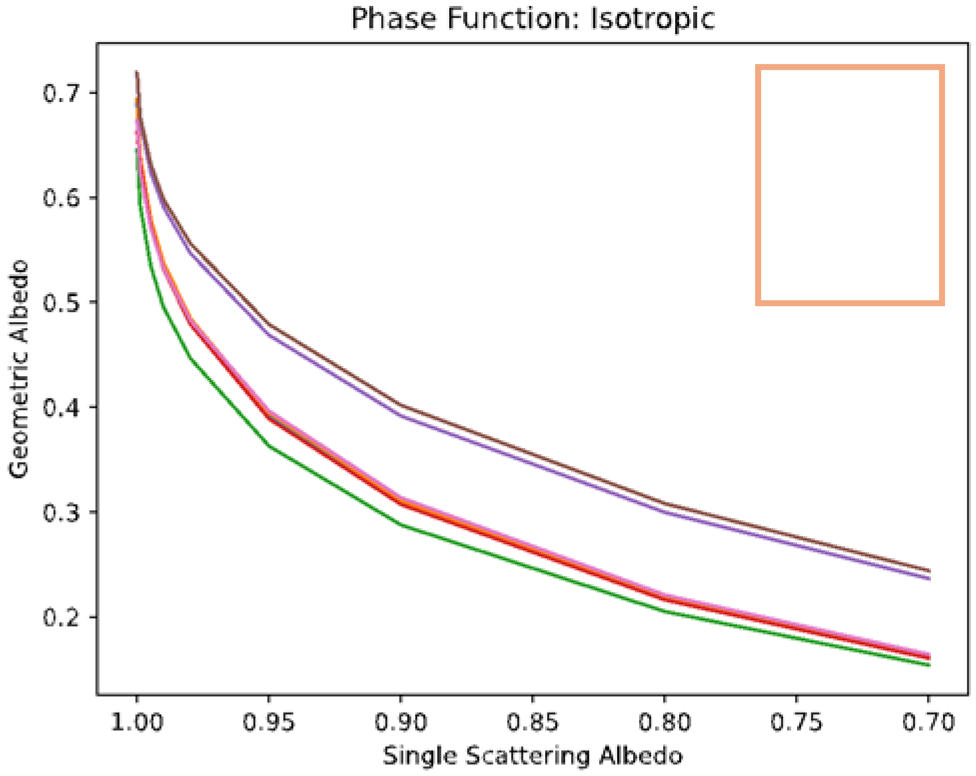
Results: Rayleigh Scattering Cross Sections

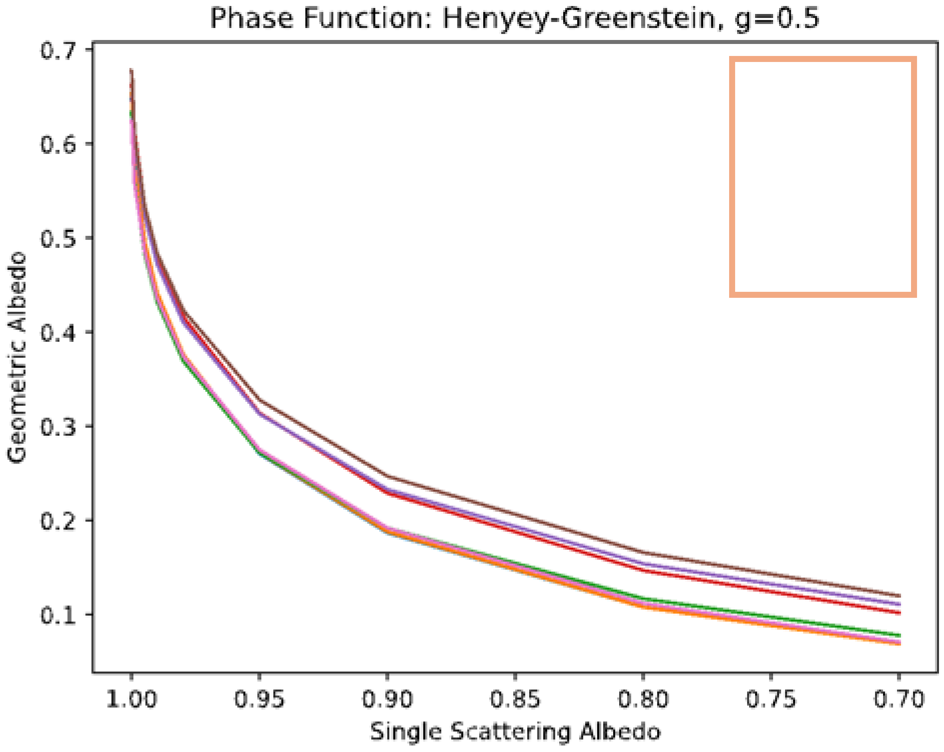


Credit: A. Tokadjian

- Strong agreement for all of:
  - CH_4, CO_2, CO, H_2, H_2O, O_2, N_2, O_3
- Small differences attributable to model assumptions.

Results: Spectral Models





Credit: A. Tokadjian

Results: Spectral Models

Credit: G.
Villa