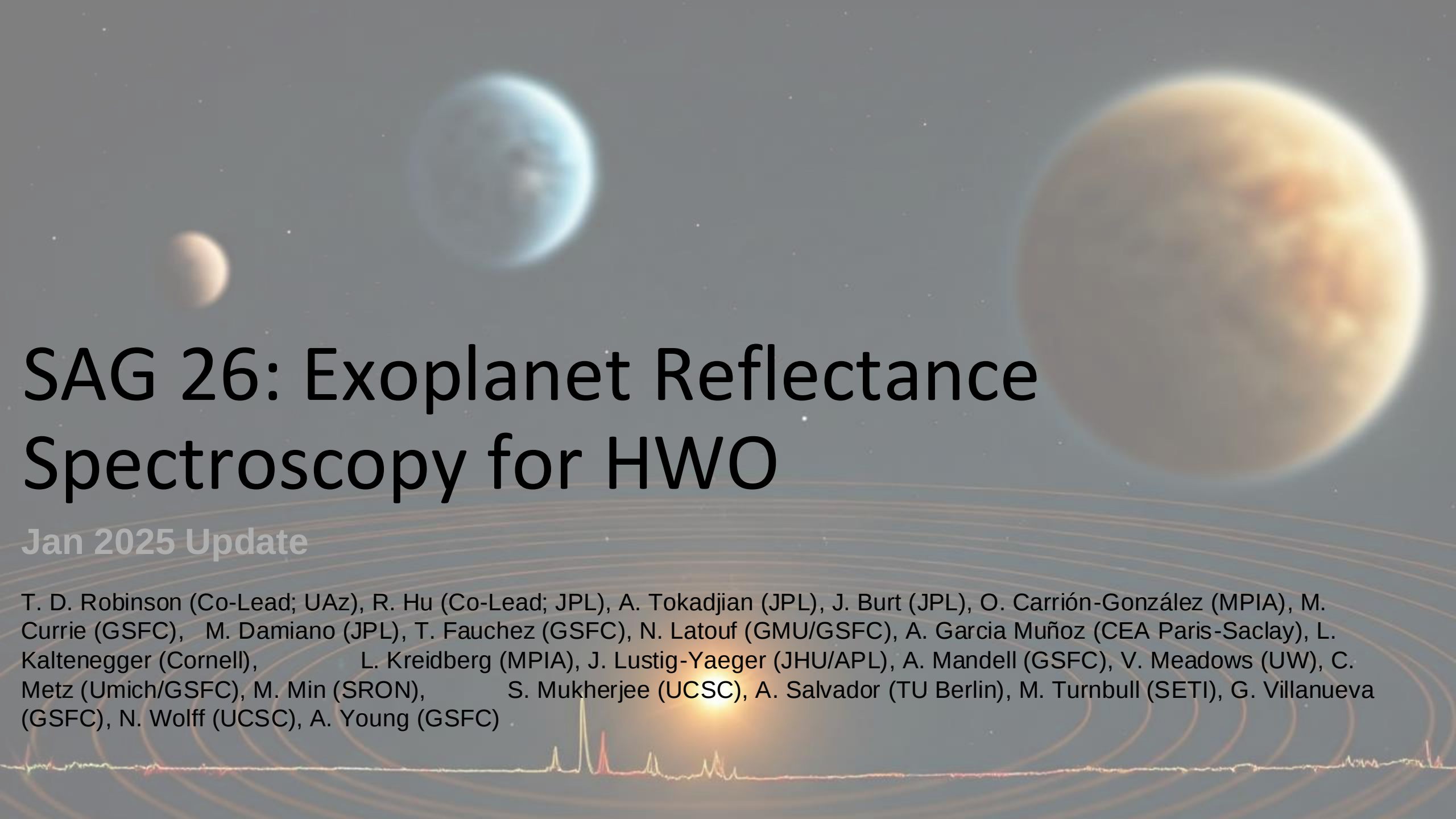




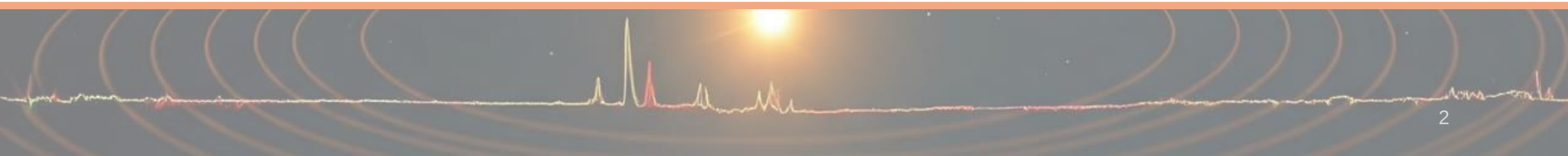
SAG 26: Exoplanet Reflectance Spectroscopy for HWO

Jan 2025 Update

T. D. Robinson (Co-Lead; UAz), R. Hu (Co-Lead; JPL), A. Tokadjian (JPL), J. Burt (JPL), O. Carrión-González (MPIA), M. Currie (GSFC), M. Damiano (JPL), T. Fauchez (GSFC), N. Latouf (GMU/GSFC), A. Garcia Muñoz (CEA Paris-Saclay), L. Kaltenegger (Cornell), L. Kreidberg (MPIA), J. Lustig-Yaeger (JHU/APL), A. Mandell (GSFC), V. Meadows (UW), C. Metz (Umich/GSFC), M. Min (SRON), S. Mukherjee (UCSC), A. Salvador (TU Berlin), M. Turnbull (SETI), G. Villanueva (GSFC), N. Wolff (UCSC), A. Young (GSFC)

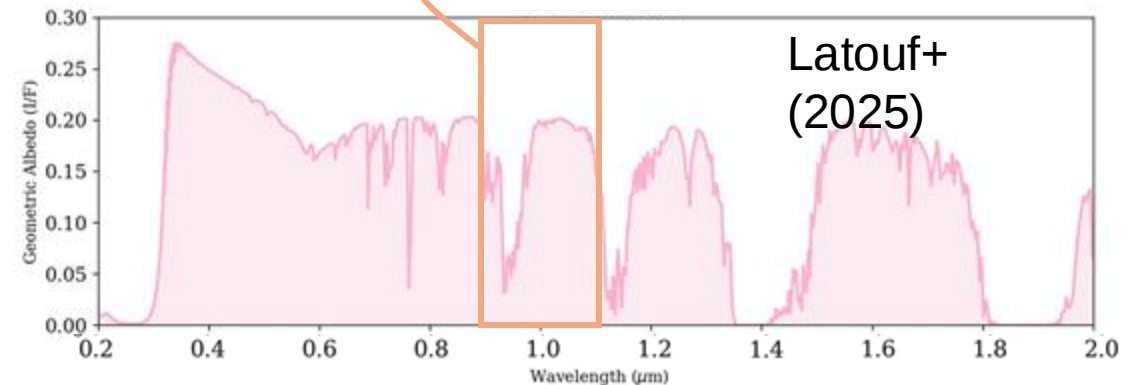
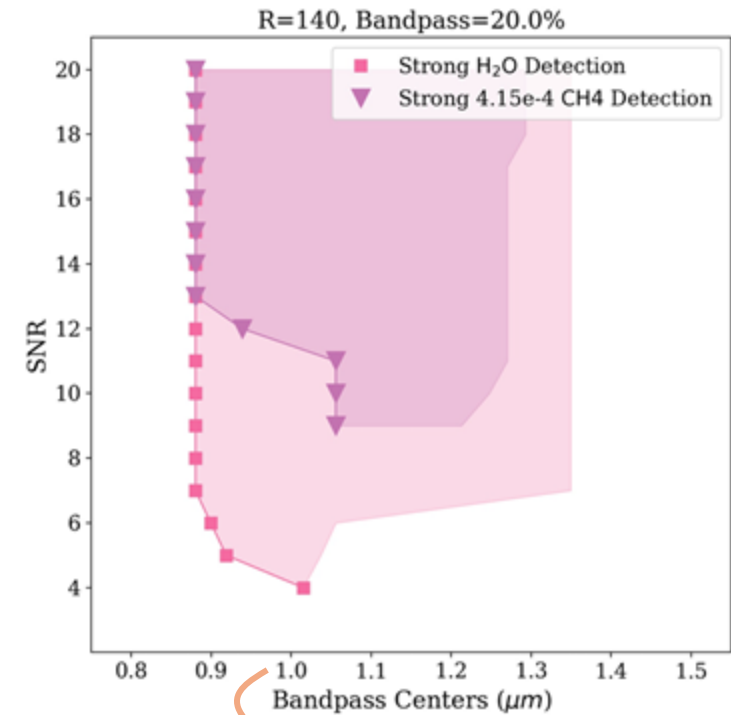
Lightning Summary

- **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.



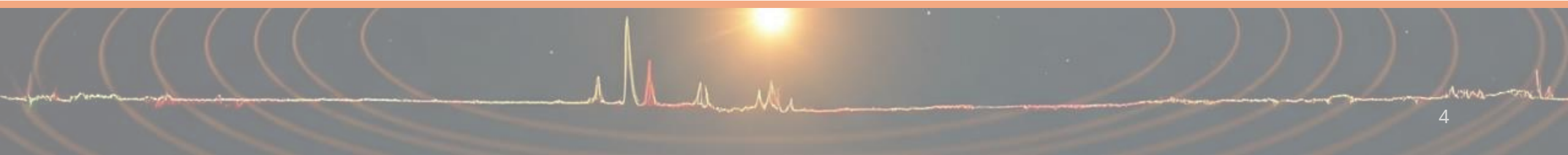
Motivation

- 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**.



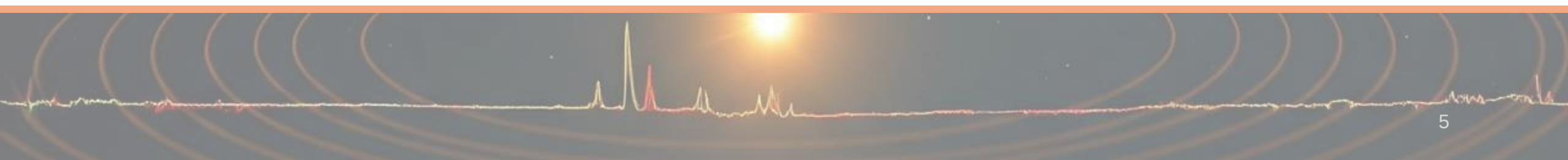
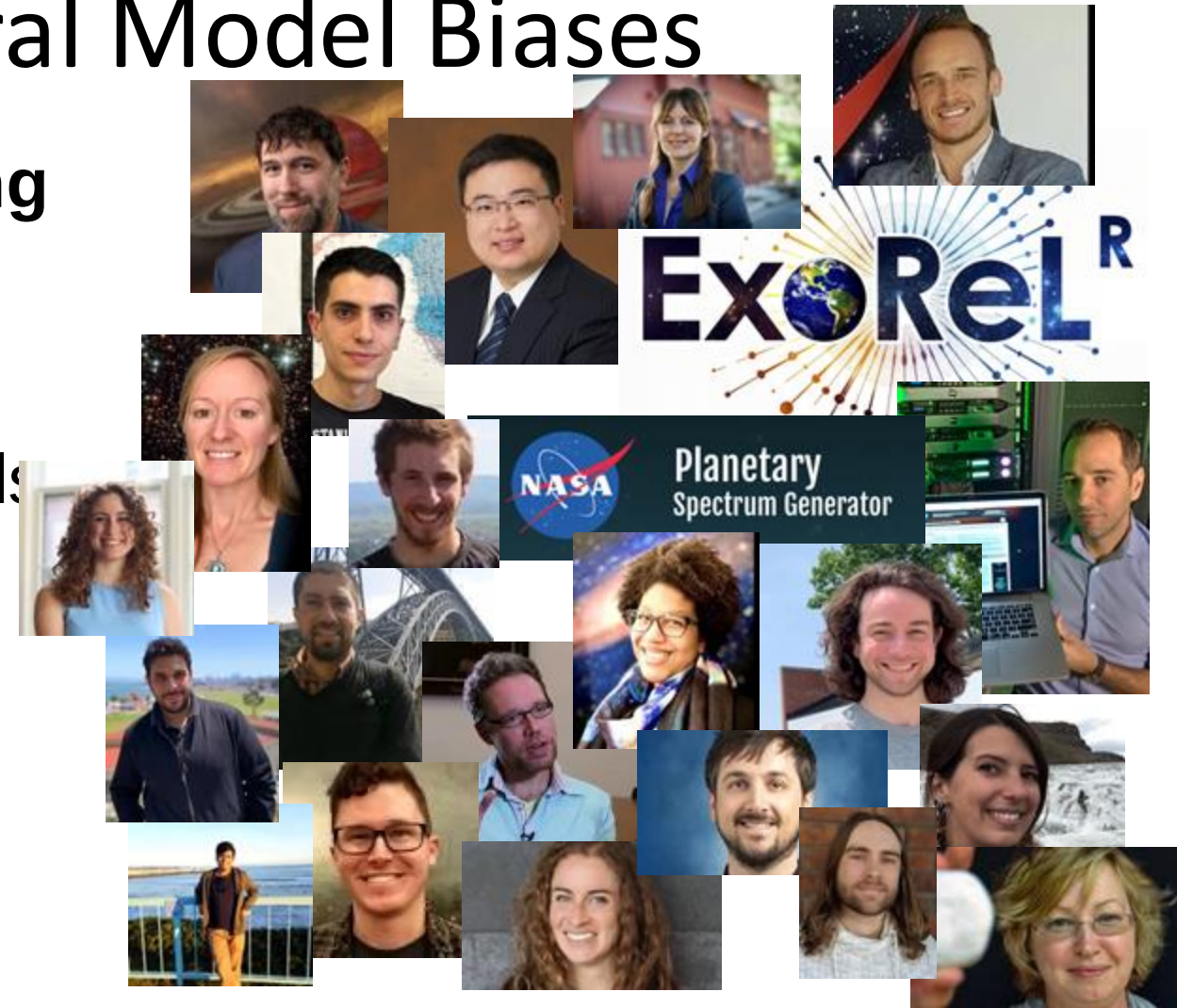
Risk

- 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 $1.1\ \mu\text{m}$ yields a strong H_2O detection while Model Y says that SNR of 20 is required.



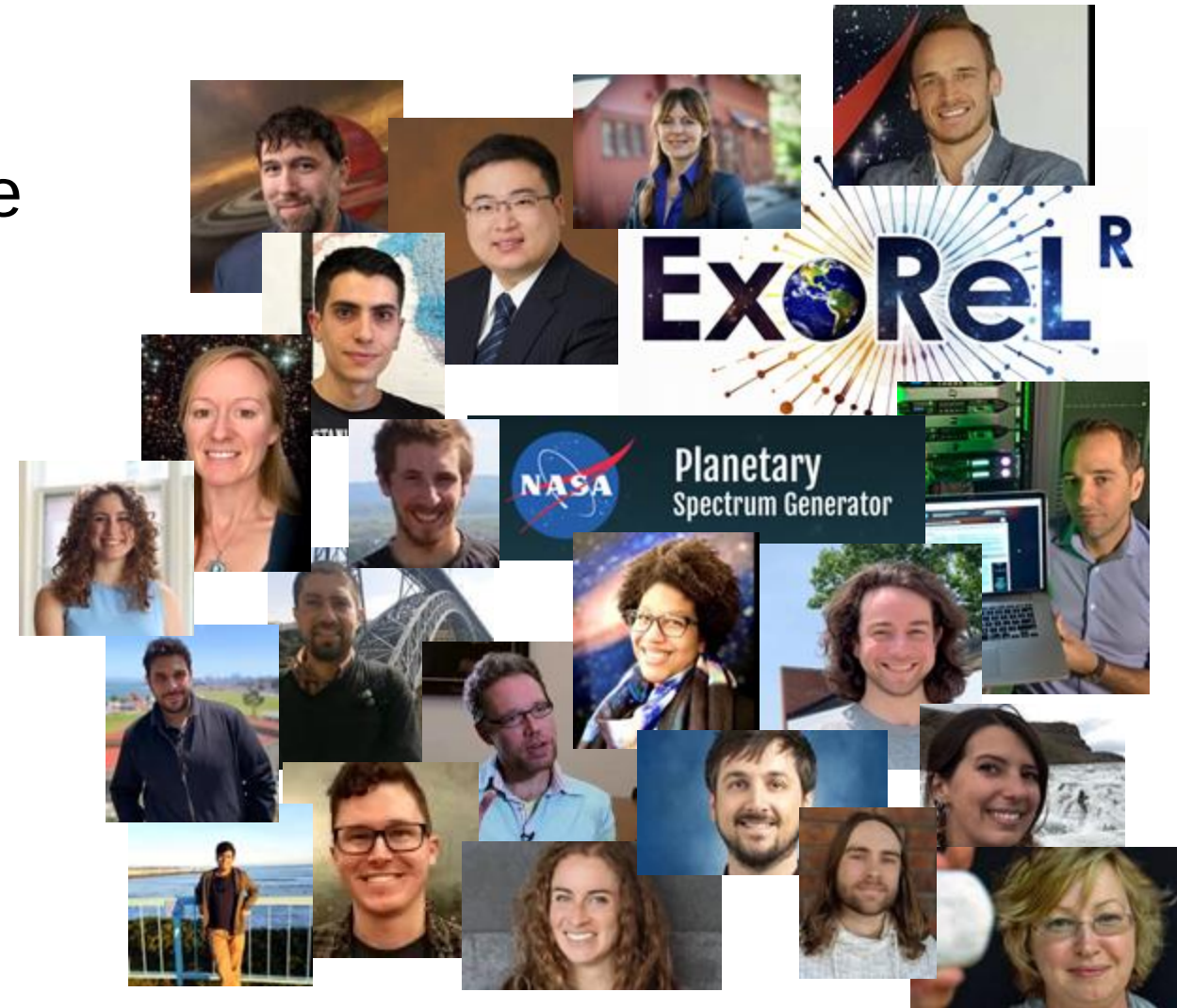
SAG 26: Addressing Spectral Model Biases

- 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 (μm): 0.2–5.0

Resolving Power: >10,000 (cross sections); >1,000 (transmission)

Outputs

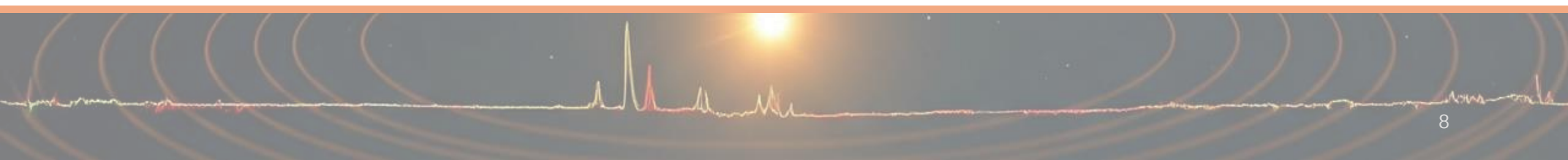
1. Cross section file
 - a. ASCII-formatted
 - b. Columns of wavelength (μm), absorption cross section (cm²/molecule)
2. Transmission file
 - a. ASCII-formatted
 - b. Columns of wavelength (μm), transmission through a column:
$$N_c = p/g/m$$
where N_c is the number of molecules per unit area, p is the pressure for this case (e.g., 1e3 Pa or 1e5 Pa), $g = 10 \text{ m s}^{-2}$, 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_hitrans2020_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

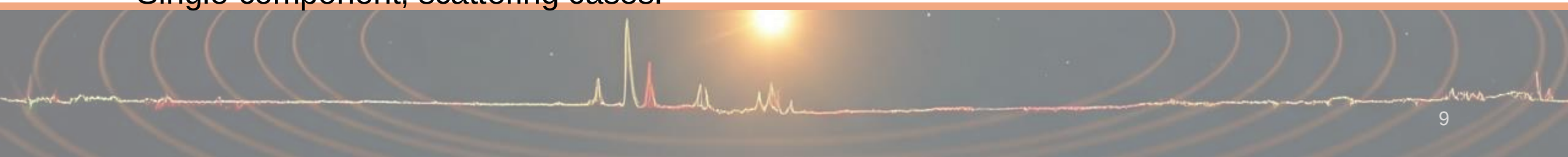
Approach

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

[illegible]

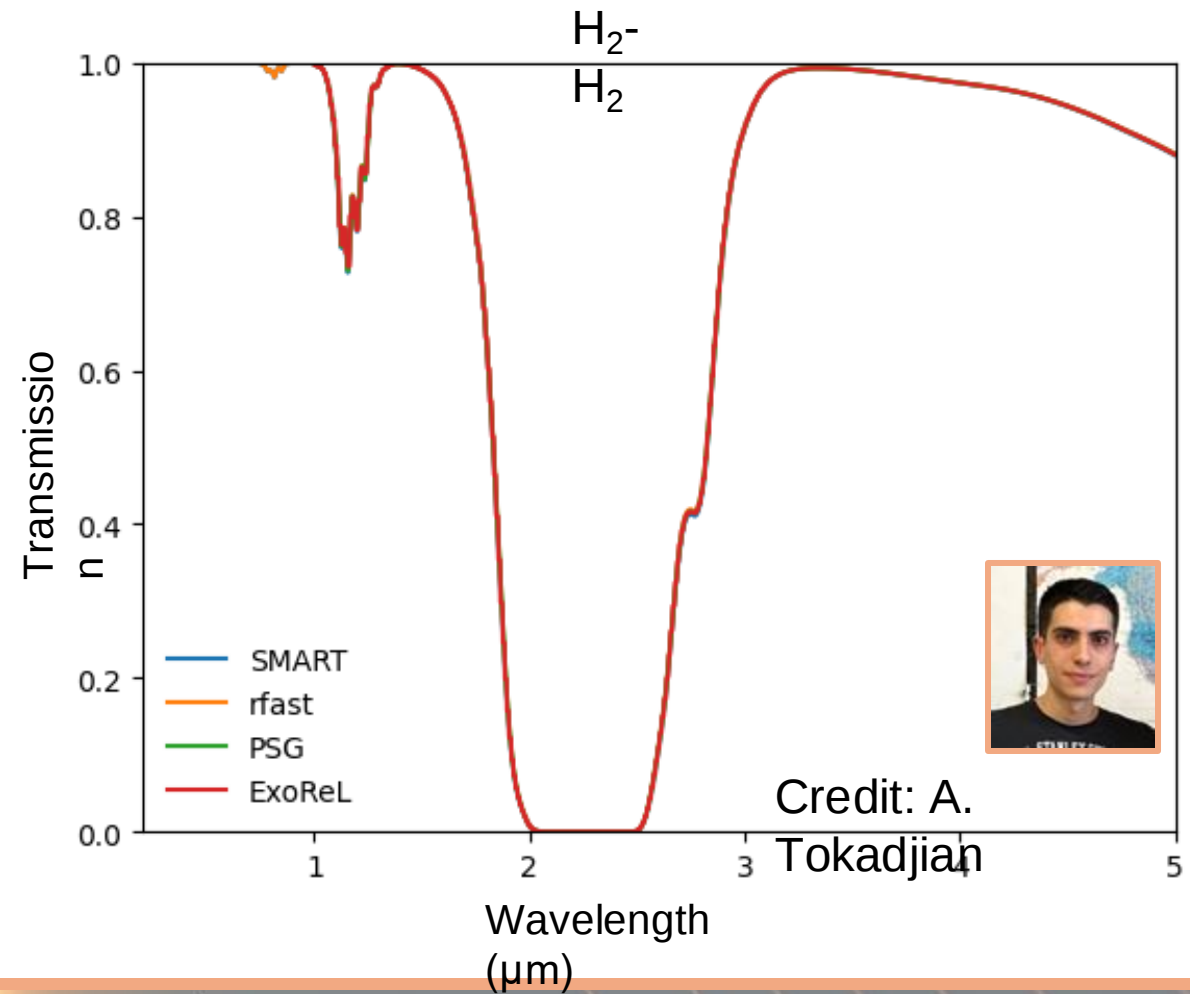
Results: Overview of Progress To-Date

- 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 ($\text{H}_2\text{-H}_2$, $\text{O}_2\text{-O}_2$, $\text{N}_2\text{-N}_2$)
- For all opacity cases, differences attributable to known model assumptions.
- Ongoing intercomparison of spectral models.
 - Single-component, scattering cases.



Results: Overview of Progress To-Date

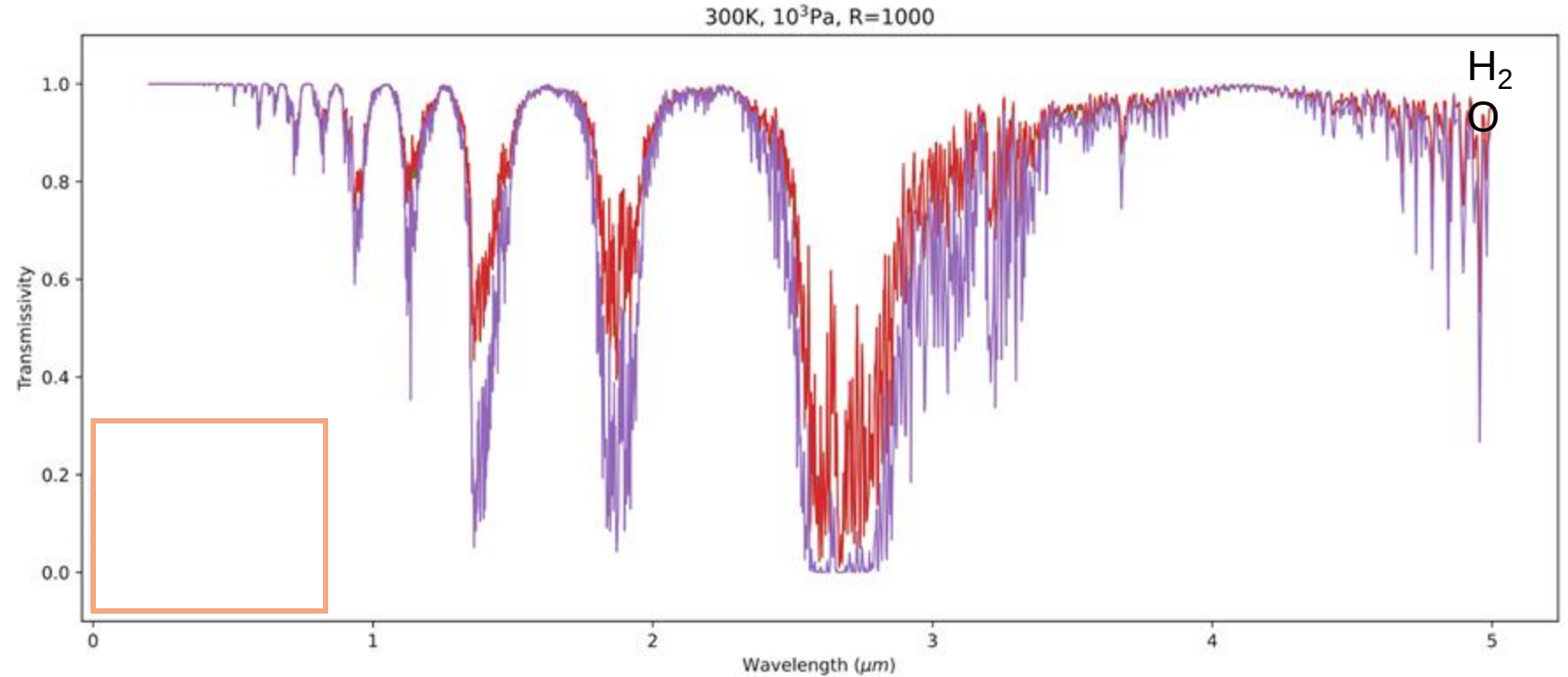
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 - Rayleigh scattering (CH_4 , CO_2 , CO , H_2 , H_2O , O_2 , N_2 , O_3)
 - Collision-Induced Absorption (H_2 - H_2 , O_2 - O_2 , N_2 - N_2)
- For all opacity cases, differences attributable to known model assumptions.
- Ongoing intercomparison of spectral models.
 - Single-component, scattering cases.



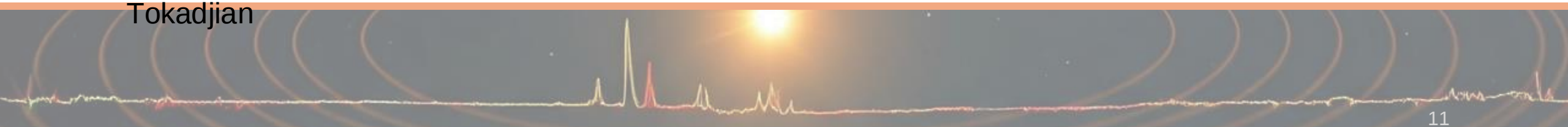
Results: Line Absorption

Earliest comparisons revealed:

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



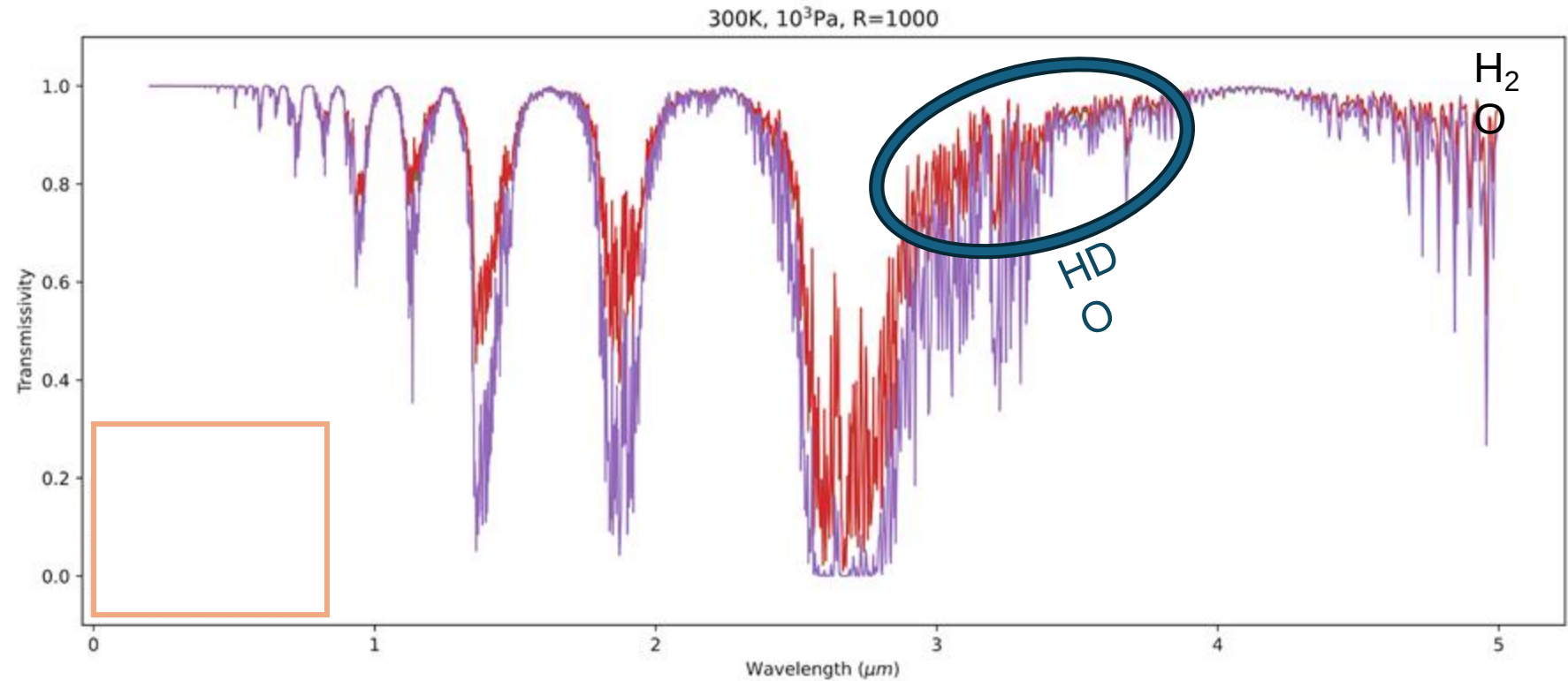
Credit: A.
Tokadjian



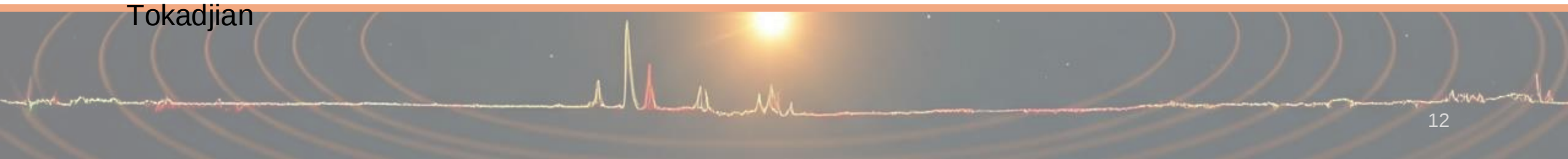
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Tokadjian

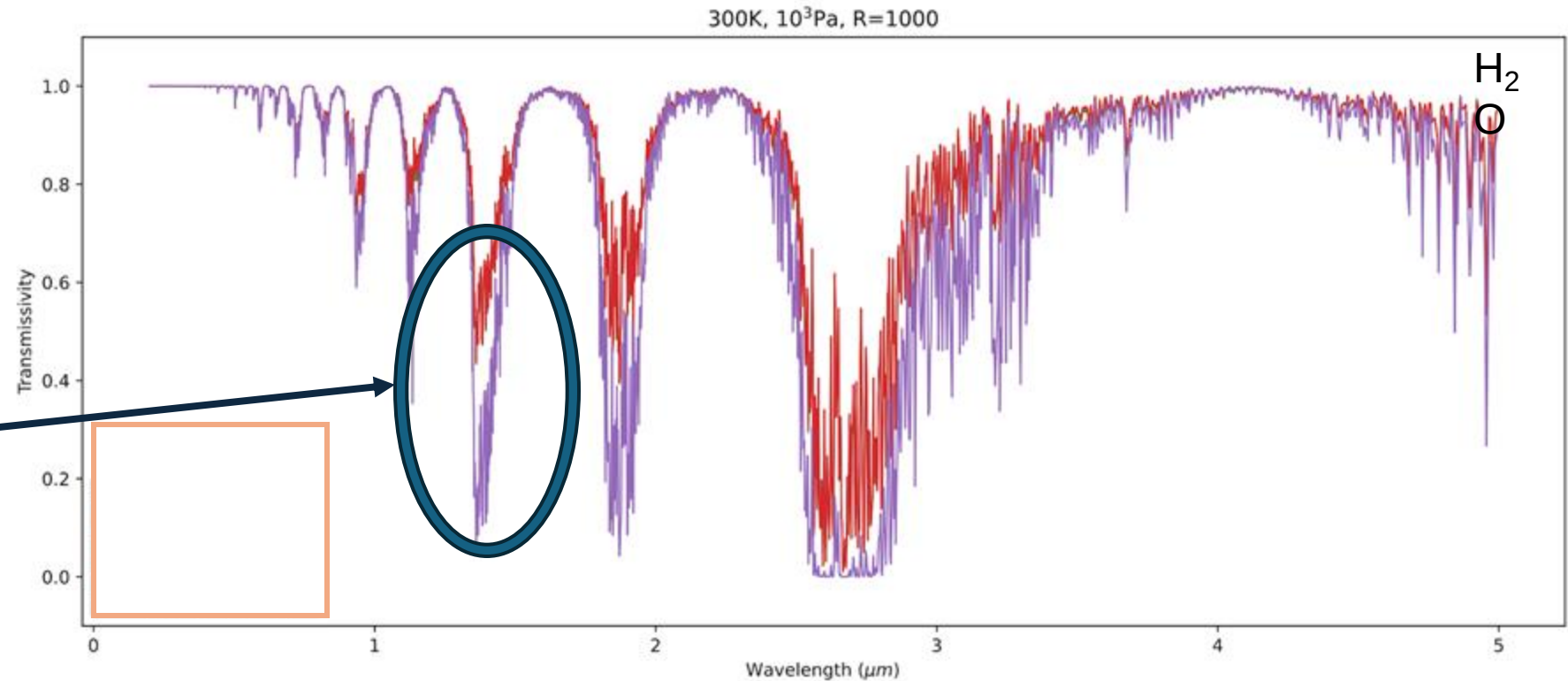


Results: Line Absorption

Earliest comparisons revealed:

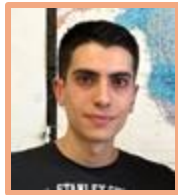
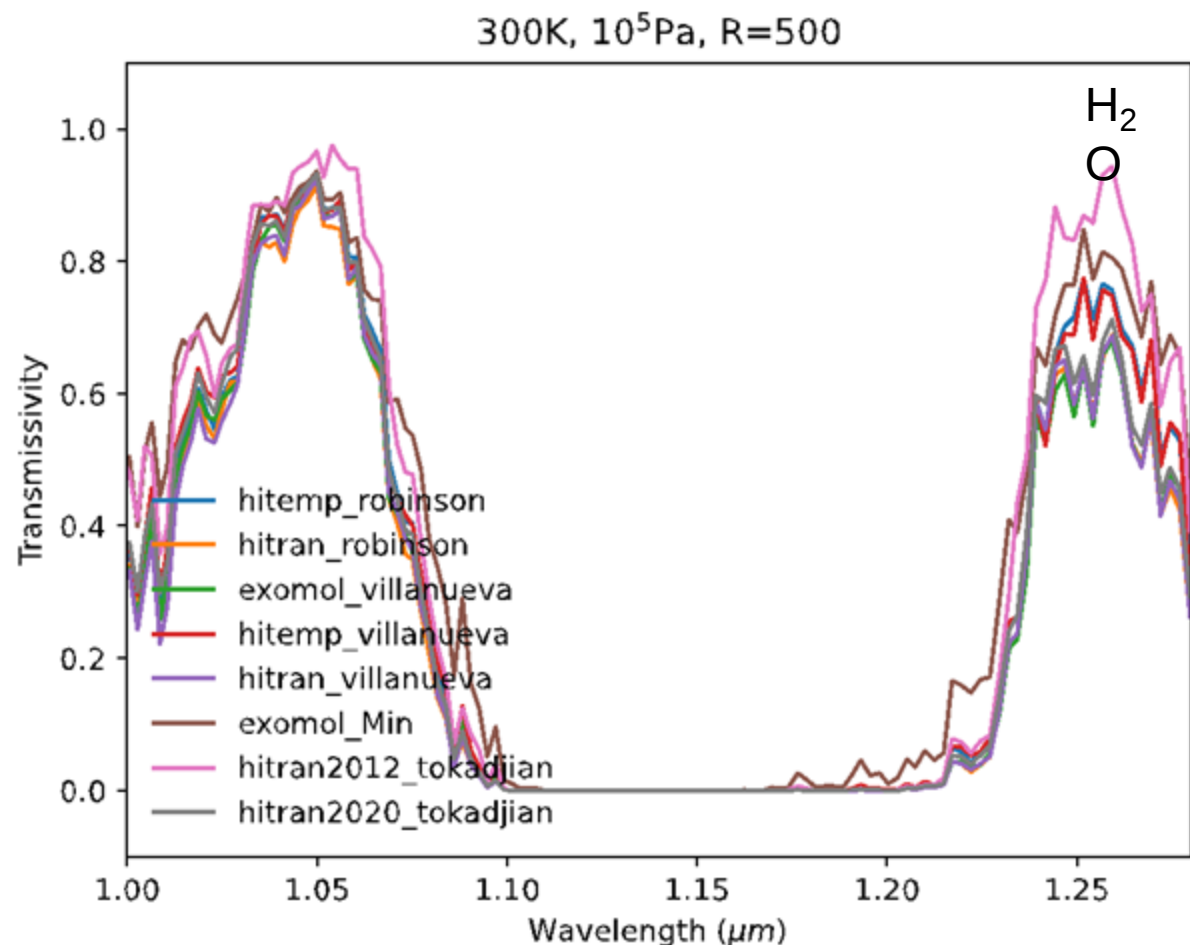
- major model differences, and
- flaws in experiment design.

sensitive to resolution of
participant-provided opacities

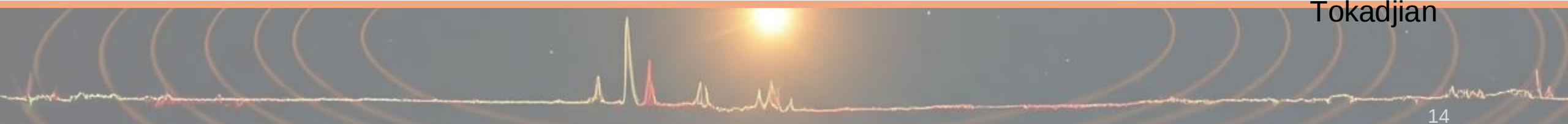


Credit: A.
Tokadjian

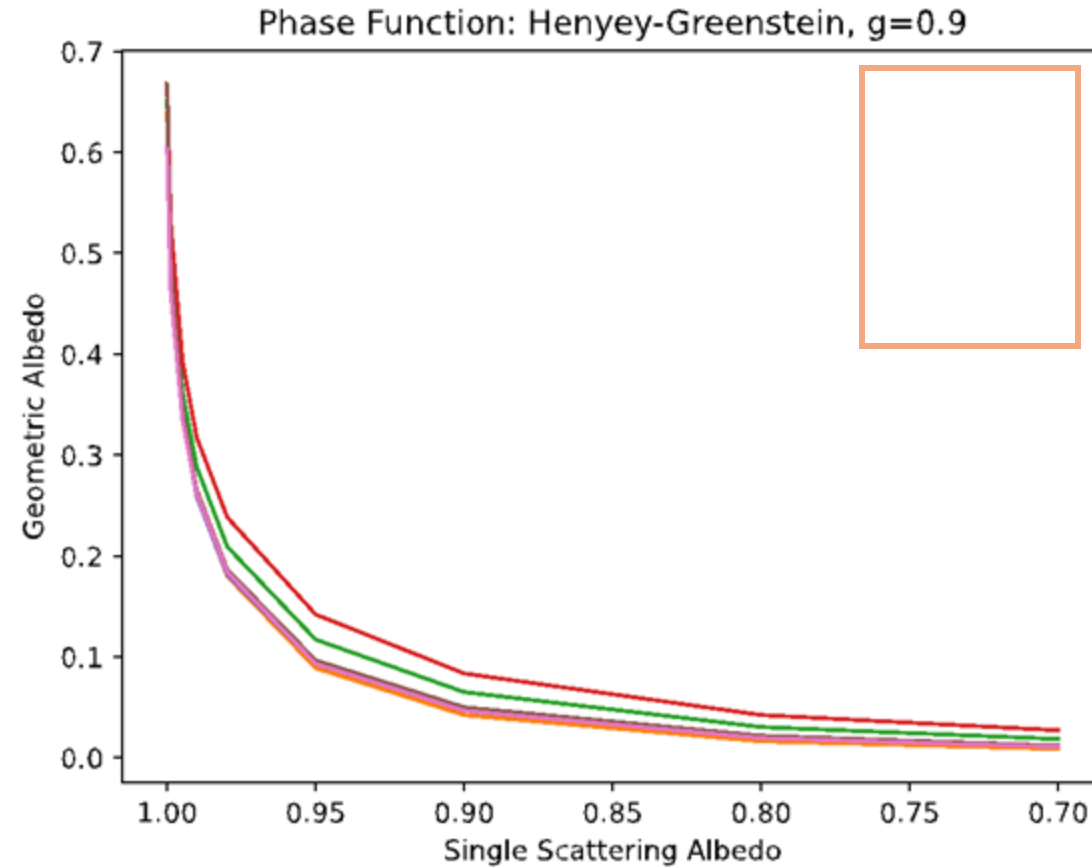
Results: Line Absorption



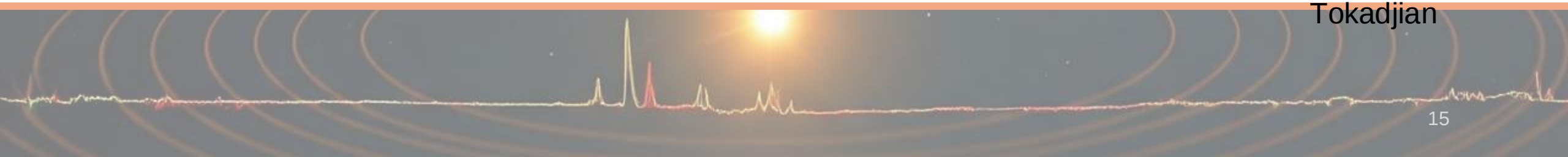
Credit: A.
Tokadjian



Results: Spectral Models

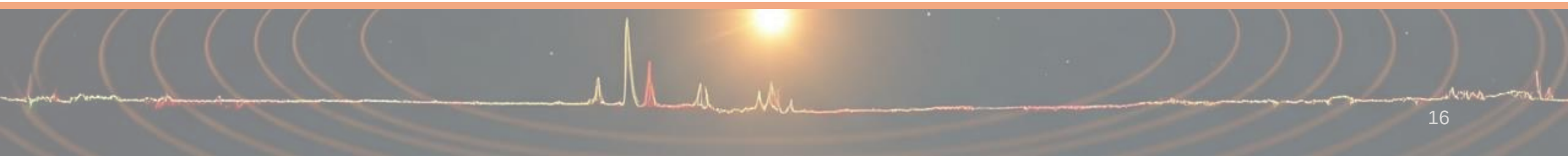


Credit: A.
Tokadjian



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).

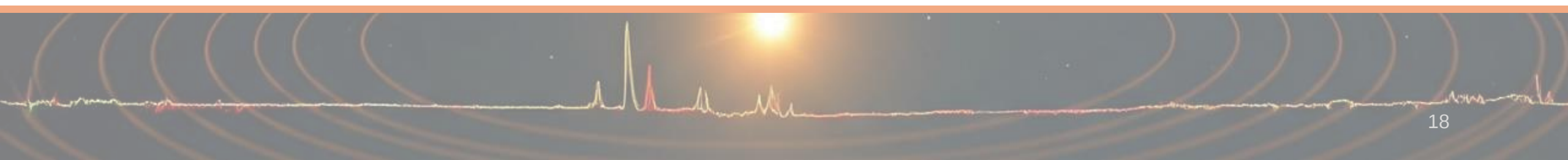


Next Steps

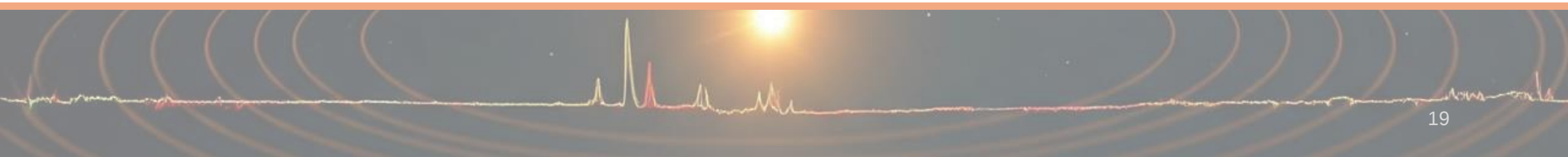
- Complete ongoing comparisons of forward (spectral) models. (Sp25)
 - Propagate opacity spread through RT models.
 - Consider cases w/cloud scattering.
- Design, execute retrieval intercomparison. (Su25)
 - Work with ongoing RISOTTO intercomparison (Young/A1e1).
- Update and complete SAG 26 report. (Sp25-Fa25)
- Package results for long-term preservation and long-lived utility.

Summary Redux

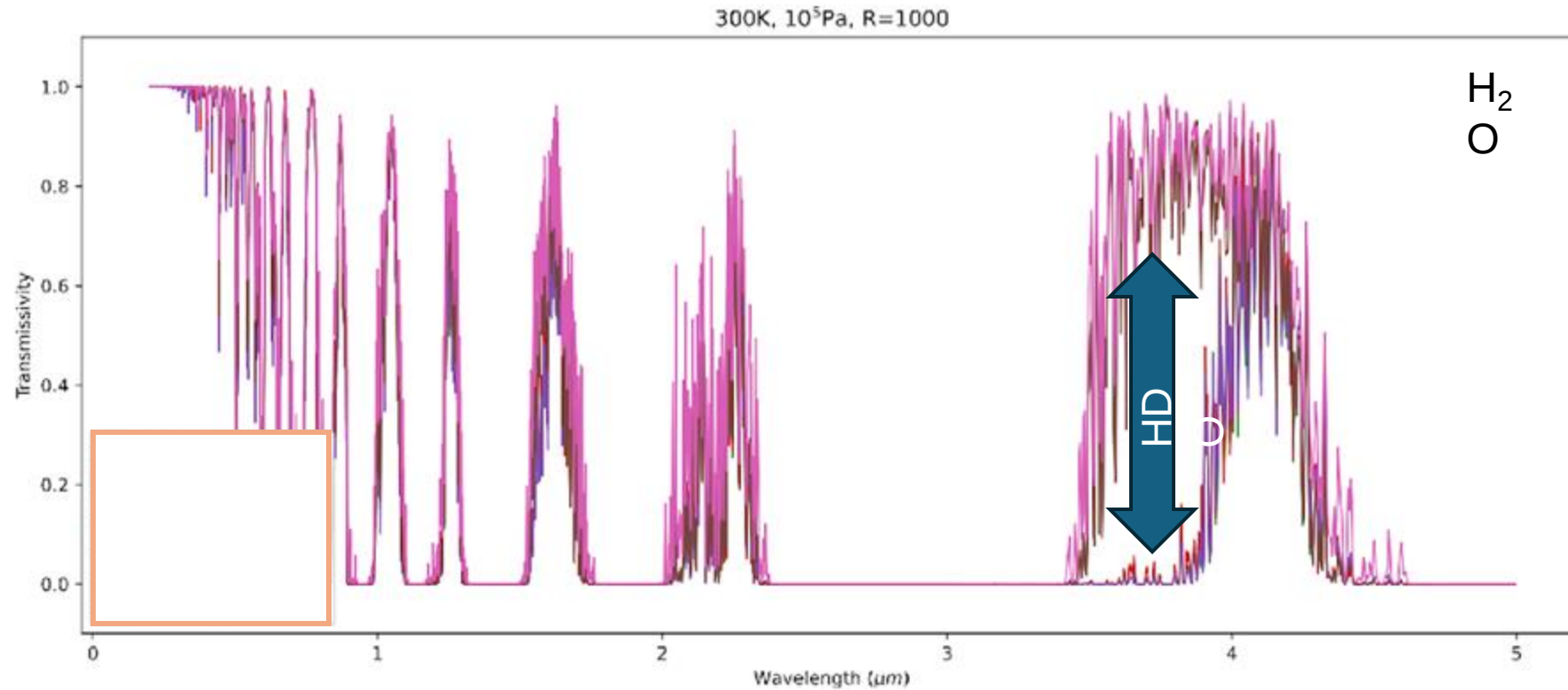
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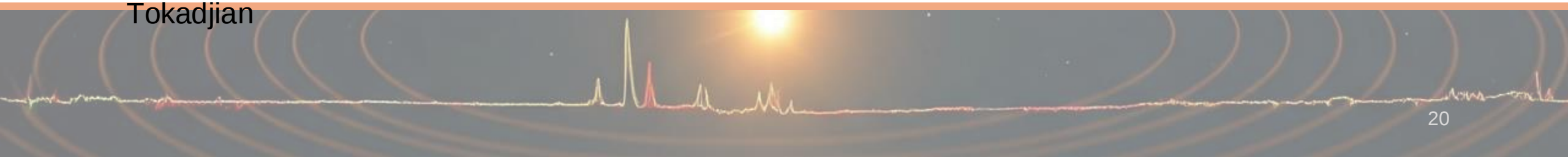
Begin Backup Slides



Results: Line Absorption

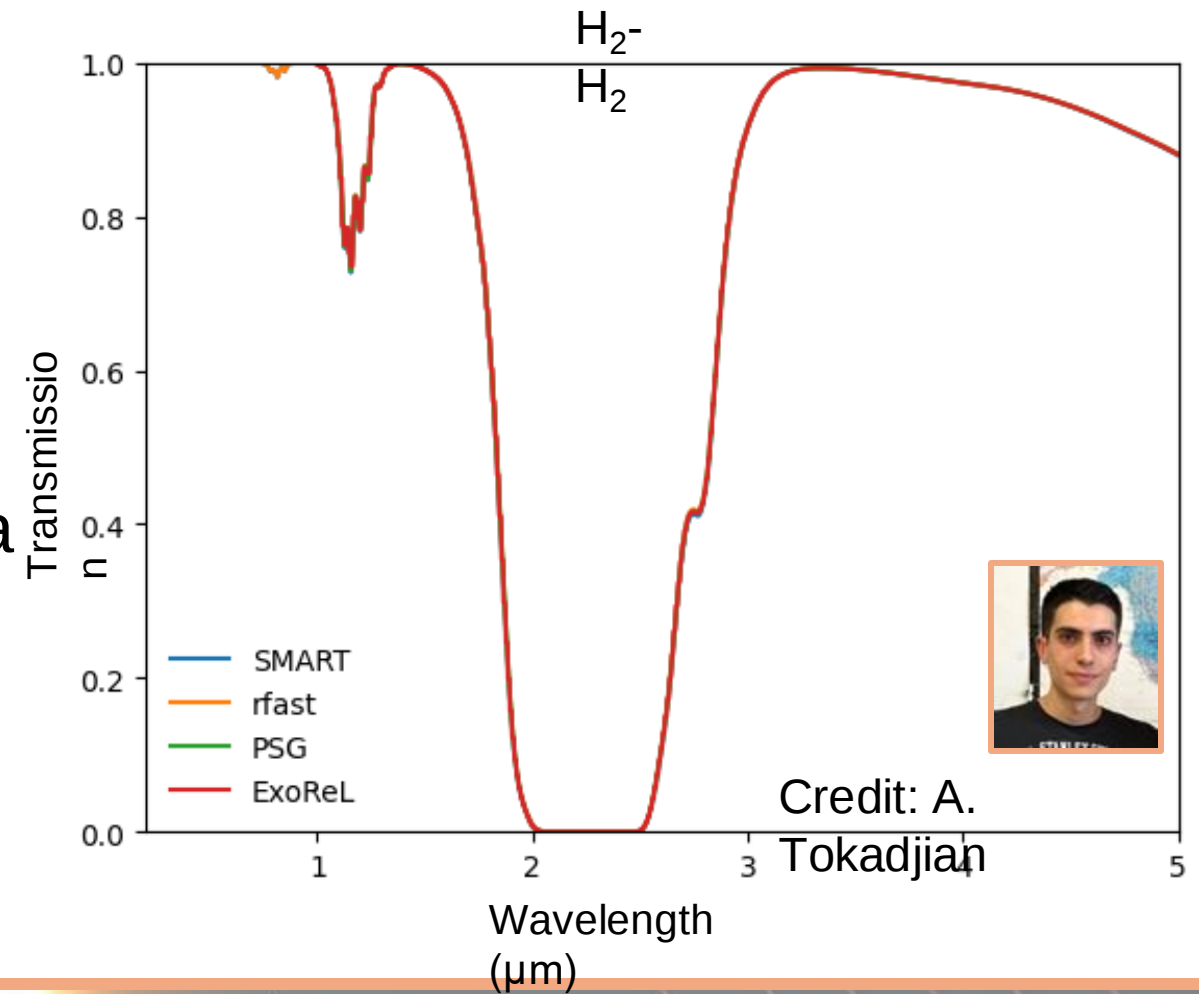


Credit: A.
Tokadjian

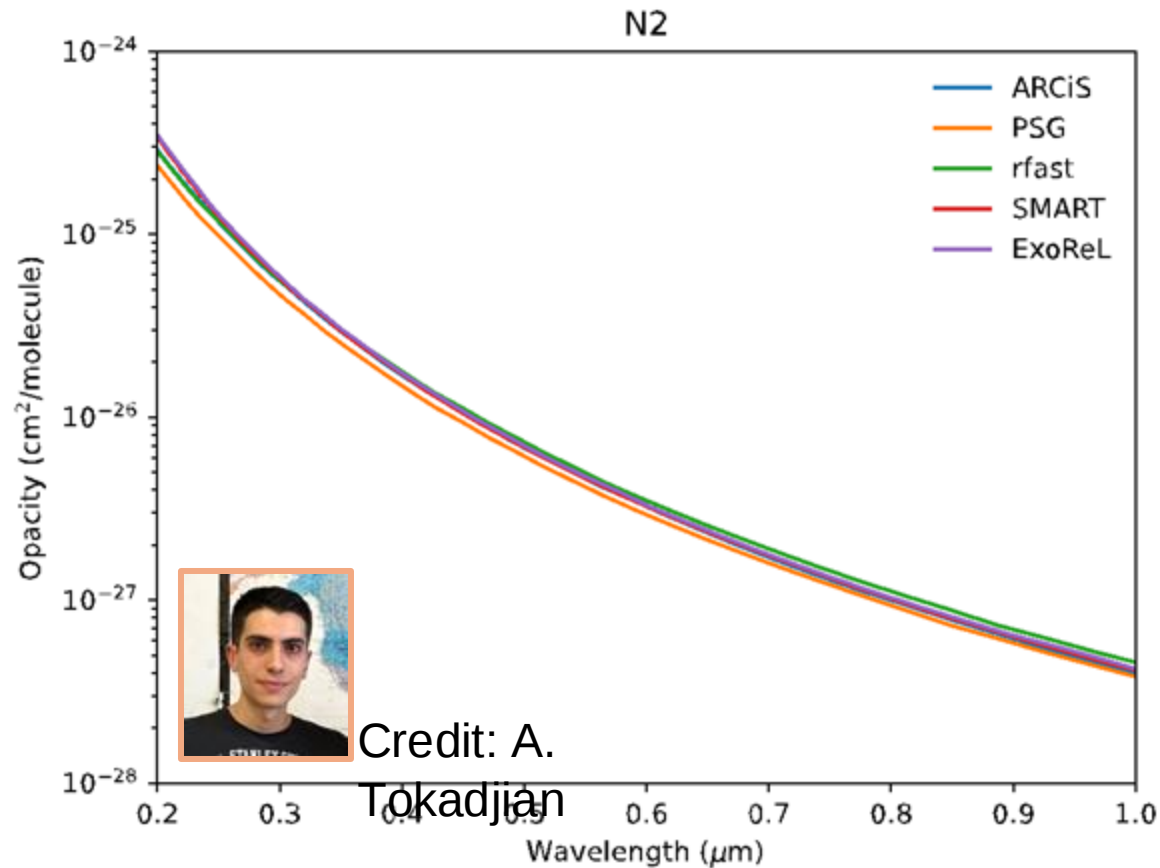


Results: Collision-Induced Absorption

- Compared all of:
 - $\text{H}_2\text{-H}_2$, $\text{O}_2\text{-O}_2$, $\text{N}_2\text{-N}_2$
- Small differences attributable to data augmentations beyond HITRAN.

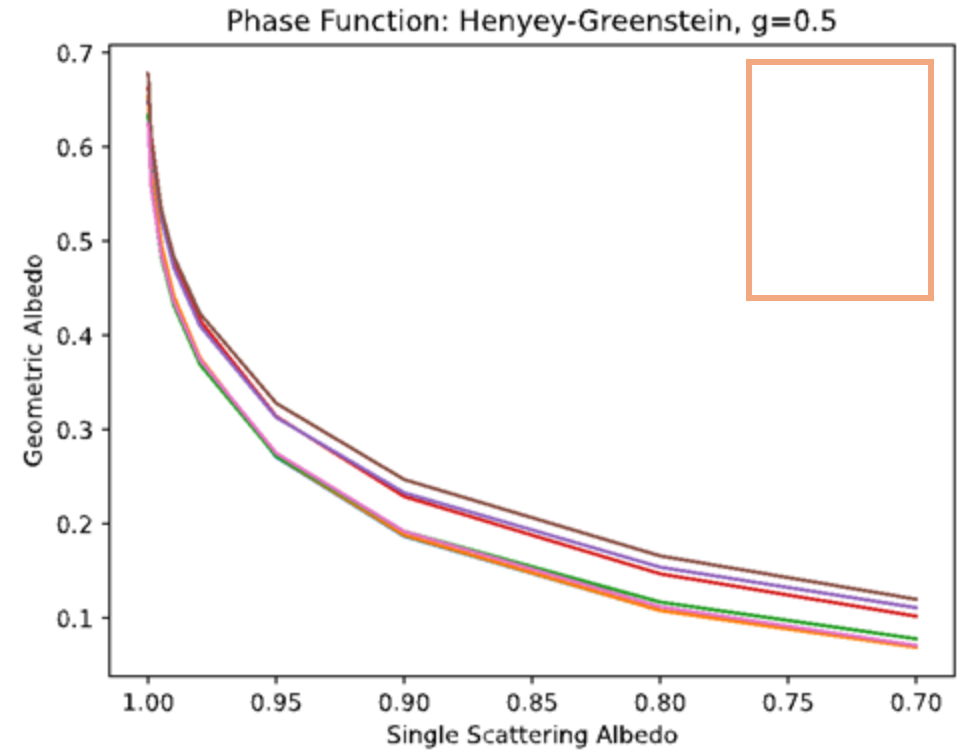
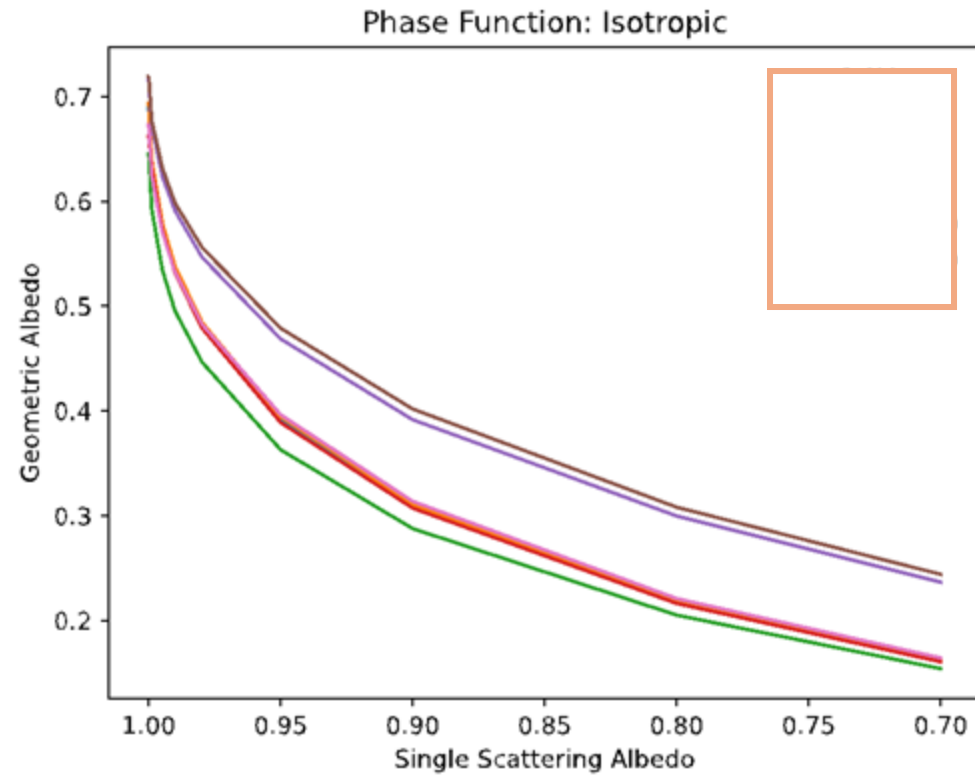


Results: Rayleigh Scattering Cross Sections

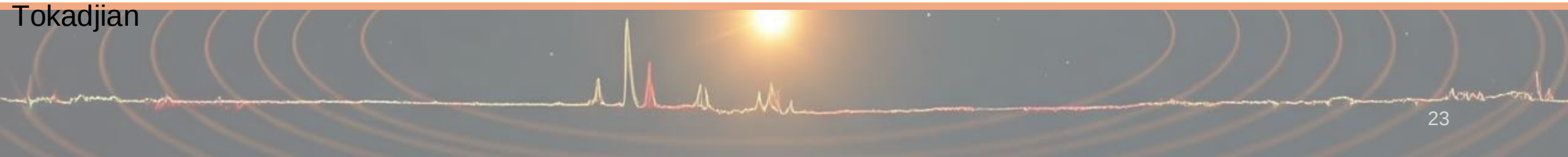


- Strong agreement for all of:
 - CH₄, CO₂, CO, H₂, H₂O, O₂, N₂, O₃
- Small differences attributable to model assumptions.

Results: Spectral Models



Credit: A.
Tokadjian



Results: Spectral Models

