# Cosmic-Ray Astrochemistry

## Why chemistry matters and what it tells you


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ADS Library

Website

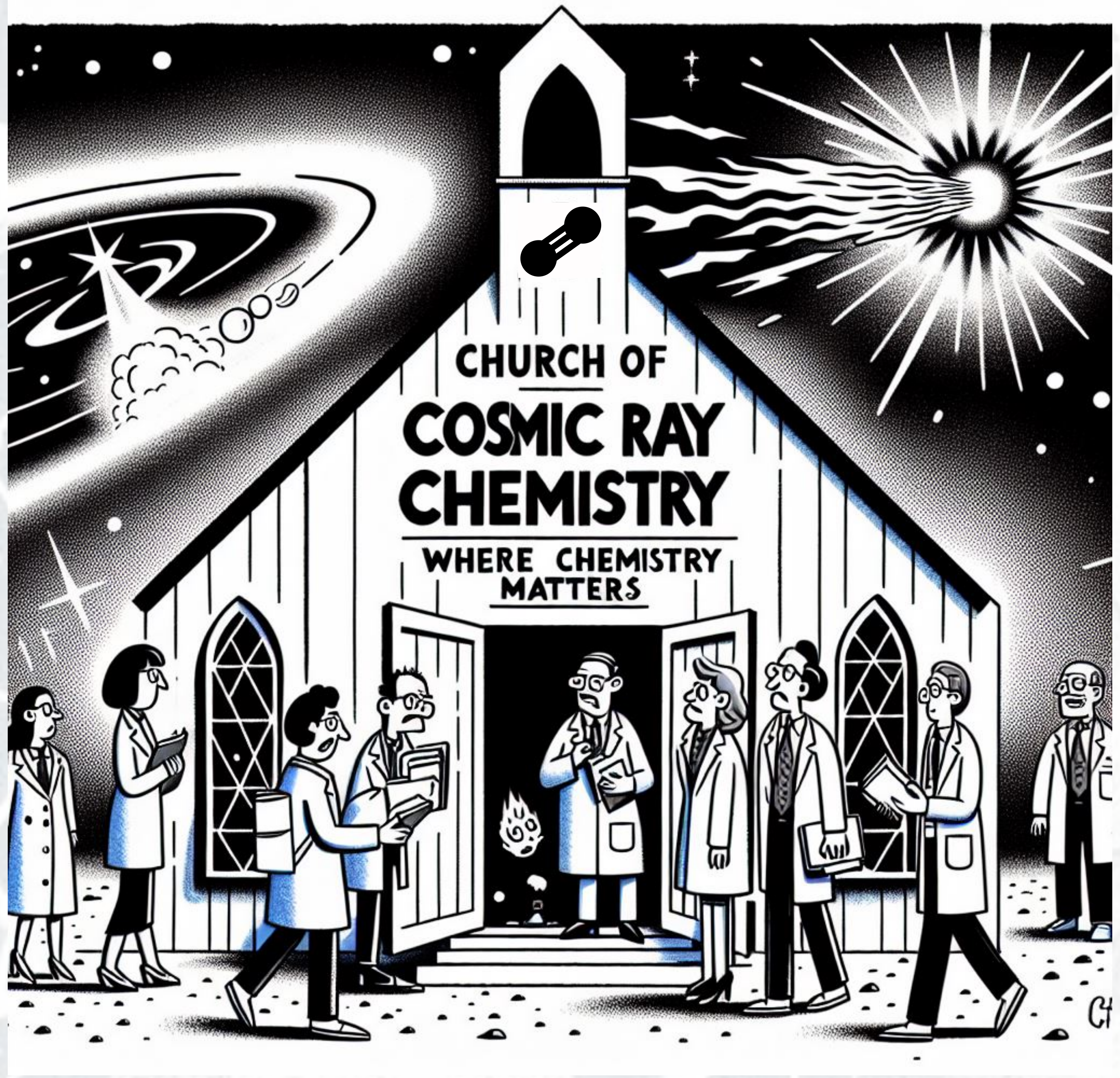
Referring to his 1926 Bakerian Lecture

*…having not yet rid myself of the tradition that "atoms are physics, but molecules are chemistry"*

- Sir Arthur S. Eddington, 1937

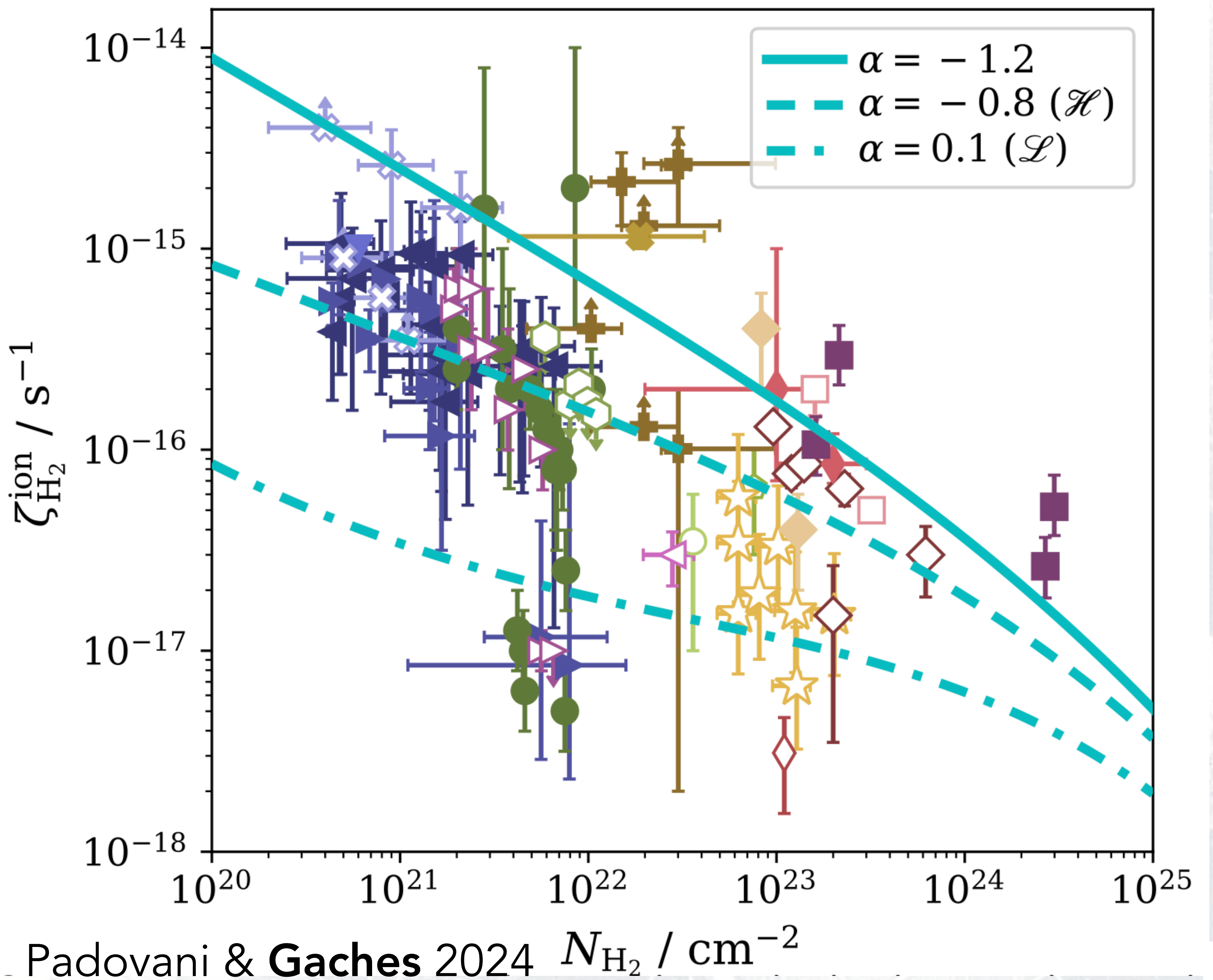
*~~…having not yet rid myself of the tradition that "atoms are physics, but molecules are chemistry"~~ molecules **probe** physics, molecules **enable** physics, molecules **are** physics and chemistry.*

~~*…having not yet rid myself of the tradition that "atoms are physics, but molecules are chemistry"*~~ *molecules **probe** physics, molecules **enable** physics, molecules **are** physics and chemistry.*



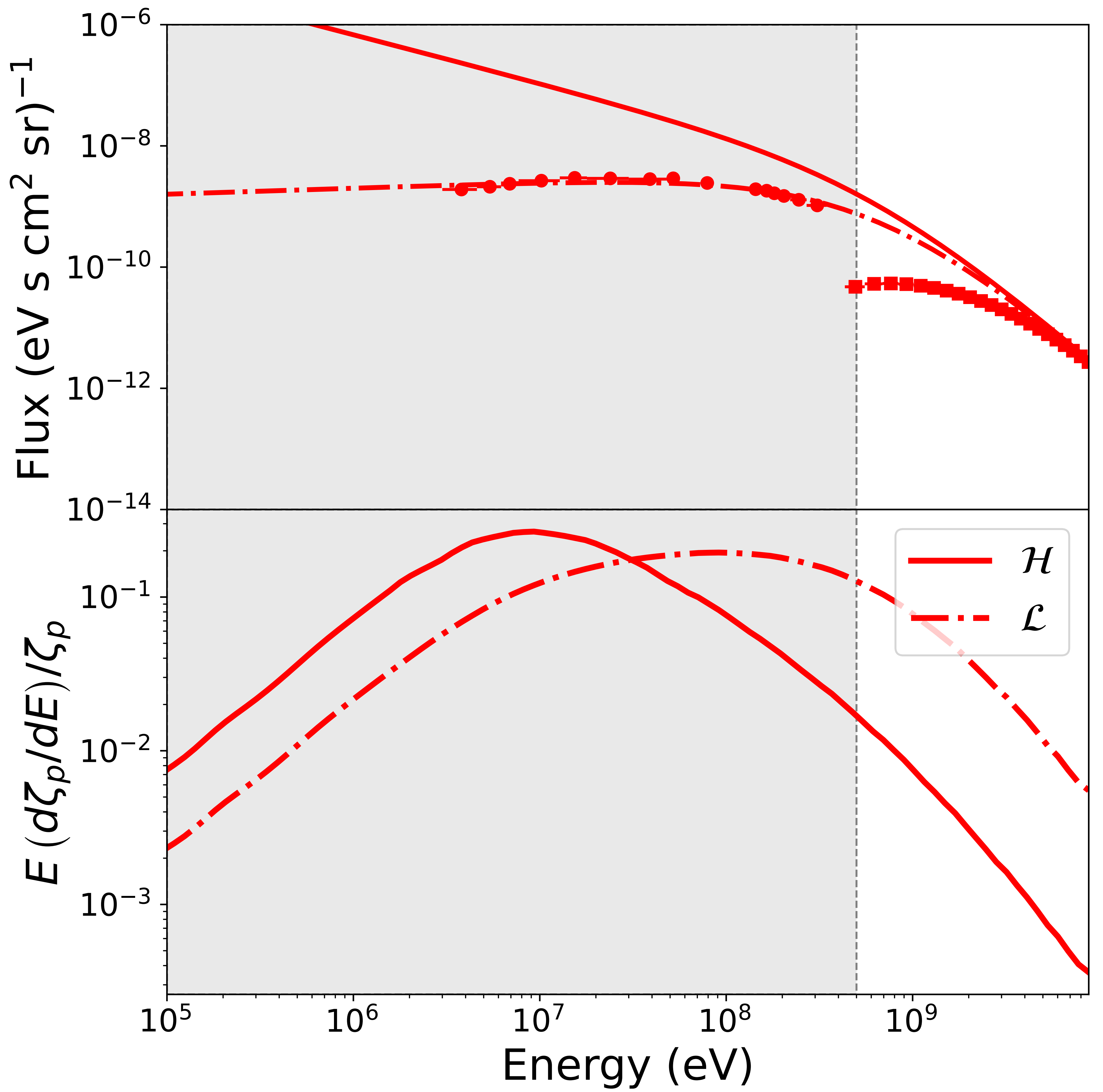
# Cosmic rays: drivers of molecular chemistry

As cosmic rays travel through clouds, they lose energy, **reducing their ionising effect**




Padovani & **Gaches** 2024

The protons with most importance are **between 1 MeV and 1 GeV**. Electrons in the 0.1 - 1 keV range.



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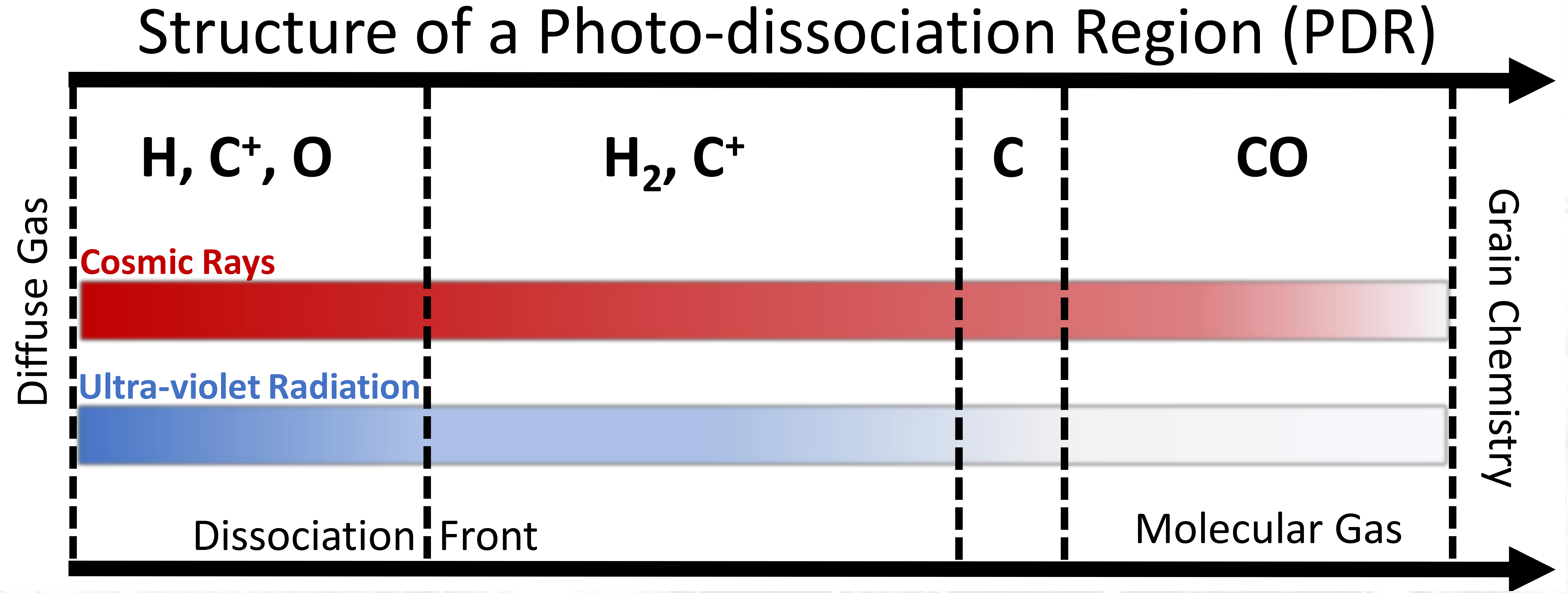
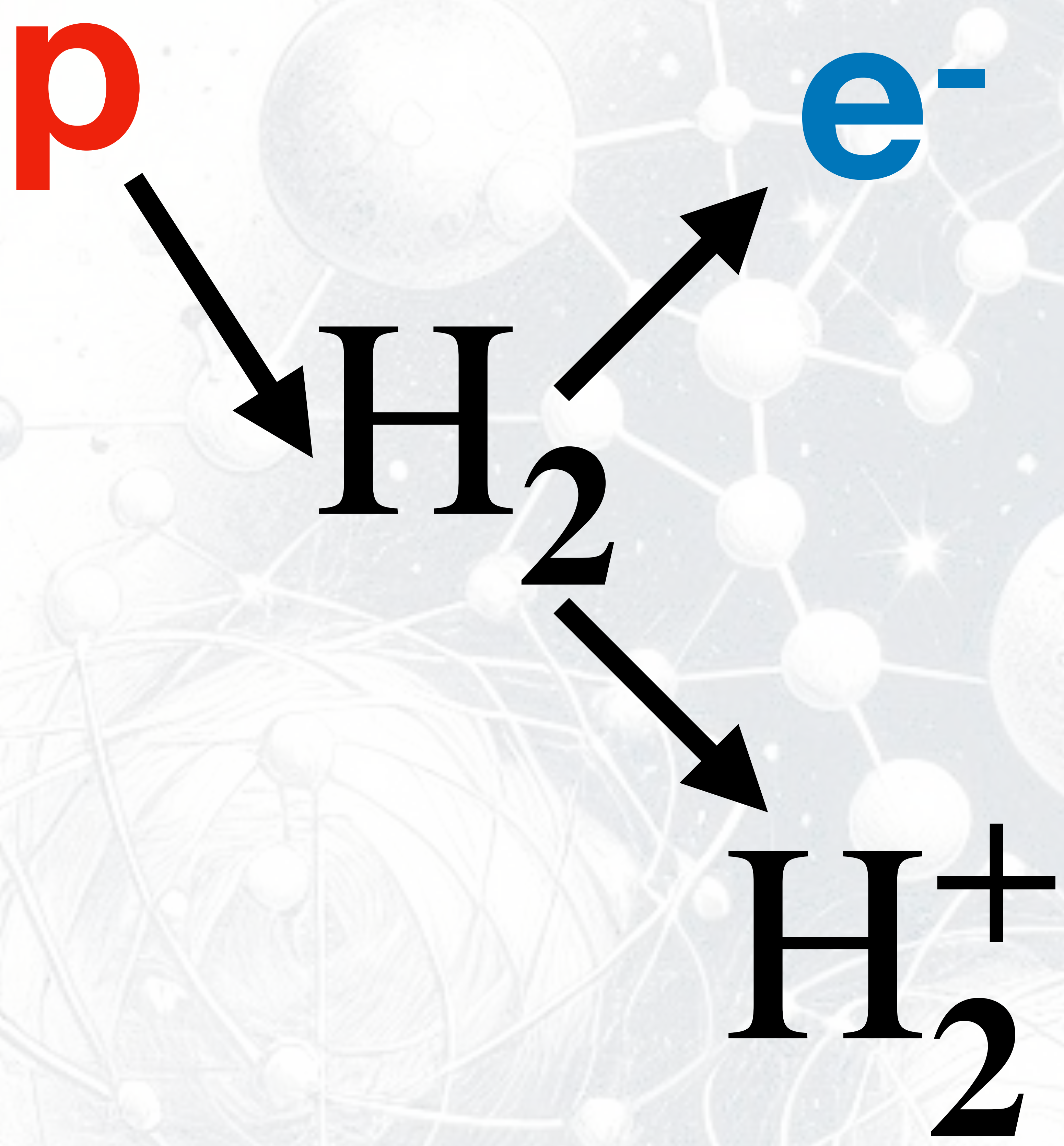
# Cake-ify a molecular cloud: what are its layers

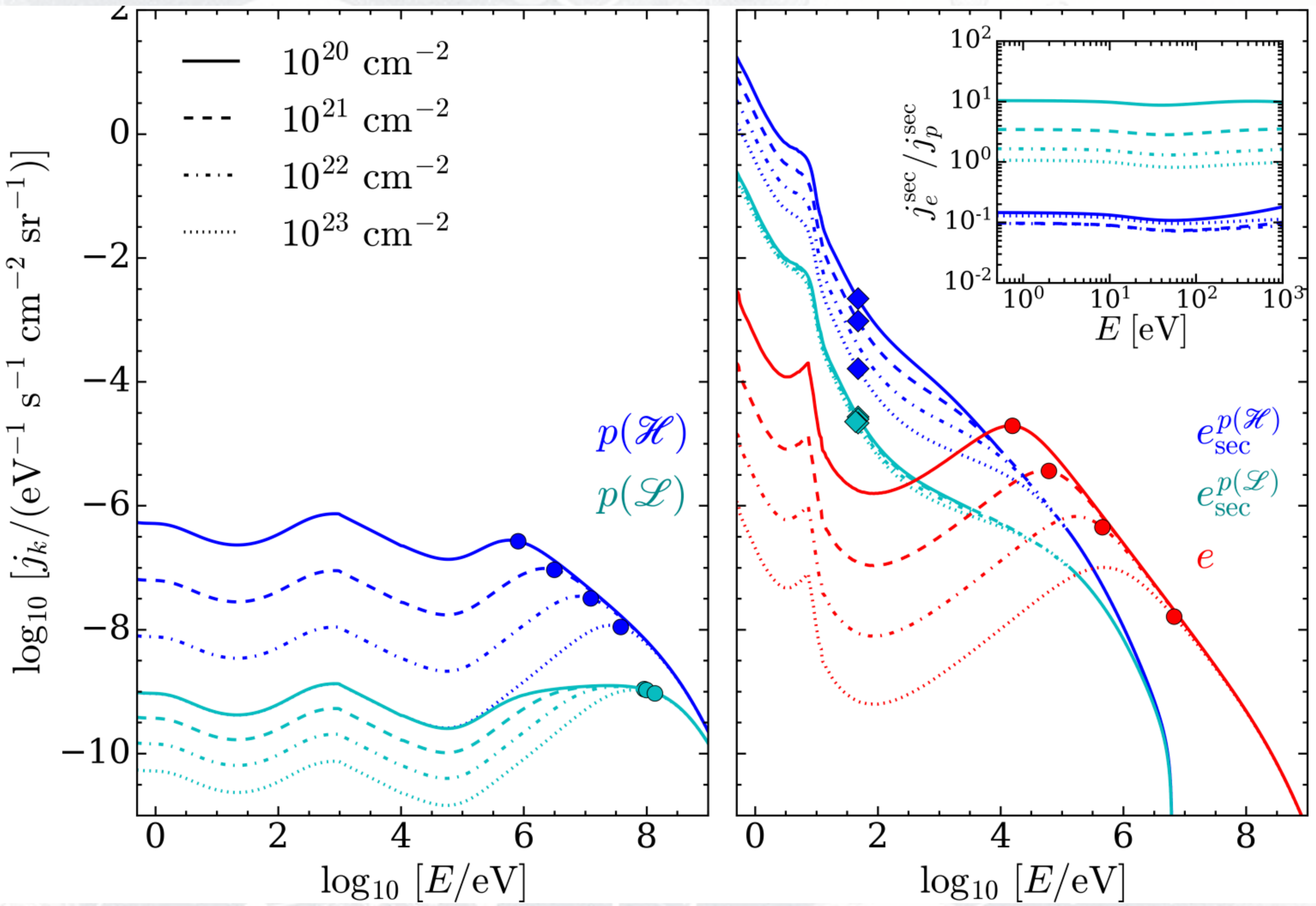
In the dense gas, shielded from UV, **cosmic rays drive** the chemistry



# Cosmic rays: Secondary electrons

Efficient secondary electron production, **ionizing and exciting molecules**

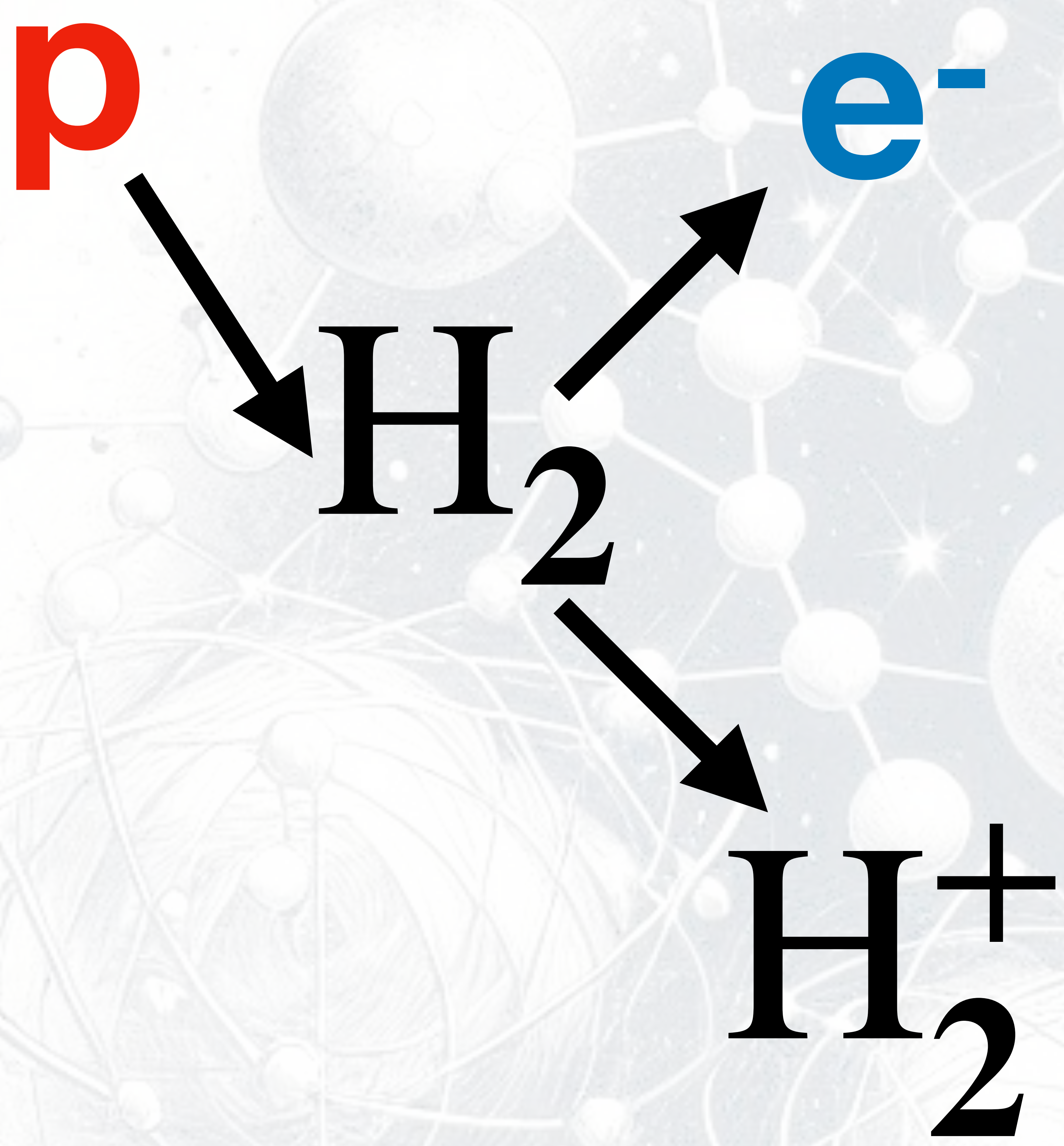


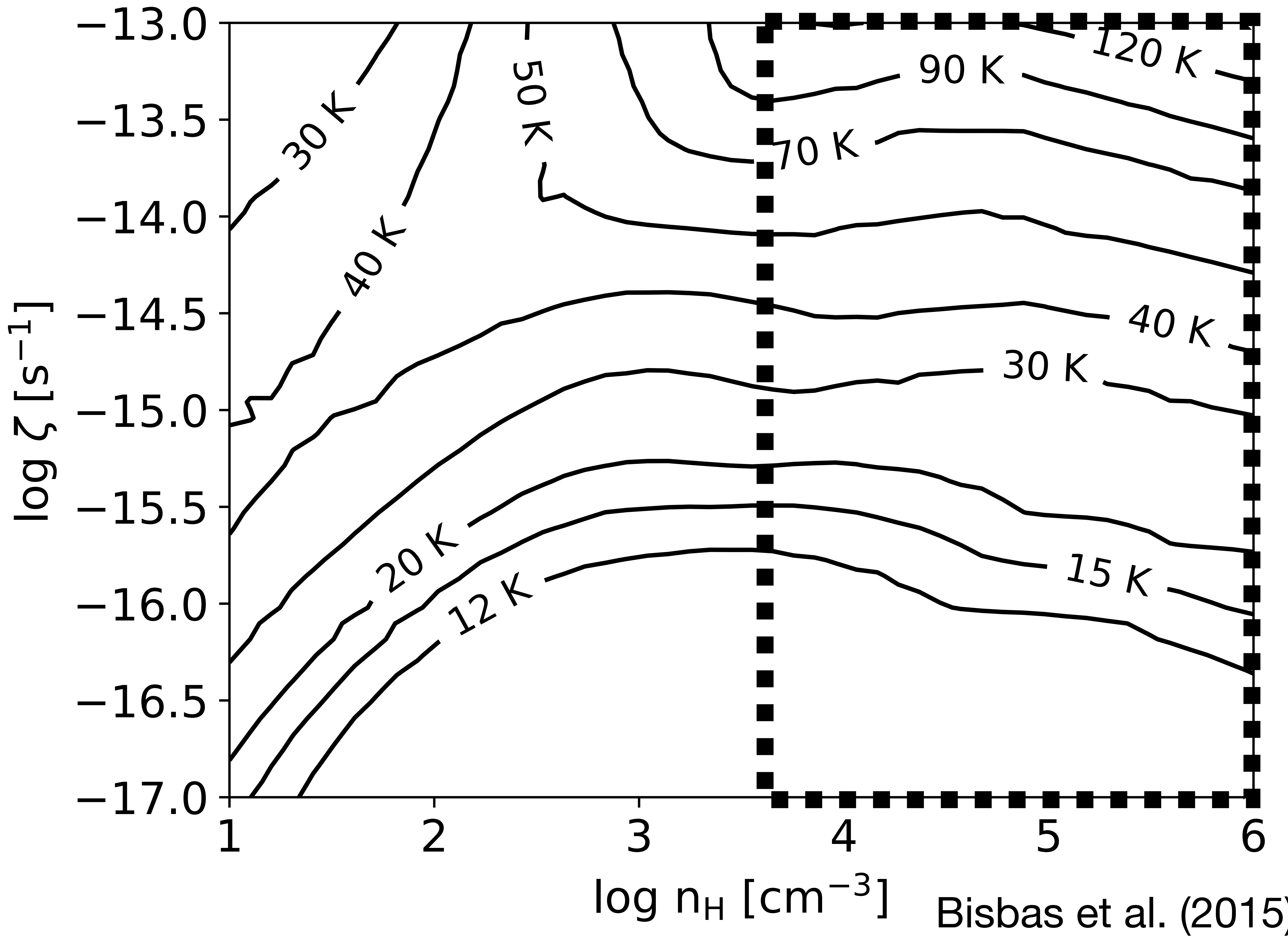




Padovani+2022

# Cosmic rays: Secondary electrons

## Electron collisional heating

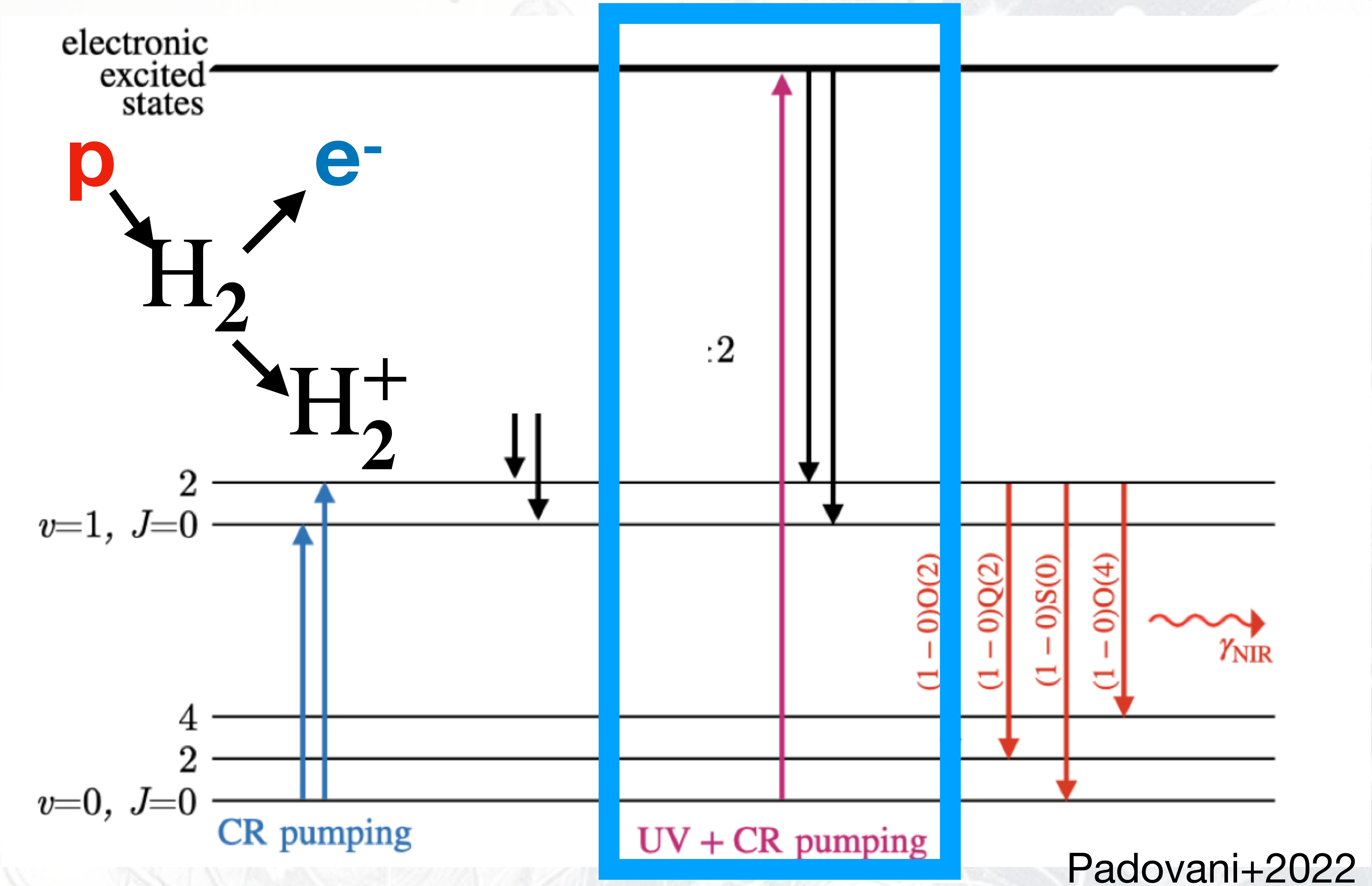



Bisbas et al. (2015)

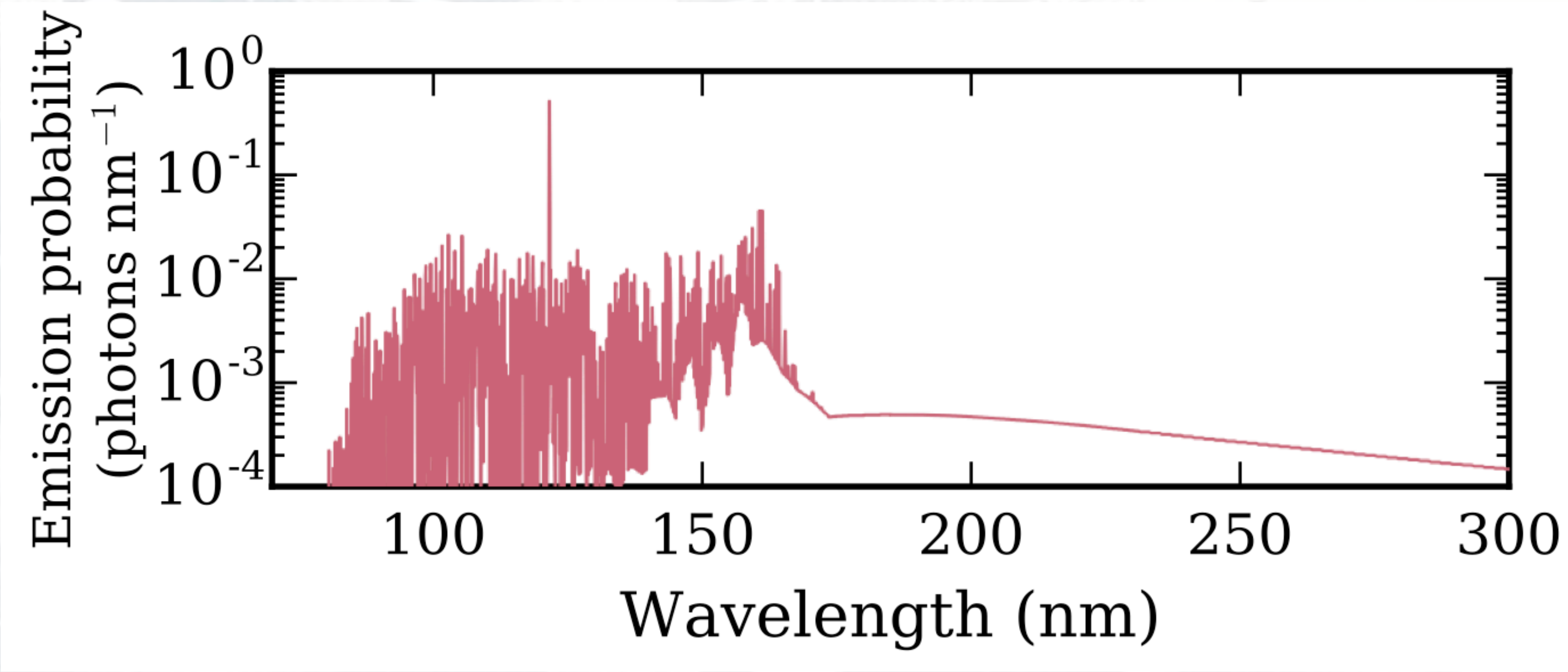
# Cosmic rays: Secondary electrons

## Ultraviolet radiation



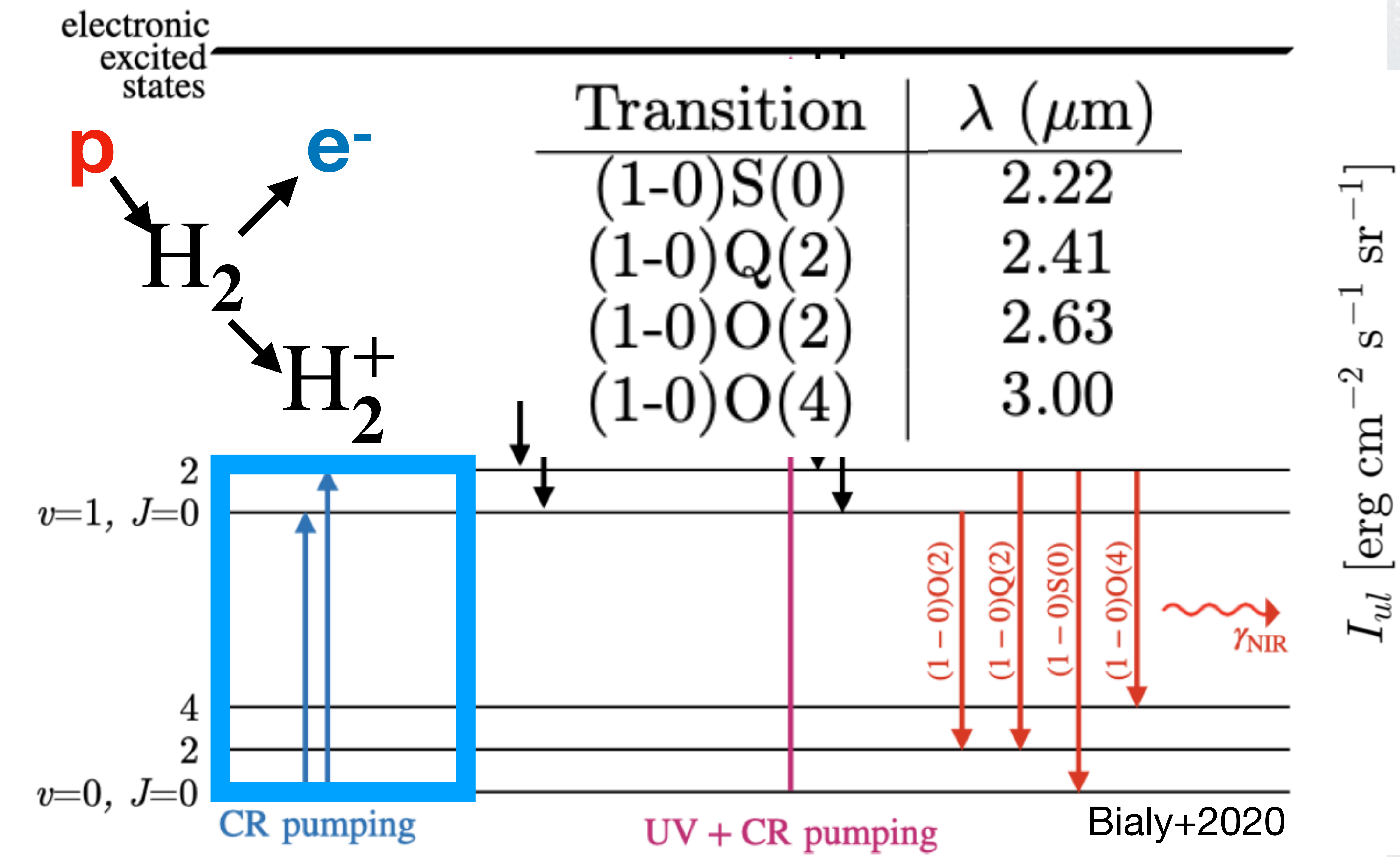

Padovani+2022

Heays+2017



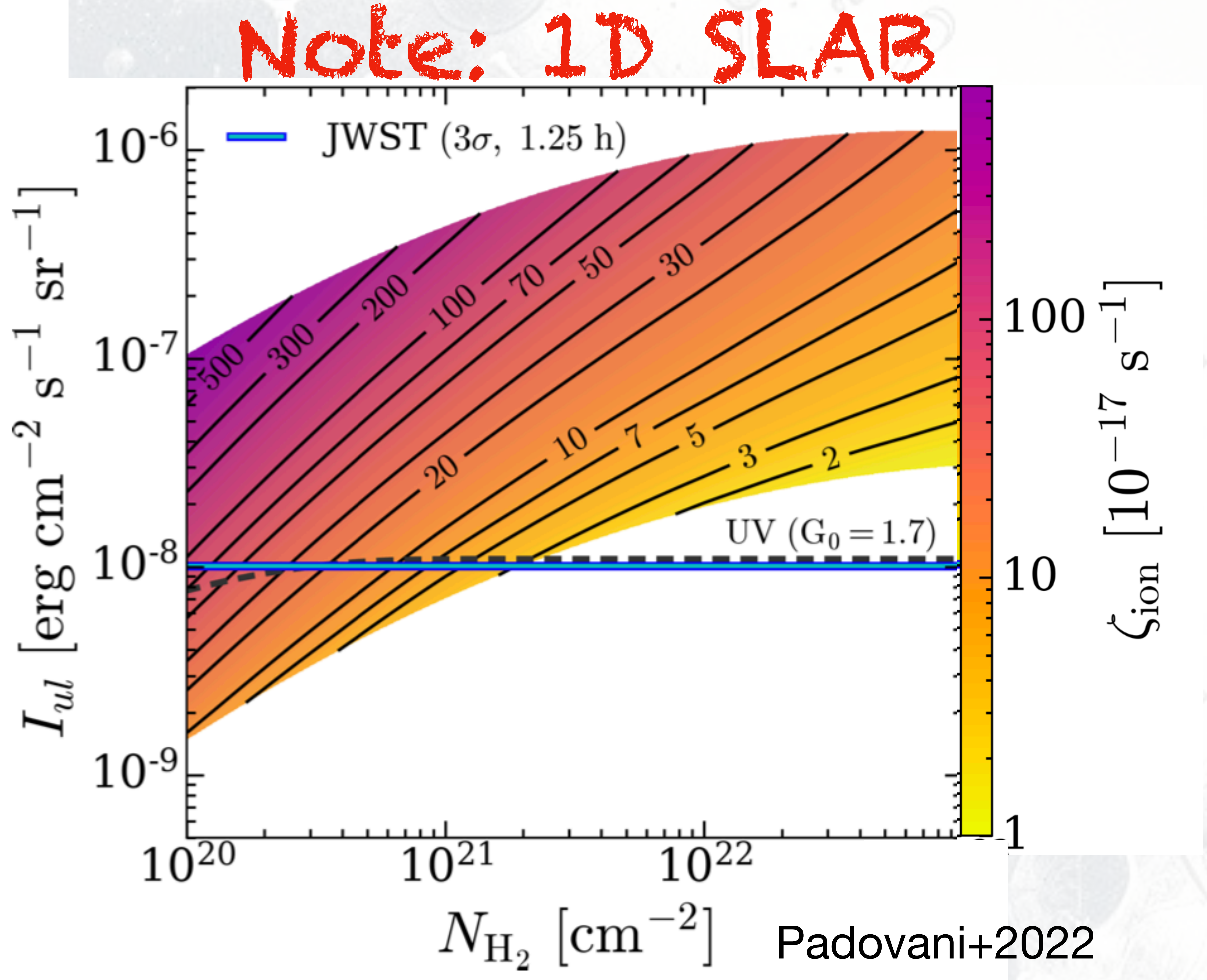

Cosmic rays can induce **ultraviolet emission** through exciting the $H_2$ molecule

# Can H2 IR emission act as a direct probe?




| Transition | λ (μm) |
|---|---|
| (1-0)S(0) | 2.22 |
| (1-0)Q(2) | 2.41 |
| (1-0)O(2) | 2.63 |
| (1-0)O(4) | 3.00 |

Bialy+2020




Padovani+2022

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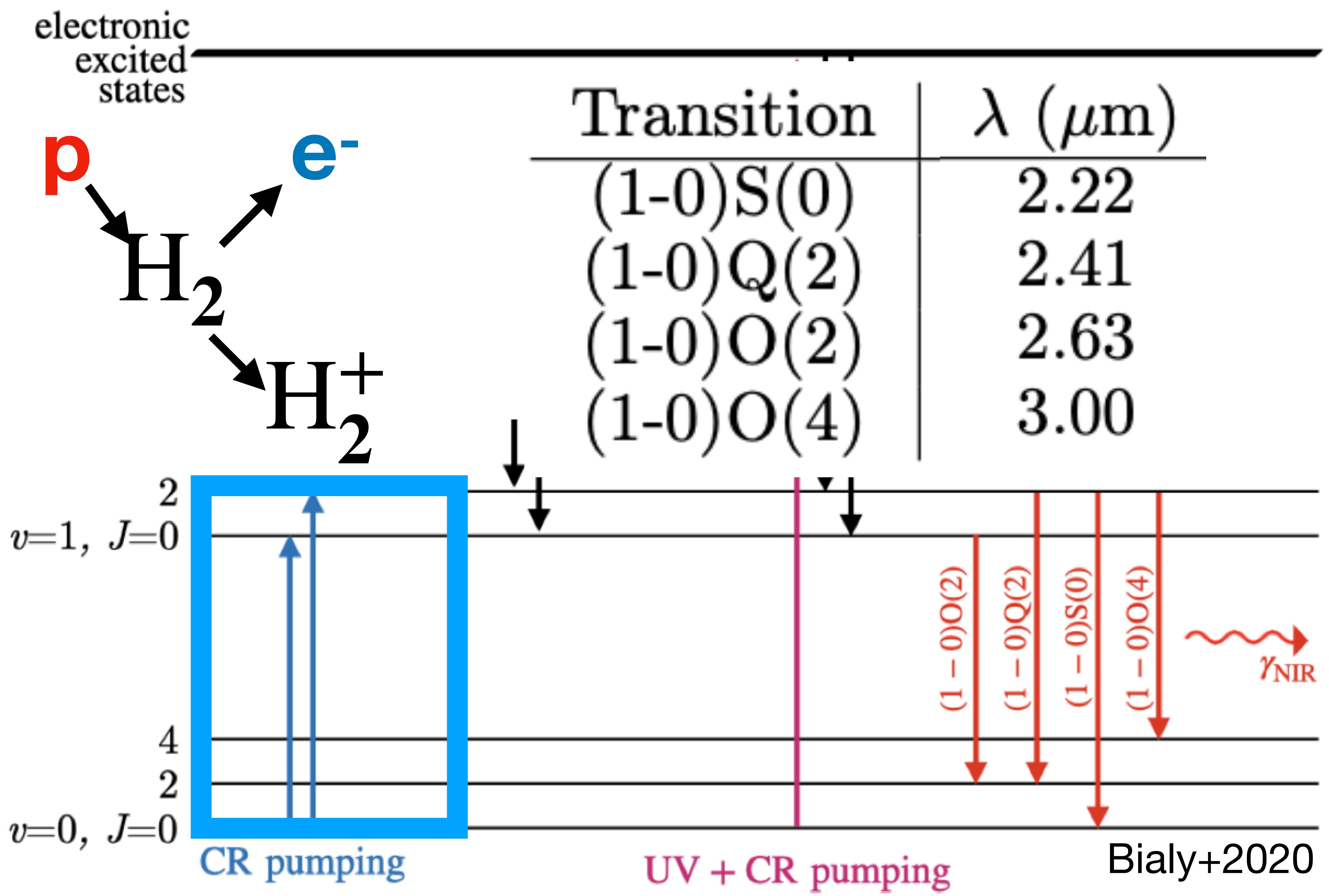


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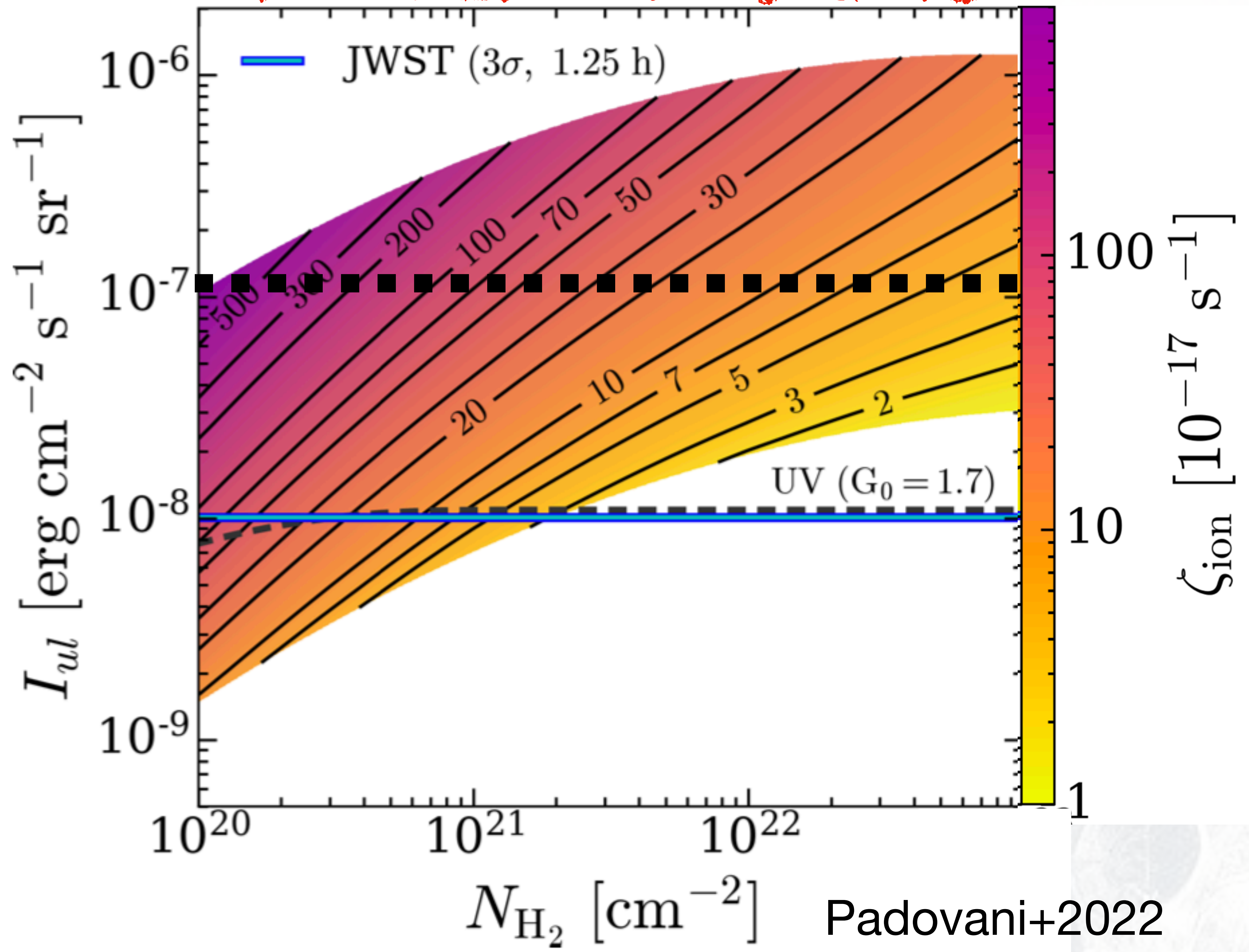
Bialy+2020

Note: 1D SLAB




Padovani+2022

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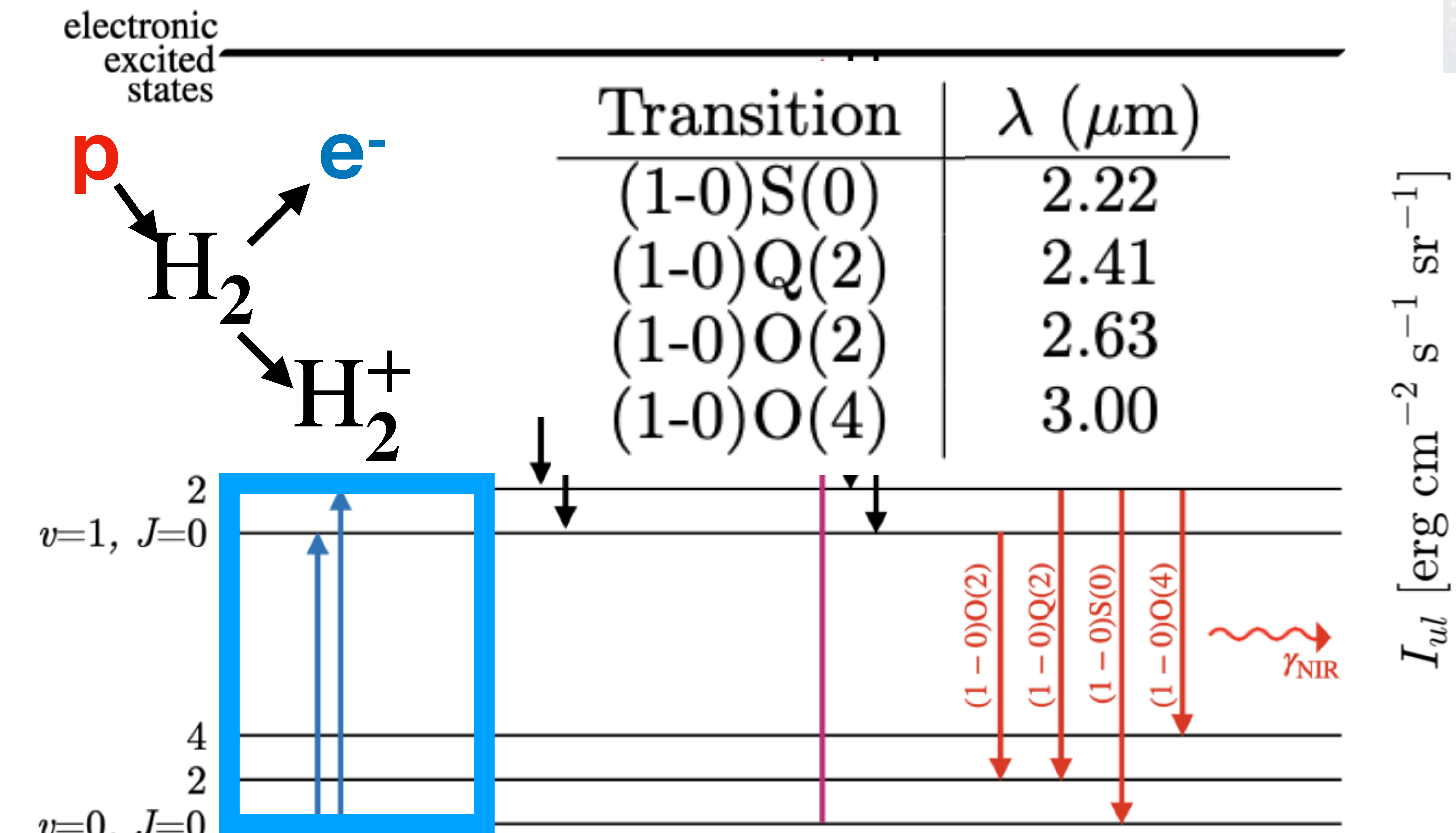


Bialy+2020

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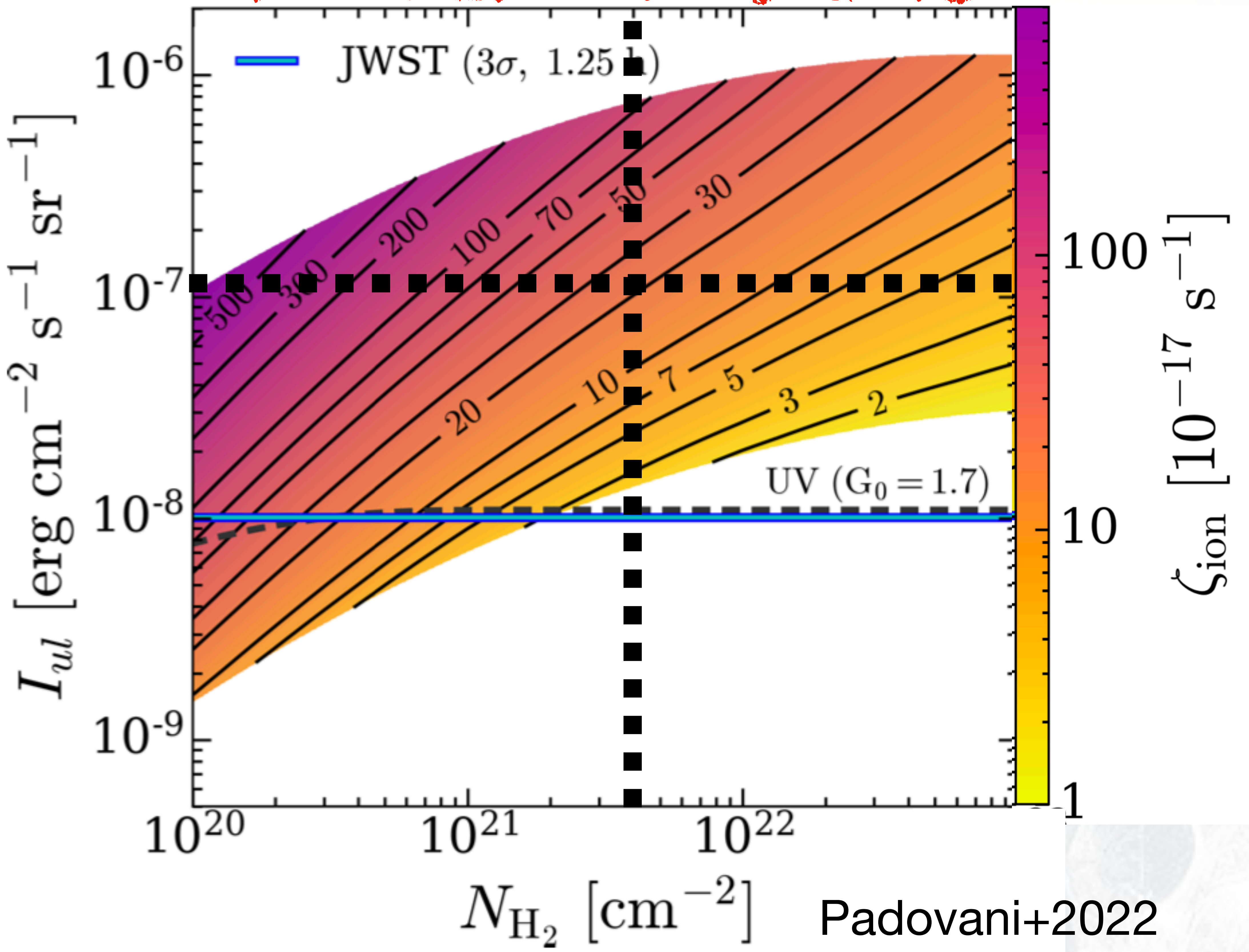
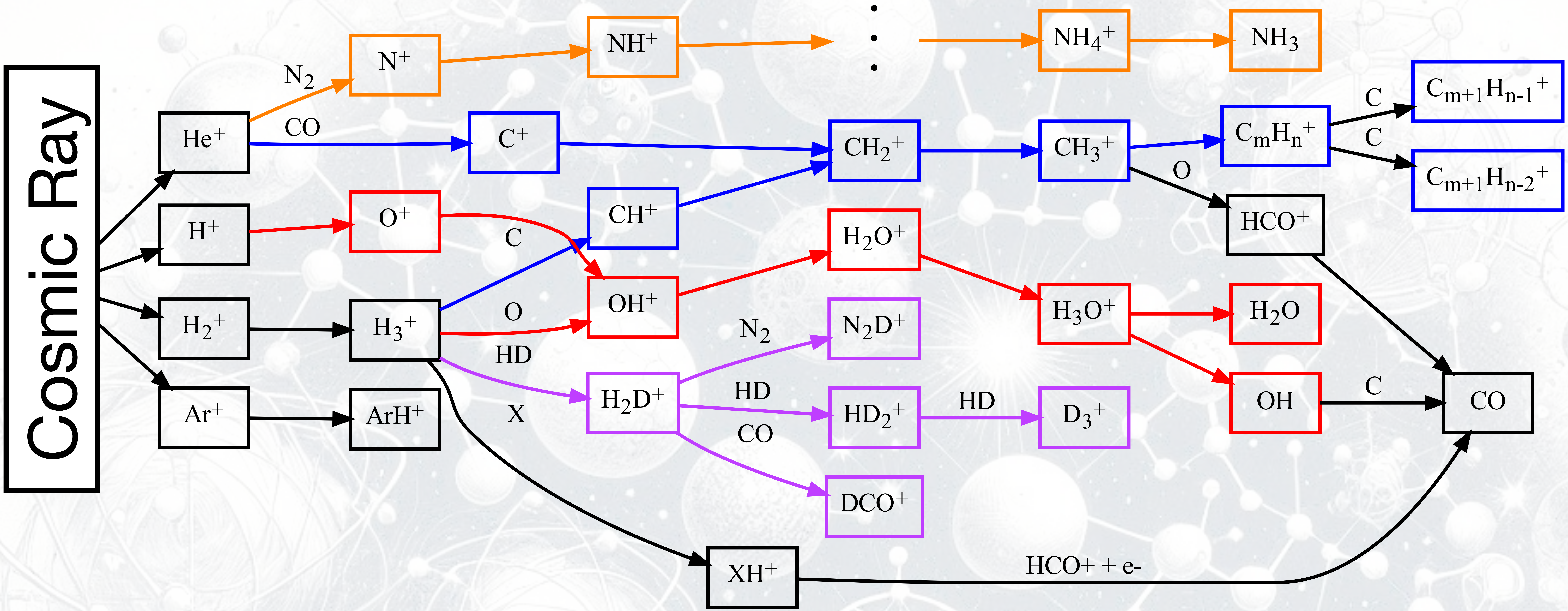



Padovani+2022

# Cosmic Rays: Drivers of Molecular Chemistry

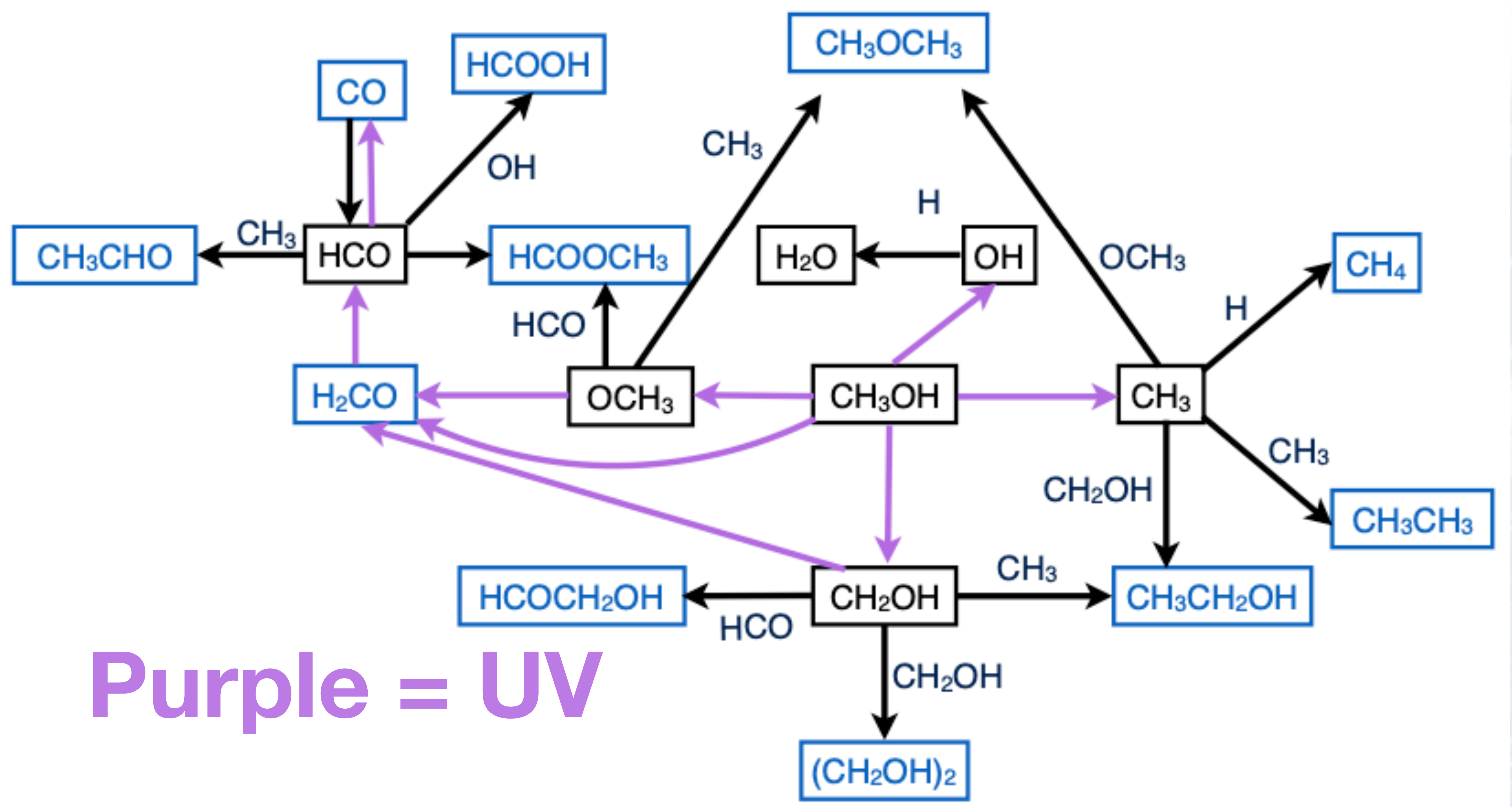
Cosmic-ray-induced ionization leads to an **explosion of gas-phase chemistry**




Adapted from Padovani & **Gaches** (2024)

# Cosmic Rays: Drivers of Molecular Chemistry

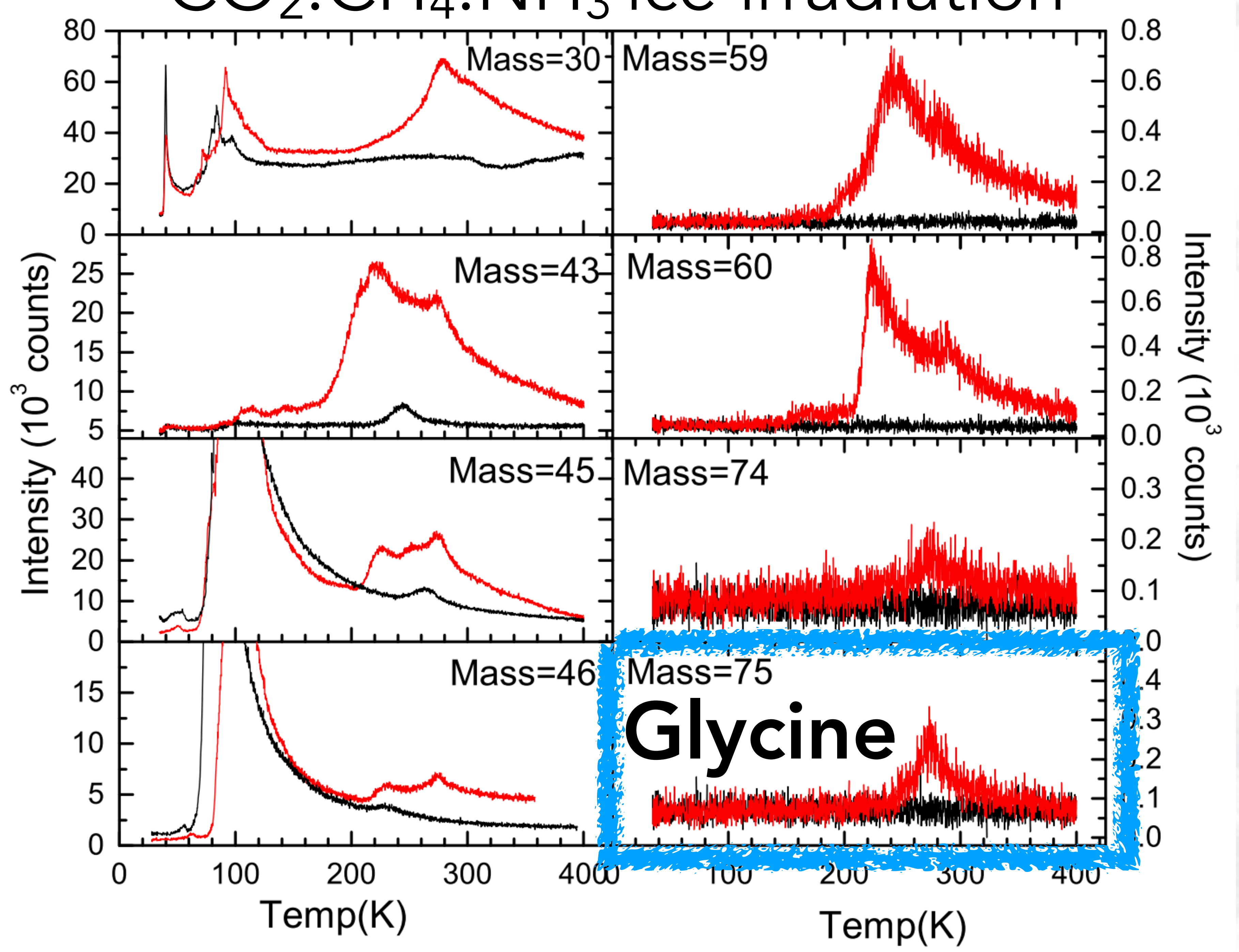
## CR-Induced UV processing




Öberg 2016

Low-energy electrons can **stimulate complex chemistry in simple ices**

$CO_2$:$CH_4$:$NH_3$ ice irradiation




Esmaili+2018



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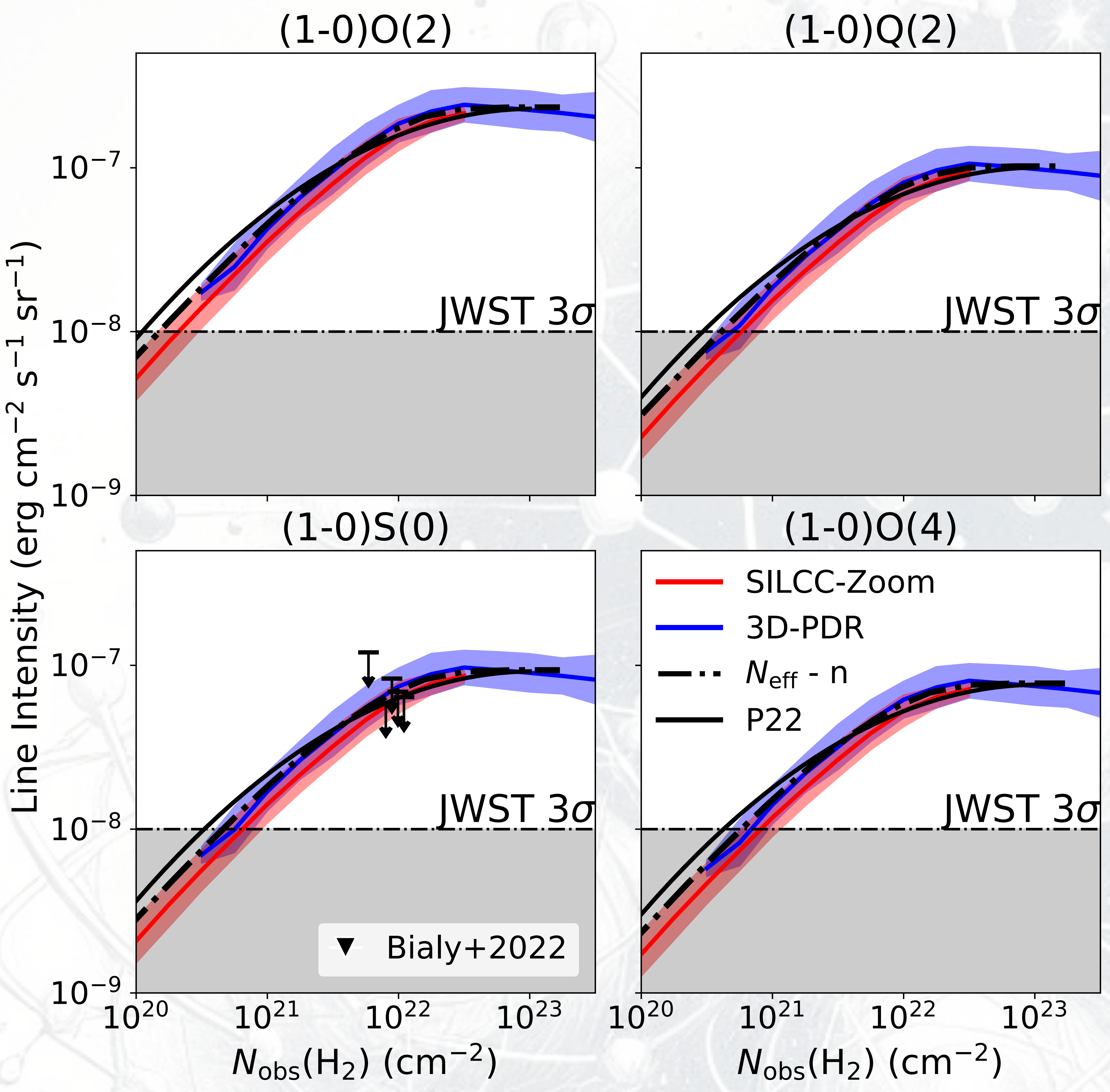
# Constraining the CRIR: "Direct" Methods

## CR-induced H2 NIR emission

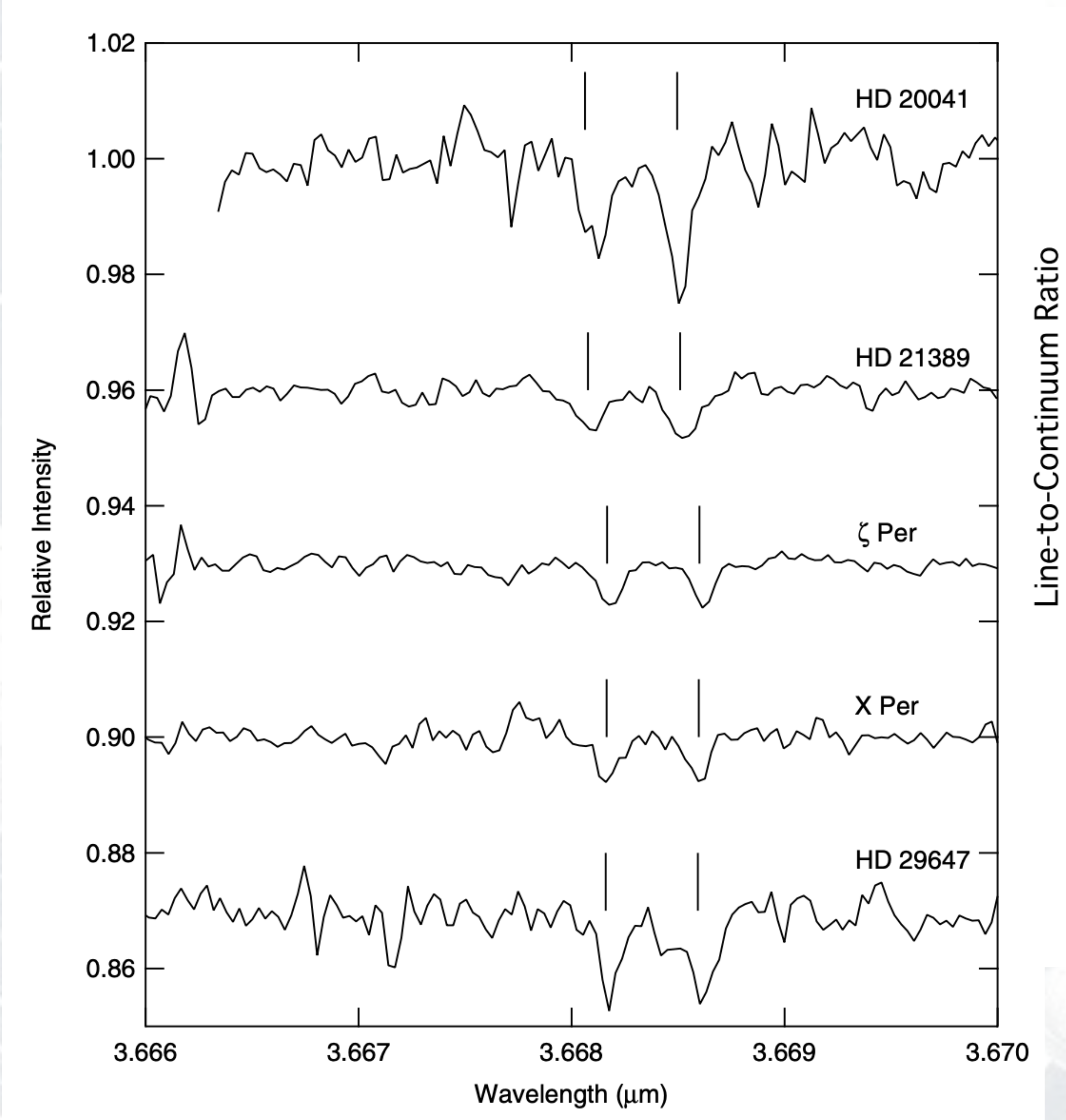



Bialy+2020, Padovani+2022, Gaches+2022b

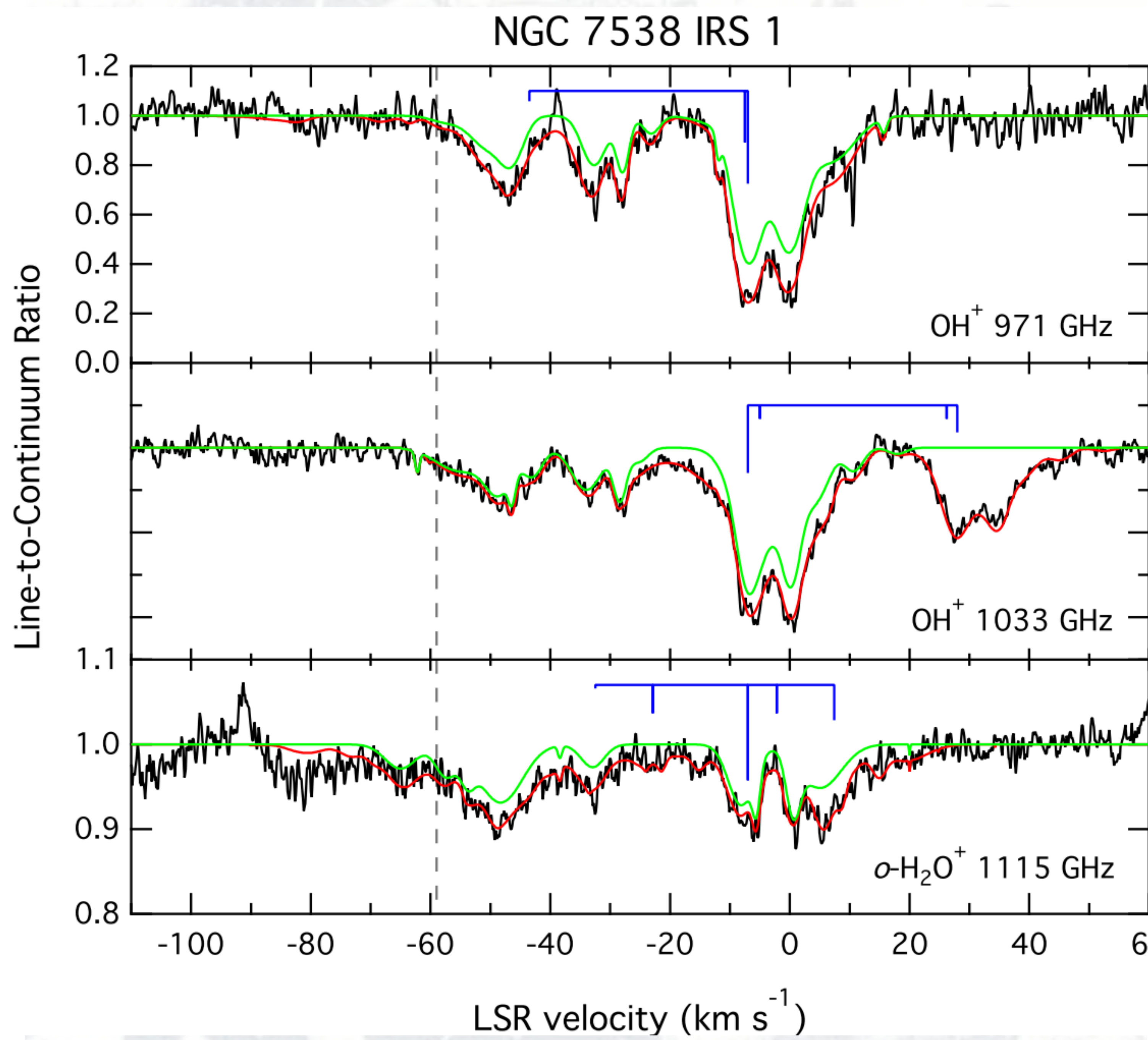
## H3+ and simply ions (OH+, H2O+..)

$$\zeta_2 = k_e x_e n_H \frac{N(H_3^+)}{N(H_2)}$$

$$\epsilon \zeta_H = \frac{N(OH^+)}{N(H)} n_H x_e \left[ \frac{k_7}{N(OH^+)/N(H_2O^+) - k_6/k_4} + k_5 \right]$$




Indriolo+2012




Indriolo+2015

# Constraining the CRIR: "Direct" Methods

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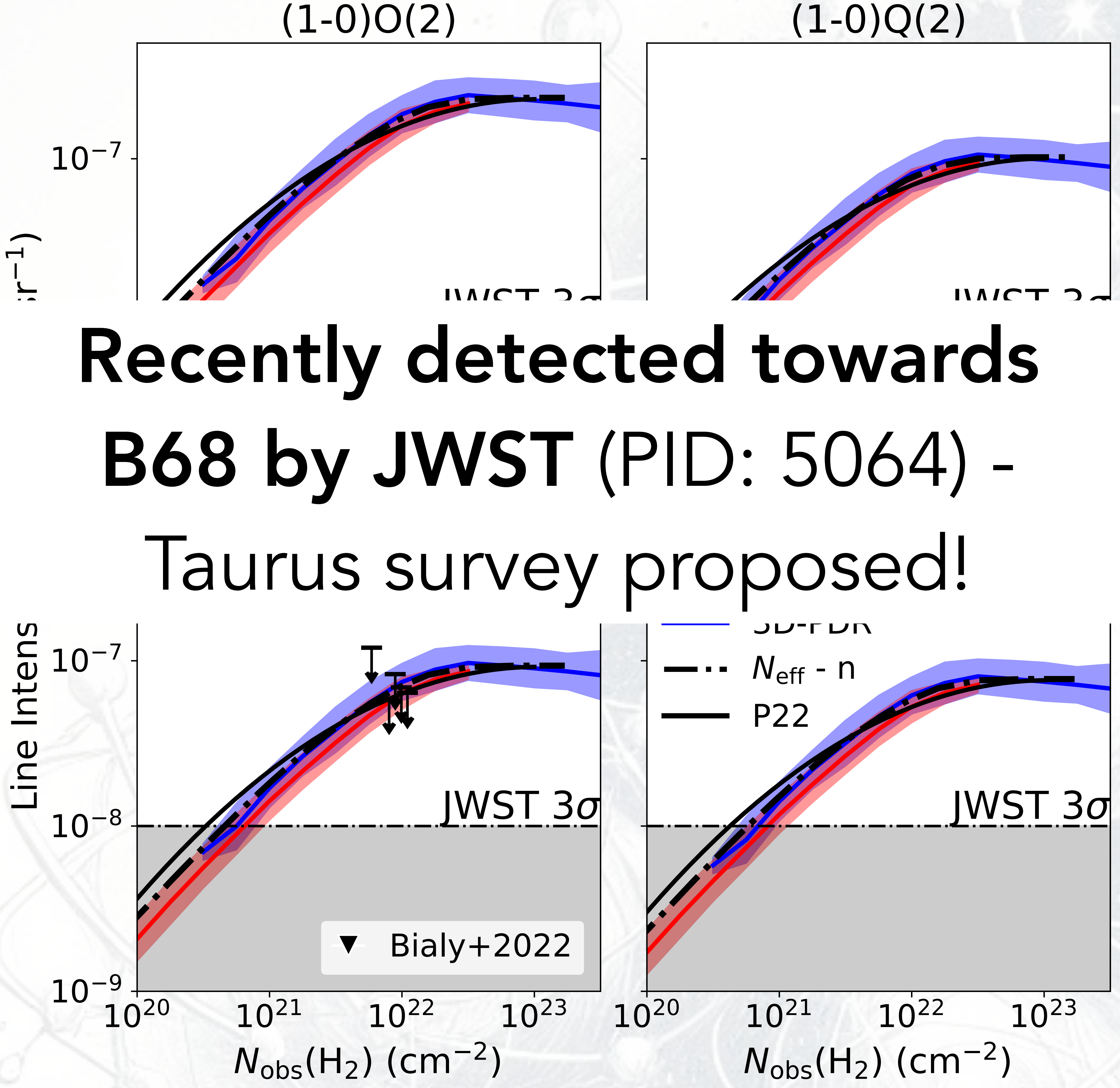


**Recently detected towards B68 by JWST** (PID: 5064) - Taurus survey proposed!

Bialy+2020, Padovani+2022, Gaches+2022b

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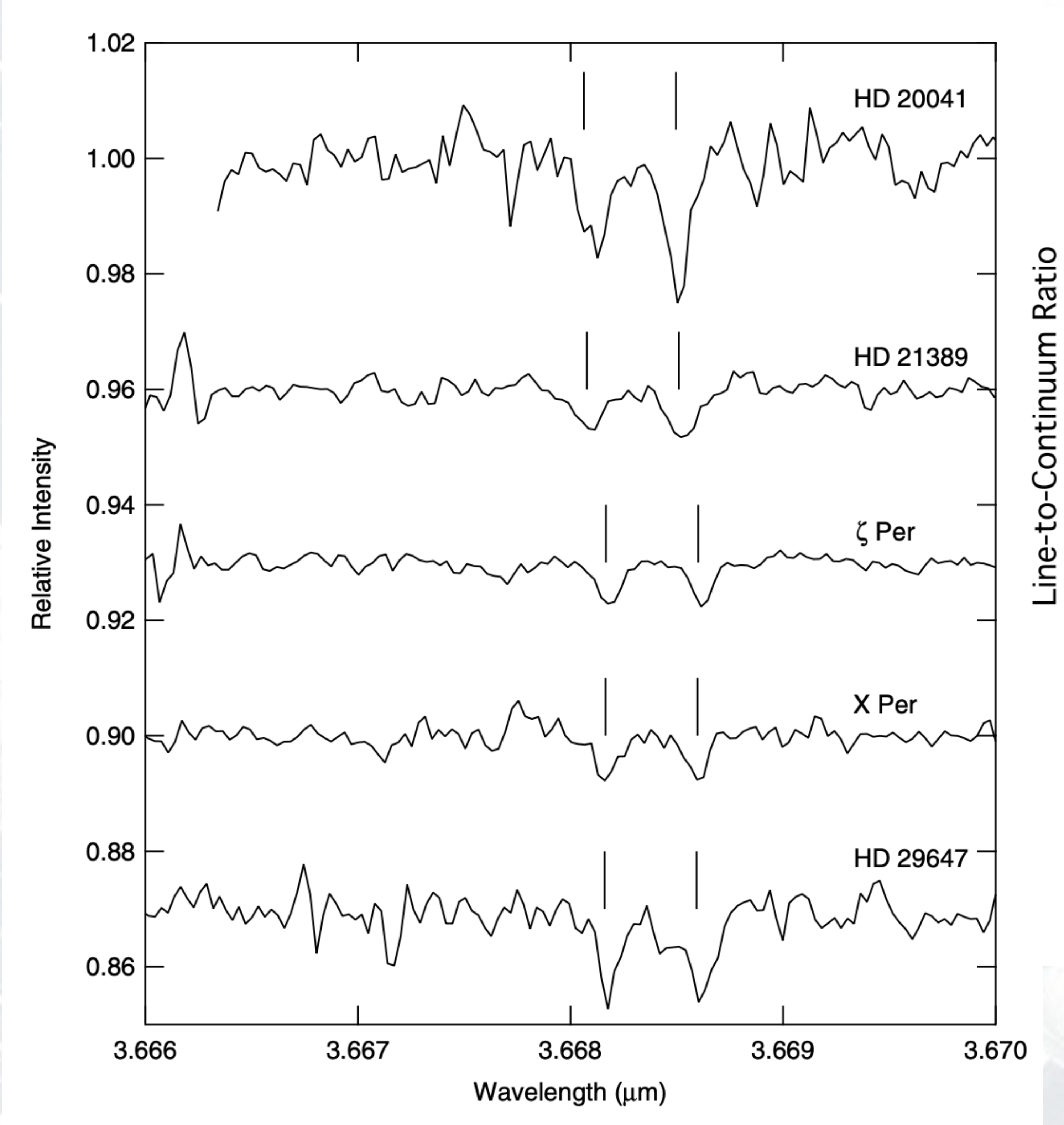
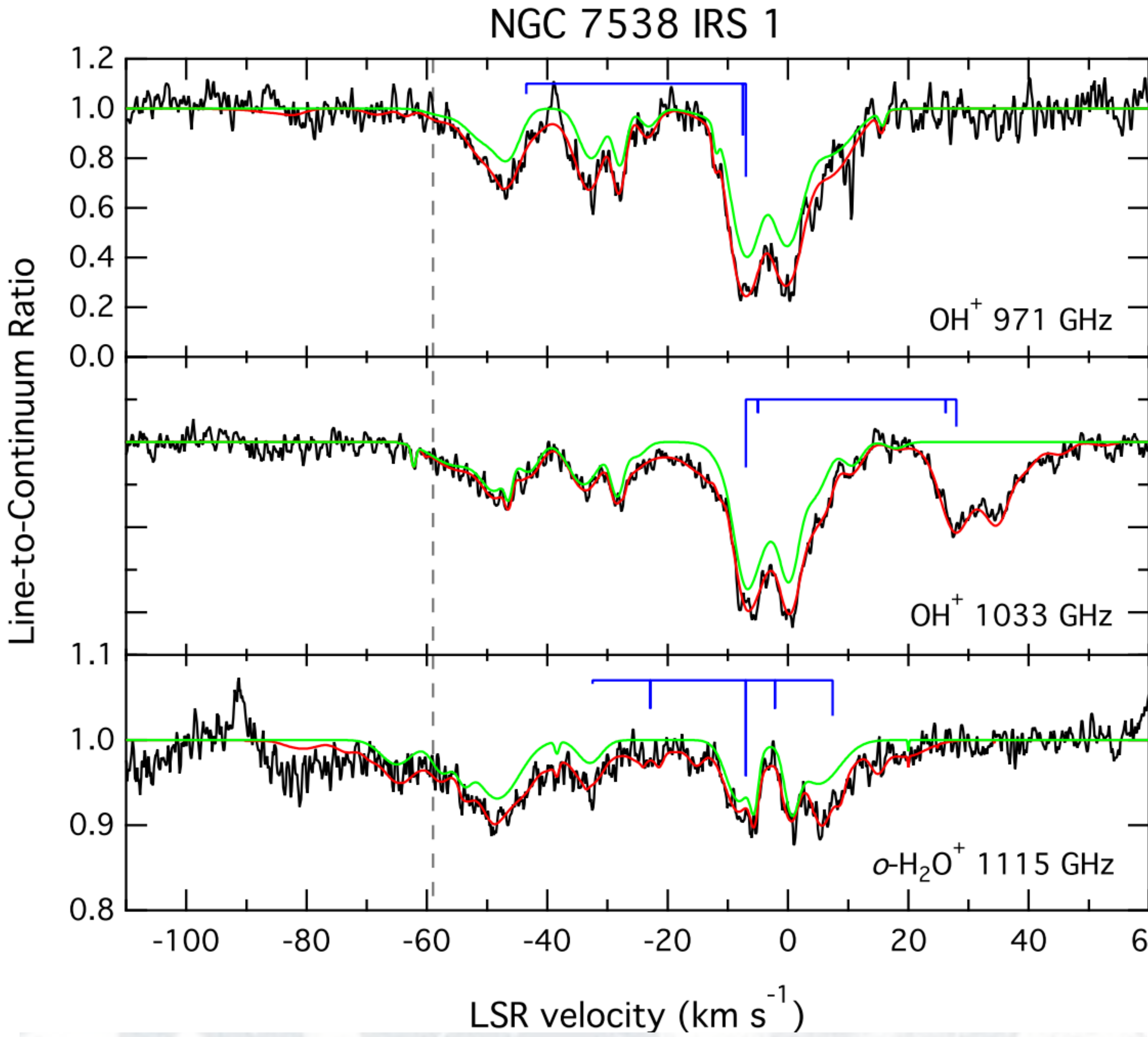



Indriolo+2012




Indriolo+2015

# Constraining the CRIR: Astrochemical models

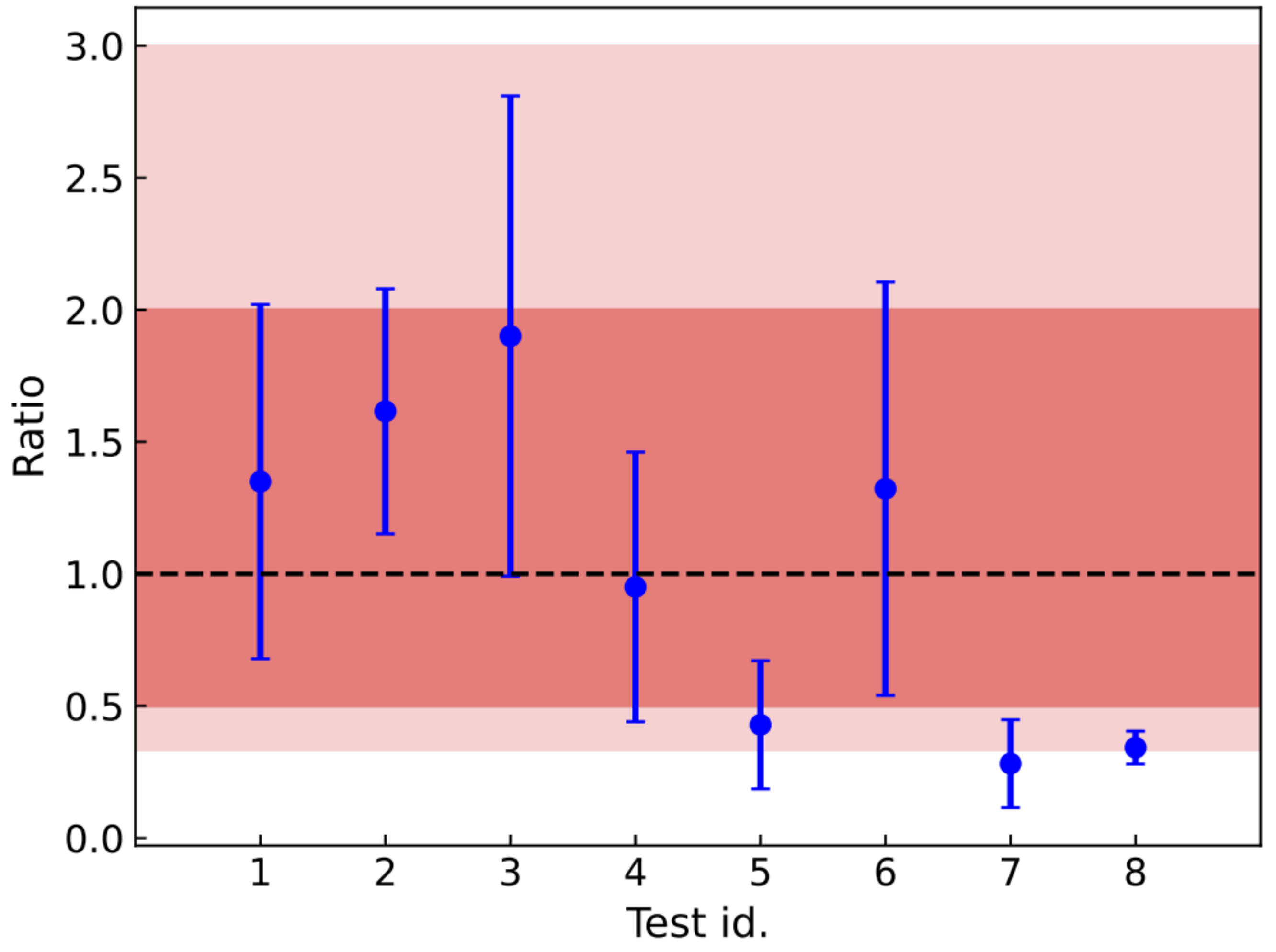
## Analytic steady-state chemistry

### Bovino+2020

$$\zeta_2 = \bar{\alpha} k_{\mathrm{CO}}^{\mathrm{H_3^+}} \frac{N[\mathrm{CO}]N[\mathrm{H_3^+}]}{N[\mathrm{H_2}]} \frac{1}{L},$$

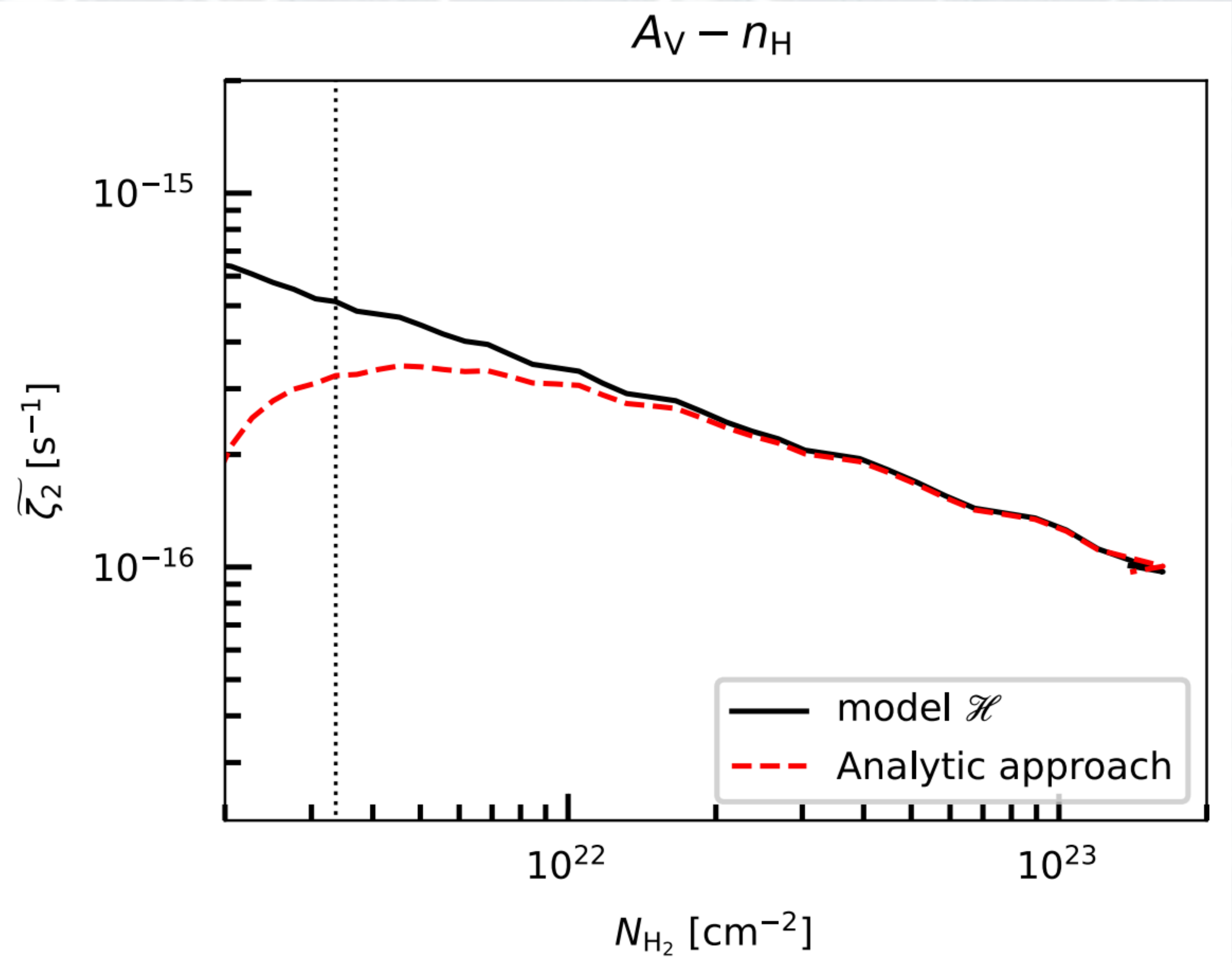
$$N[\mathrm{H_3^+}] = \frac{1}{3} \frac{D[\mathrm{H_3^+}]}{R_\mathrm{D}},$$

$$R_\mathrm{D} = \frac{N[\mathrm{DCO^+}]}{N[\mathrm{HCO^+}]}$$



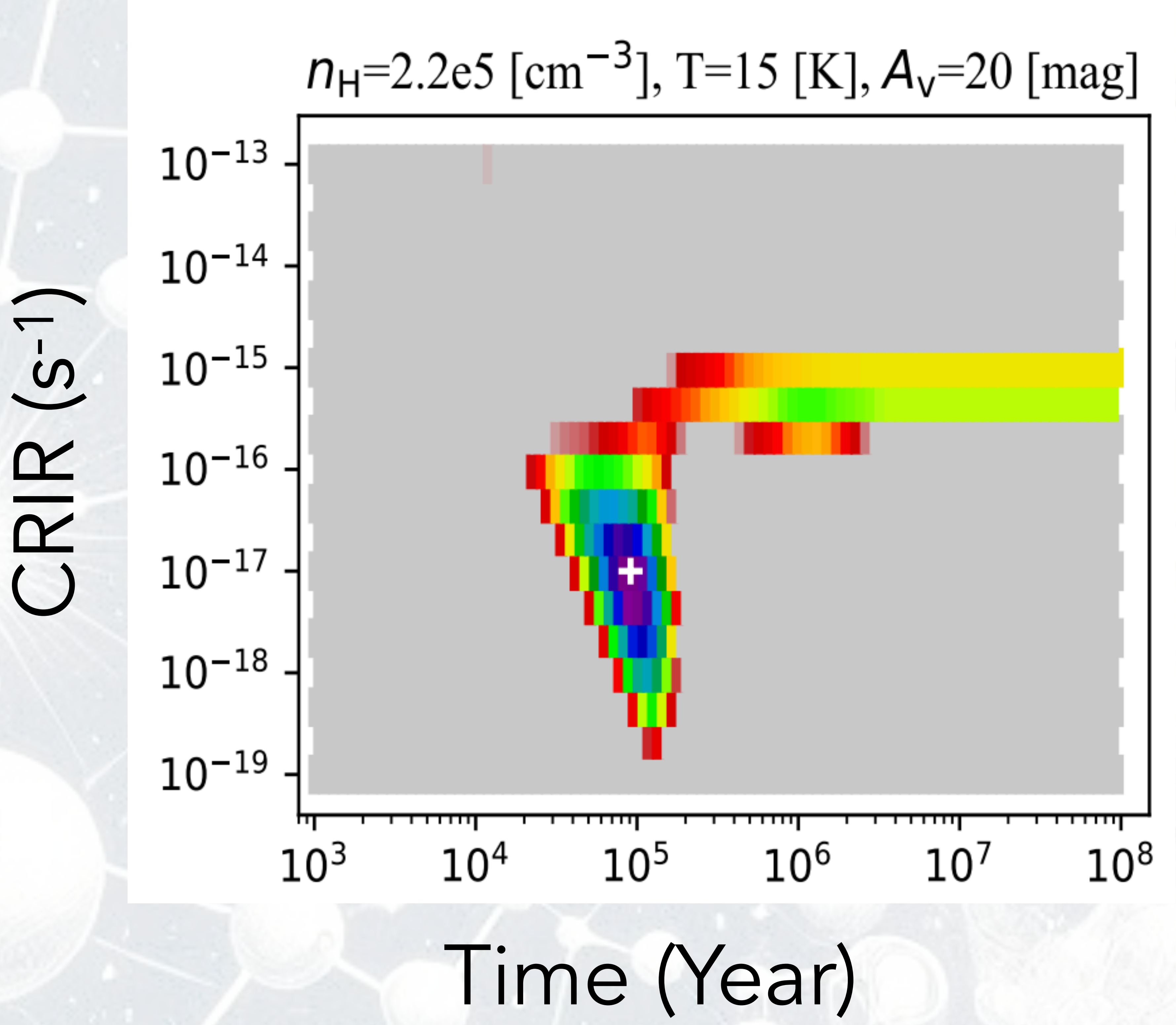

### Luo,G+2024

$$\widetilde{\zeta_2} = n(\mathrm{H_2}) f(\mathrm{H_3^+}) \left[ f(\mathrm{CO})\mathrm{k_{R3}} + f(\mathrm{N_2})\mathrm{k_{R4}} + f(\mathrm{O})\mathrm{k_{R5}} + f(\mathrm{e^-})\mathrm{k_{R6}} \right]$$



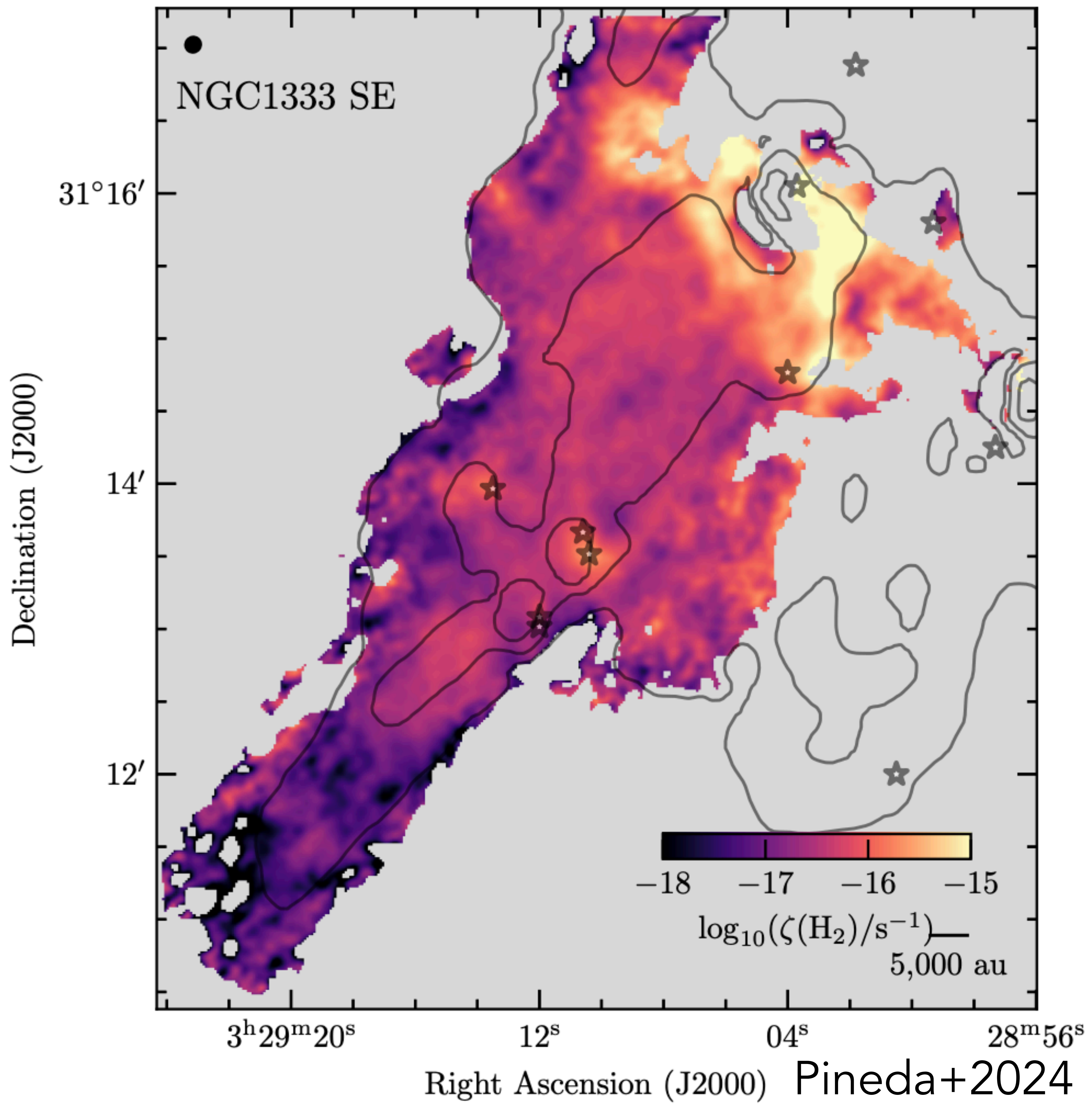

## Chemical model grids

### Entekhabi+2022

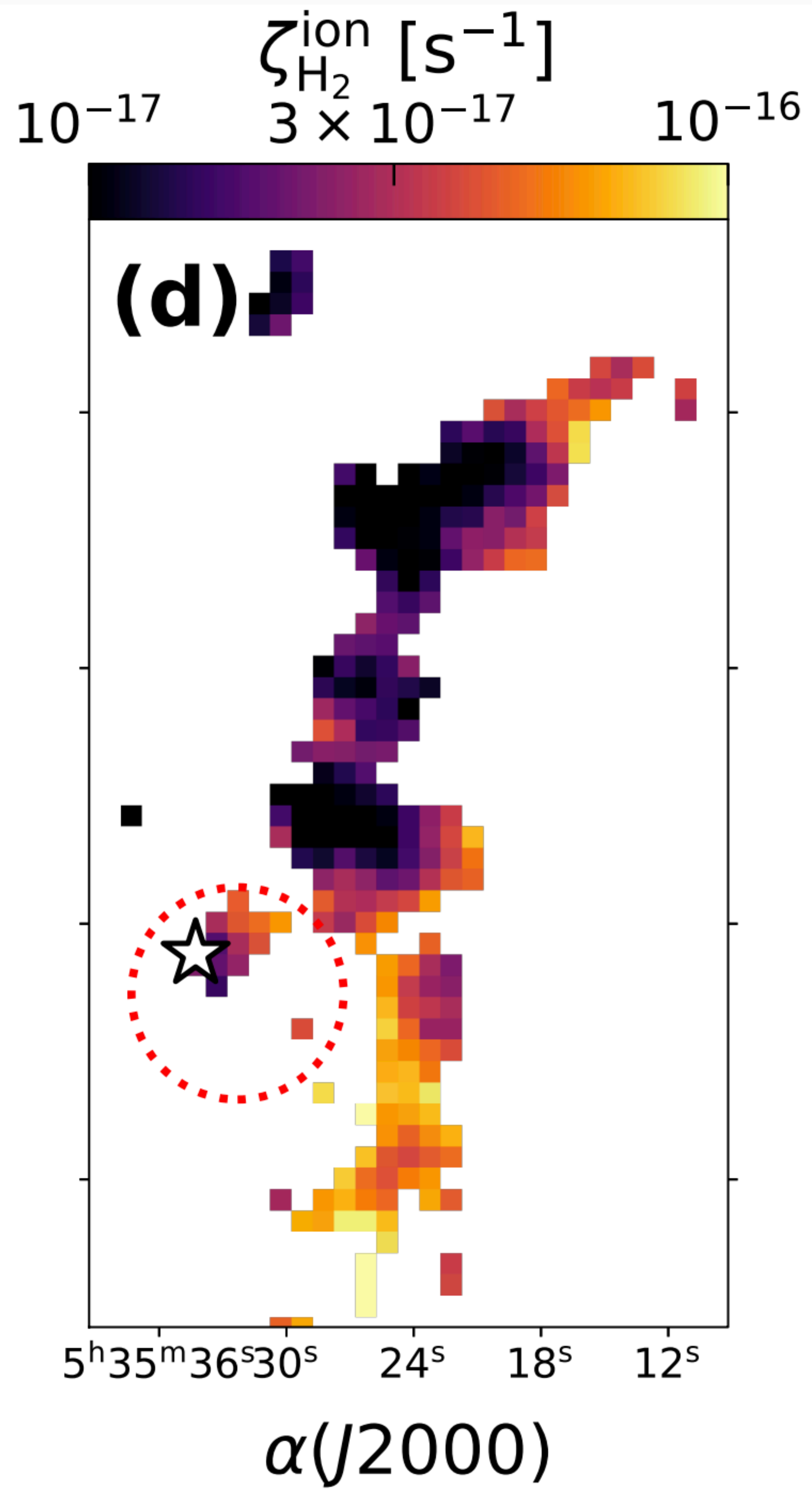


# Observations Clearly Show CRs are Not Uniform!

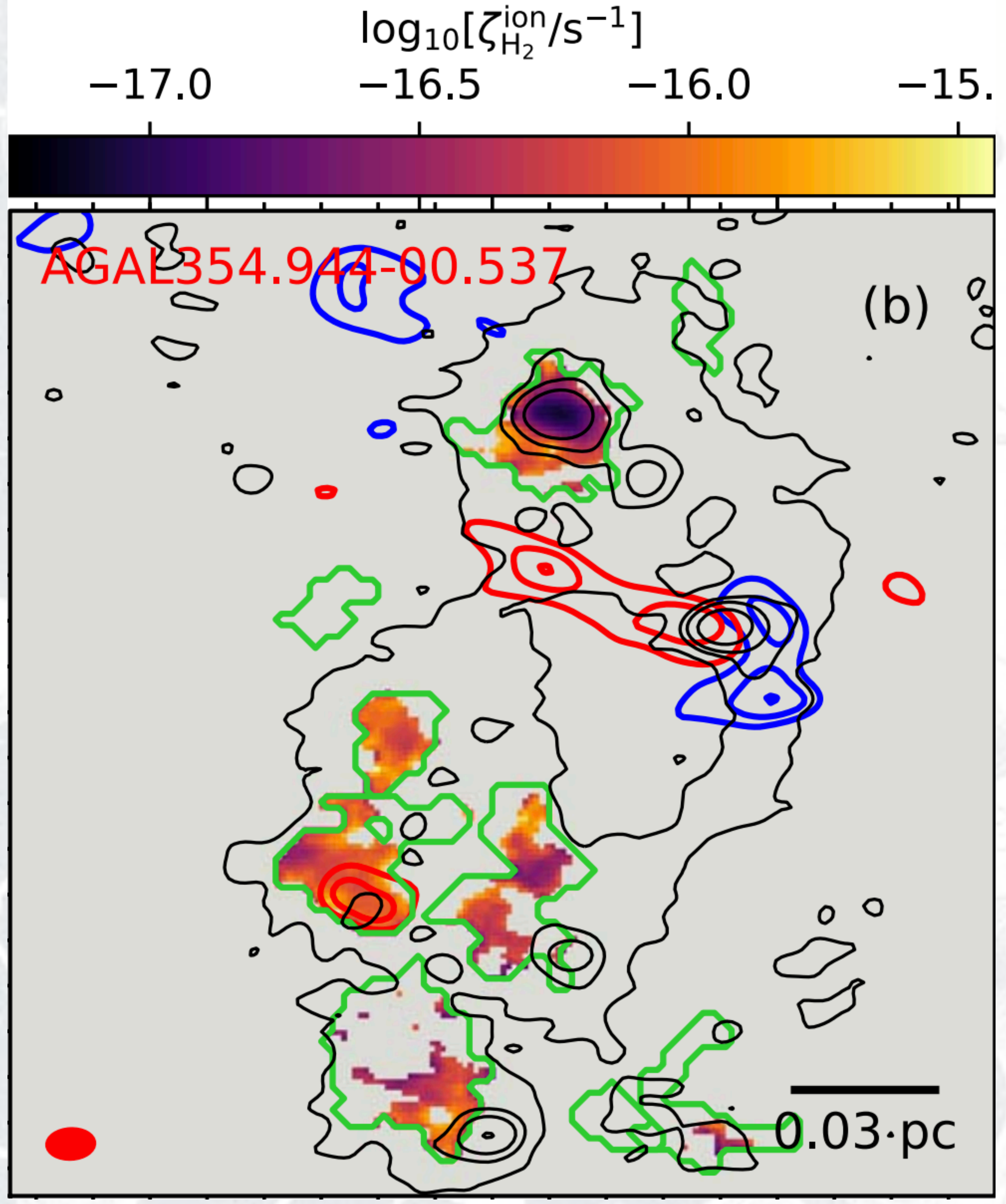
Observations also show signatures of **embedded sources**.




Pineda+2024

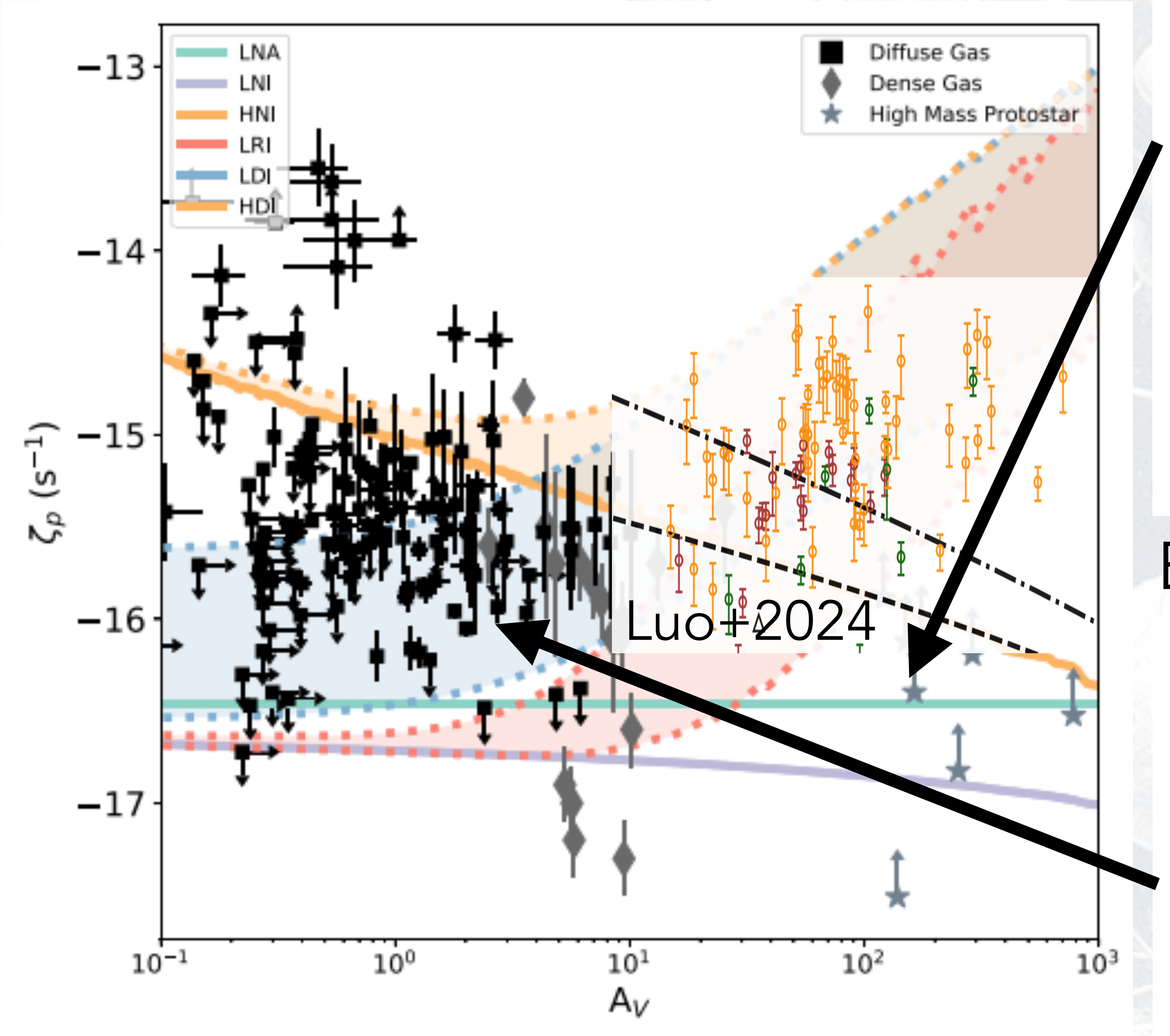



Socci+2024



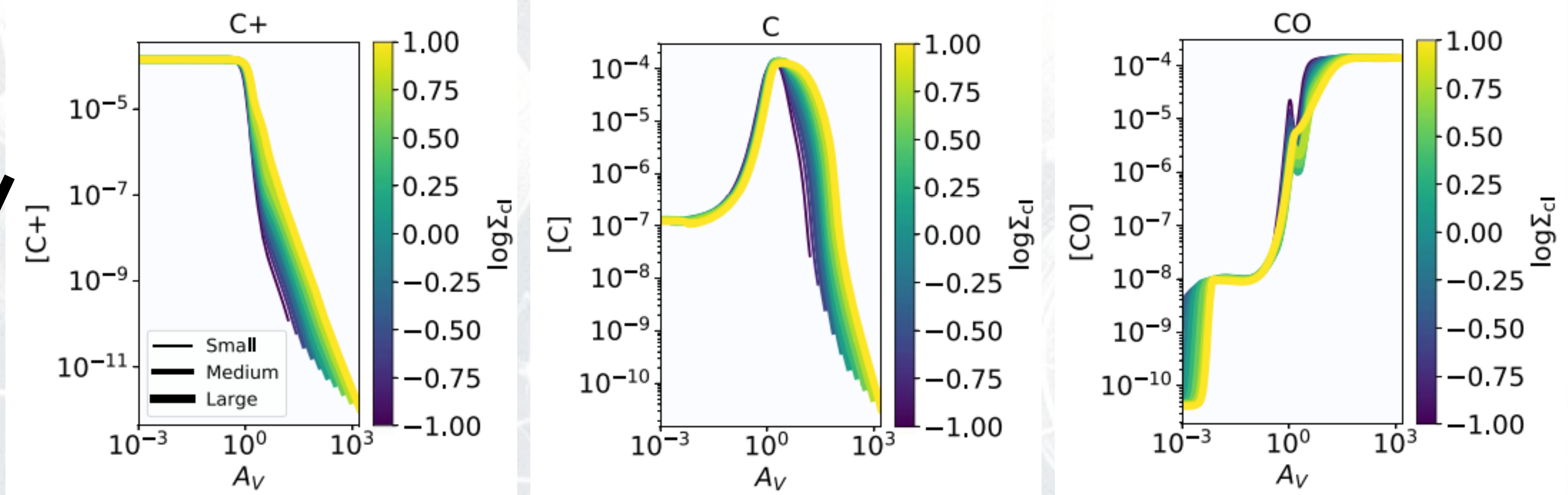

Sabatini+2023

# Chemical models with protostellar CRs

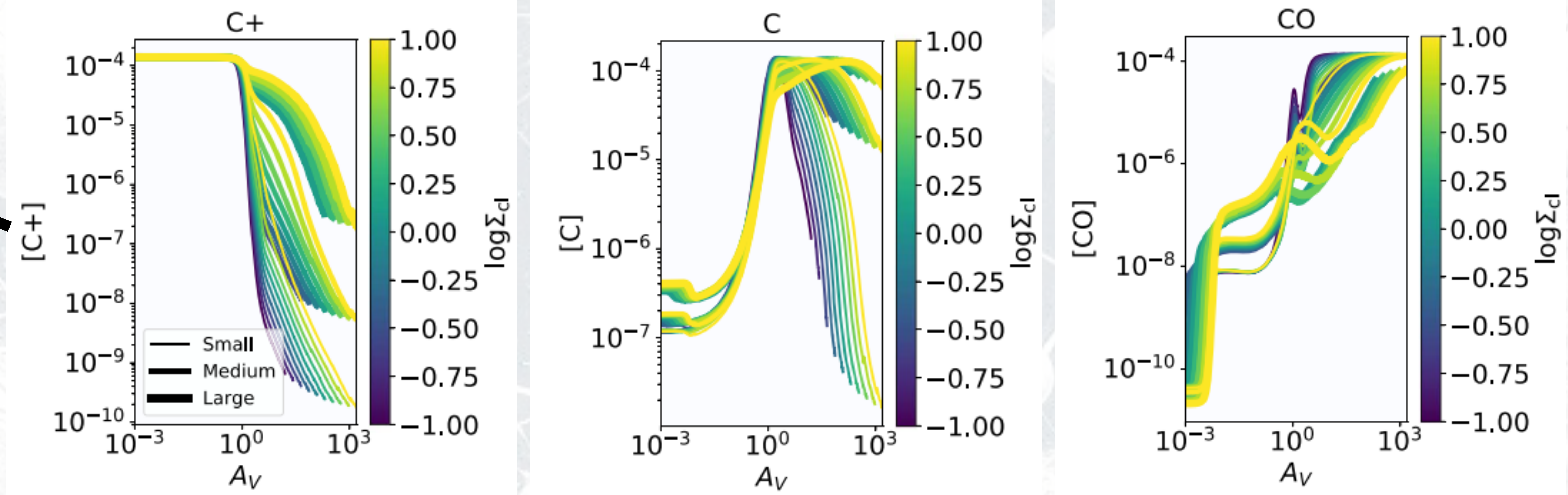



Gaches+2019a,b

Without embedded CRs, recover the "layered cake" PDR model

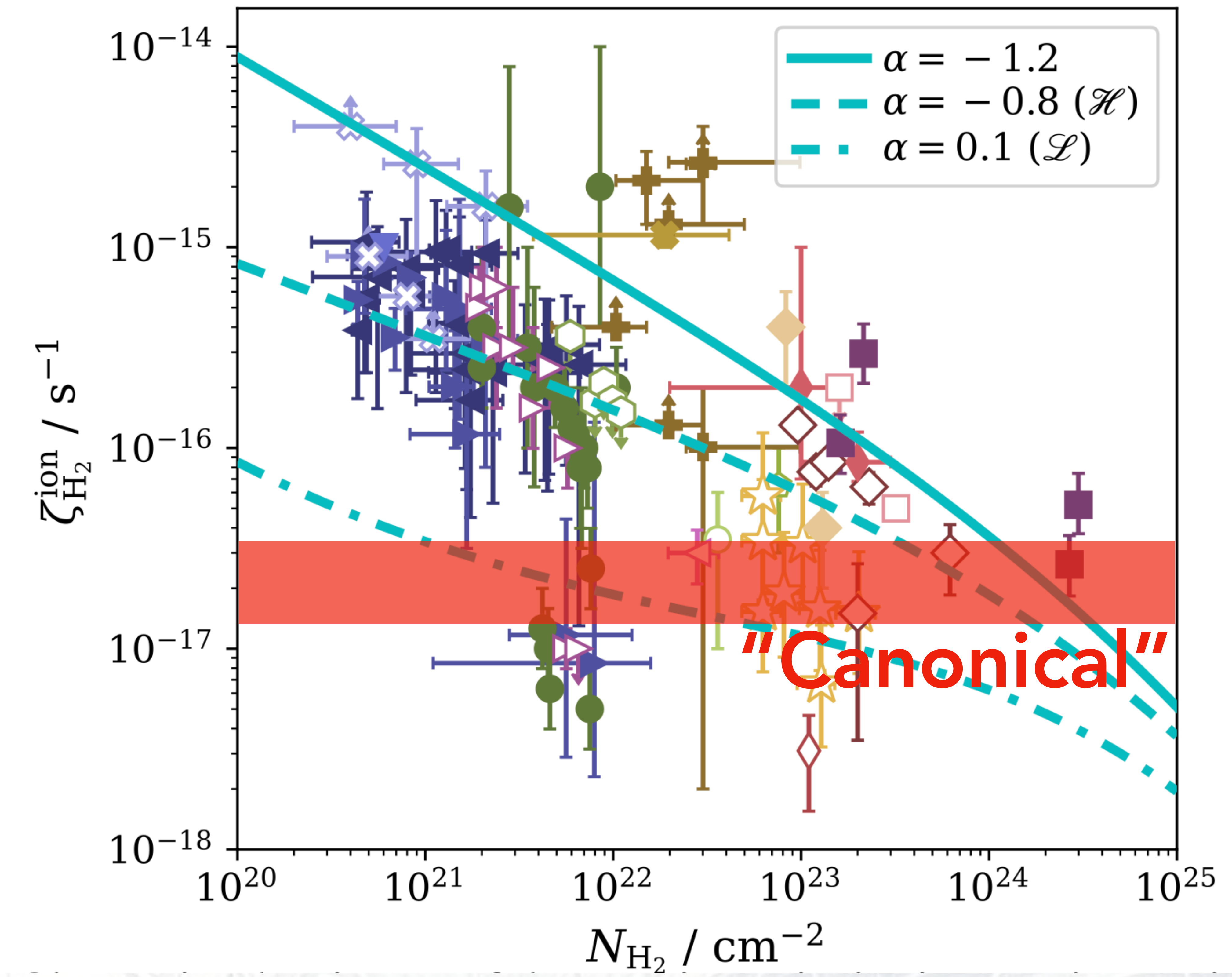



Embedded CRs reduce CO and inject atomic C in dense gas



# How are cosmic rays treated in cloud chemistry?

## Constant ionization rates




## UMIST + KIDA Chemical rates

| Atoms | 2 atoms |
|---|---|
| H | $H_2$ |
| He | $N_2$ |
| C | CO |
| N | |
| O | |
| Cl | |
| Ar | |

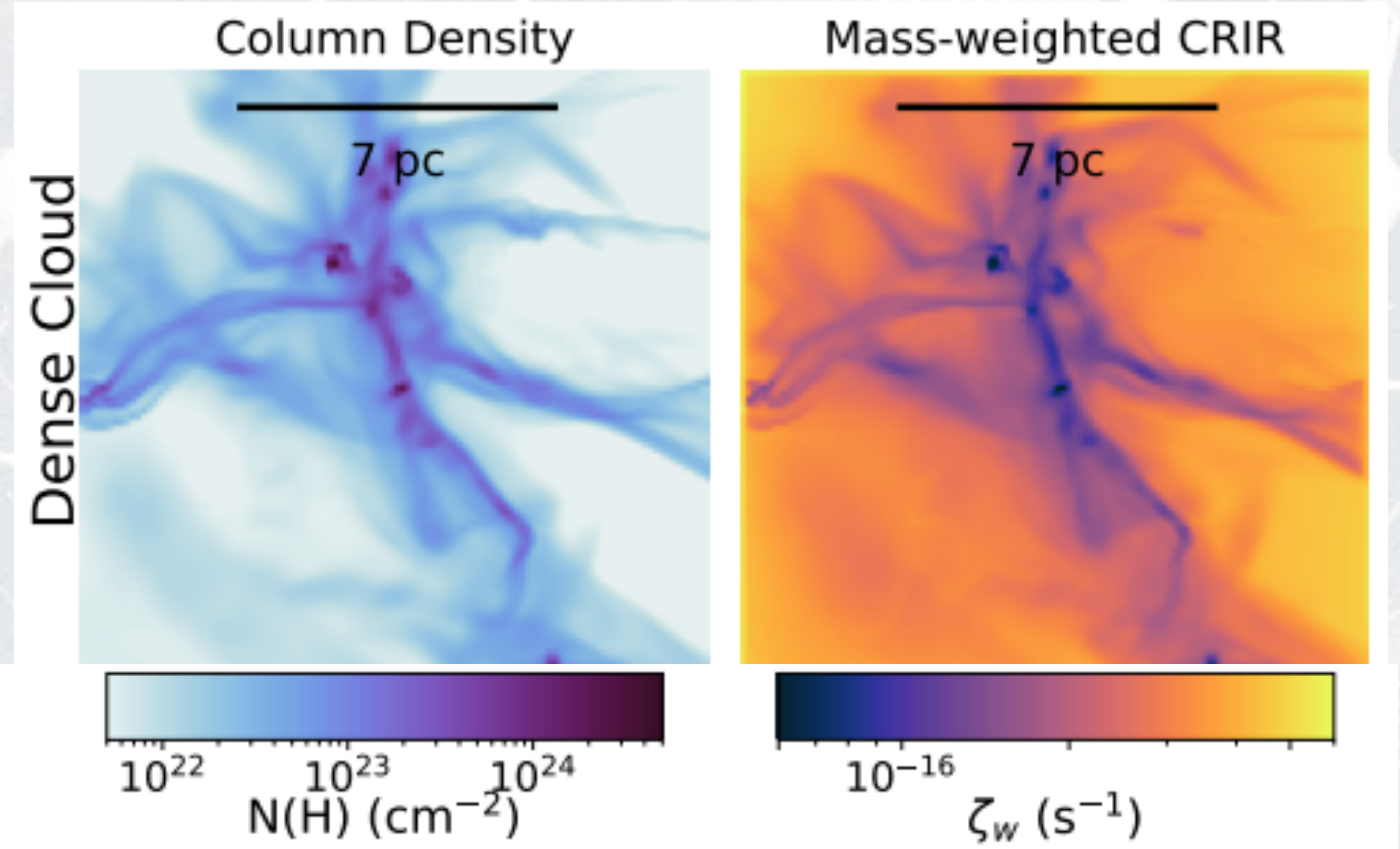
## Lab: NIST ionization cross sections

| Small molecules | Atmospheric molecules | Oxygenates |
|---|---|---|
| $H_2$ $H_2^+$ $HO_2$ $H_2O$ $H_3O^+$ | $H_2S$ $N_2O$ $NO_2$ | CHO |
| $N_2$ $N_2^+$ $NH_3$ NO $O_2$ | $O_3$ CS COS | $CH_2O$ |
| CO $CO^+$ $CO_2$ | $S_2$ $SO_2$ $CS_2$ | $C_2H_3O$ |

| Hydrocarbons | | | | |
|---|---|---|---|---|
| CH | $C_2H_2$ | $C_3H_3$ | $C_4H_2$ | $C_6H_2$ |
| $CH^+$ | $C_2H_2^+$ | $C_3H_4$ (allene) | $C_4H_4$ | $C_6H_6$ (benzene) |
| $CH_2$ | $C_2H_3$ | $C_3H_4$ (propyne) | $C_4H_6$ | $C_6H_6$ (fulvene) |
| $CH_2^+$ | $C_2H_4$ | $C_3H_5$ | $C_4H_8$ (1-butene) | |
| $CH_3$ | $C_2H_4^+$ | $C_3H_6$ | $C_4H_8$ (trans-2-butene) | |
| $CH_3^+$ | $C_2H_6$ | $C_3H_8$ | $C_4H_8$ (isobutene) | |
| $CH_4$ | $C_2H_6^+$ | | | |
| $CH_4^+$ | | | | |

# Astrochemical models with 3D CR physics

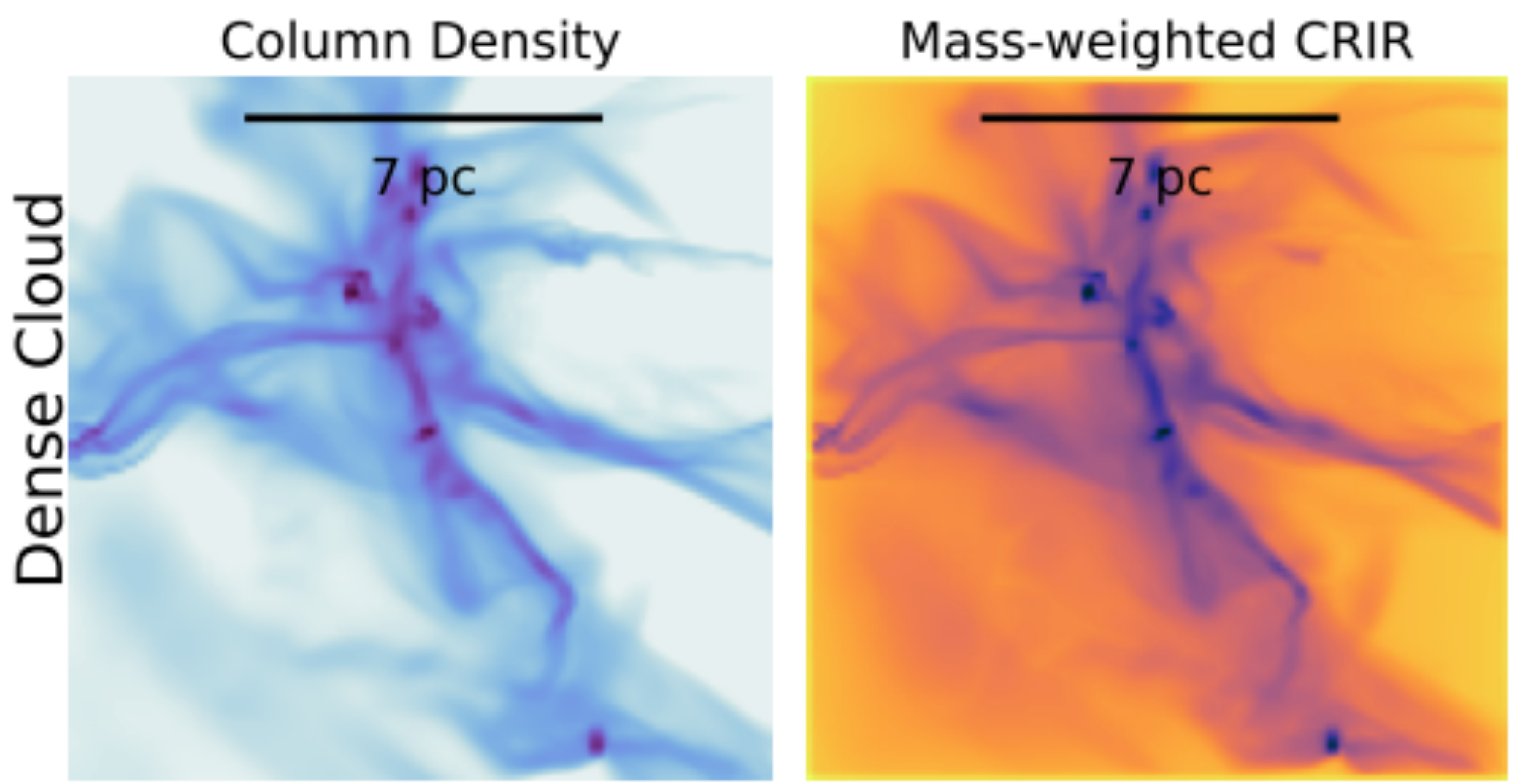
3D-PDR: First (public) astrochemistry
to include attenuated CR physics
Public at uclchem.github.io




Other codes that now include **polynomial/fit CR attenuation:** UCLCHEM, Nautilus - *only for chemical rates, not temperature!*

1D with energy-loss solver: **Gaches+2019a**
3D with ζ(N) function: **Gaches+2022a,b**
3D with energy-loss solver: on **GitHub** public
Future plans: 1D + 3D with full CR transport

# Astrochemical models with 3D CR physics



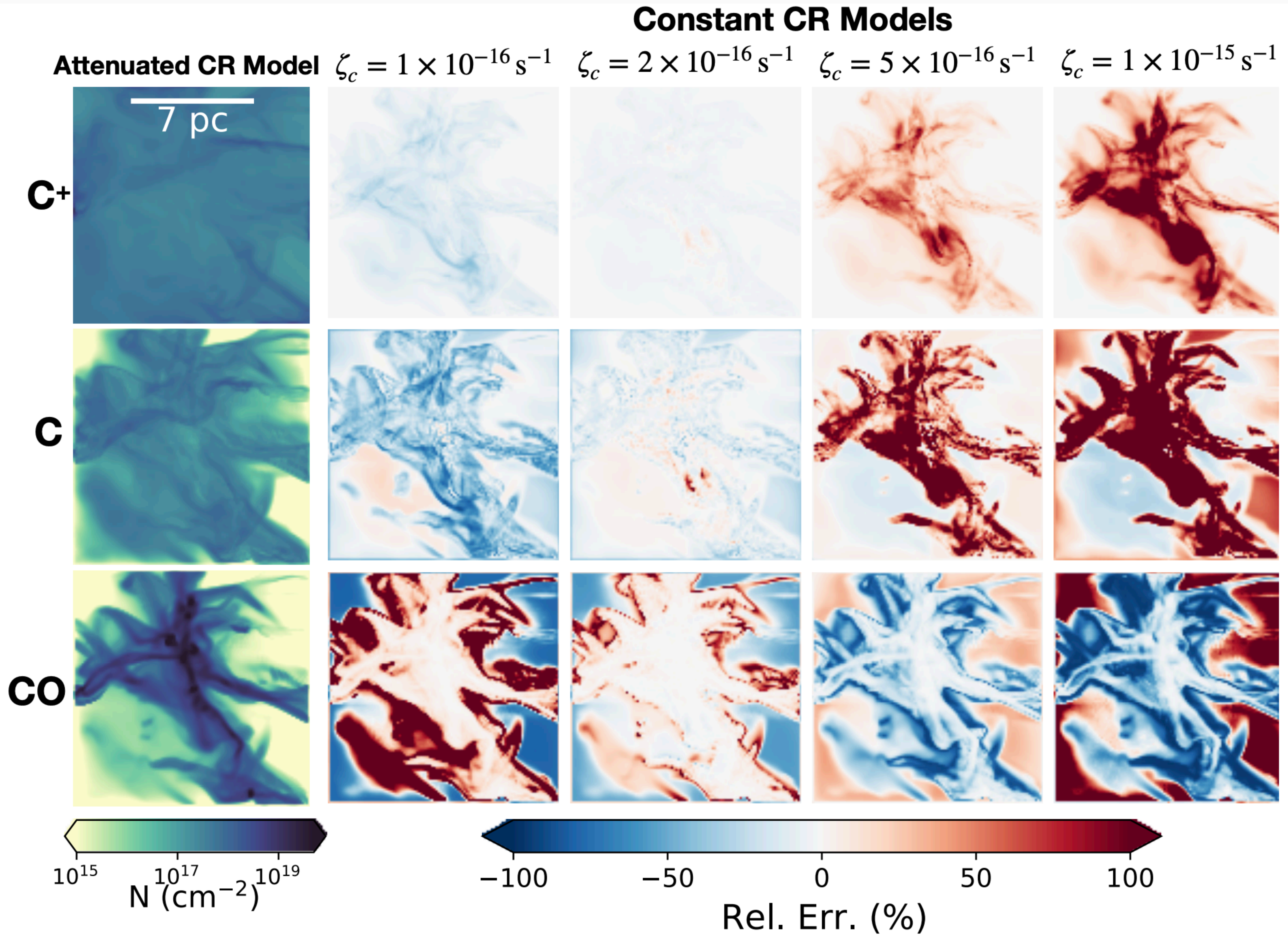

**Gaches**+2022a

Cloud-cloud collisions from Wu+2017
14 pc box
Post-processed with modified version of 3D-(CR)PDR (Bisbas+2012)
(Public at uclchem.github.io)

Model the chemistry in 3D using CR attenuation, and four constant rates.

The CRIR uses a prescribed function of $\zeta(N)$ from Padovani+2018. However, 3D-PDR **can** do the CDSA approach spectrally resolved, but for these 3D runs, a prescribed version was needed for memory concerns.

# Astrochemical models with 3D CR physics




**Gaches**+2022a

The relative errors in the chemical models due to choosing constant ionization rates versus the attenuated model are highly **sensitive to the assumed rate, and a complex function of density.**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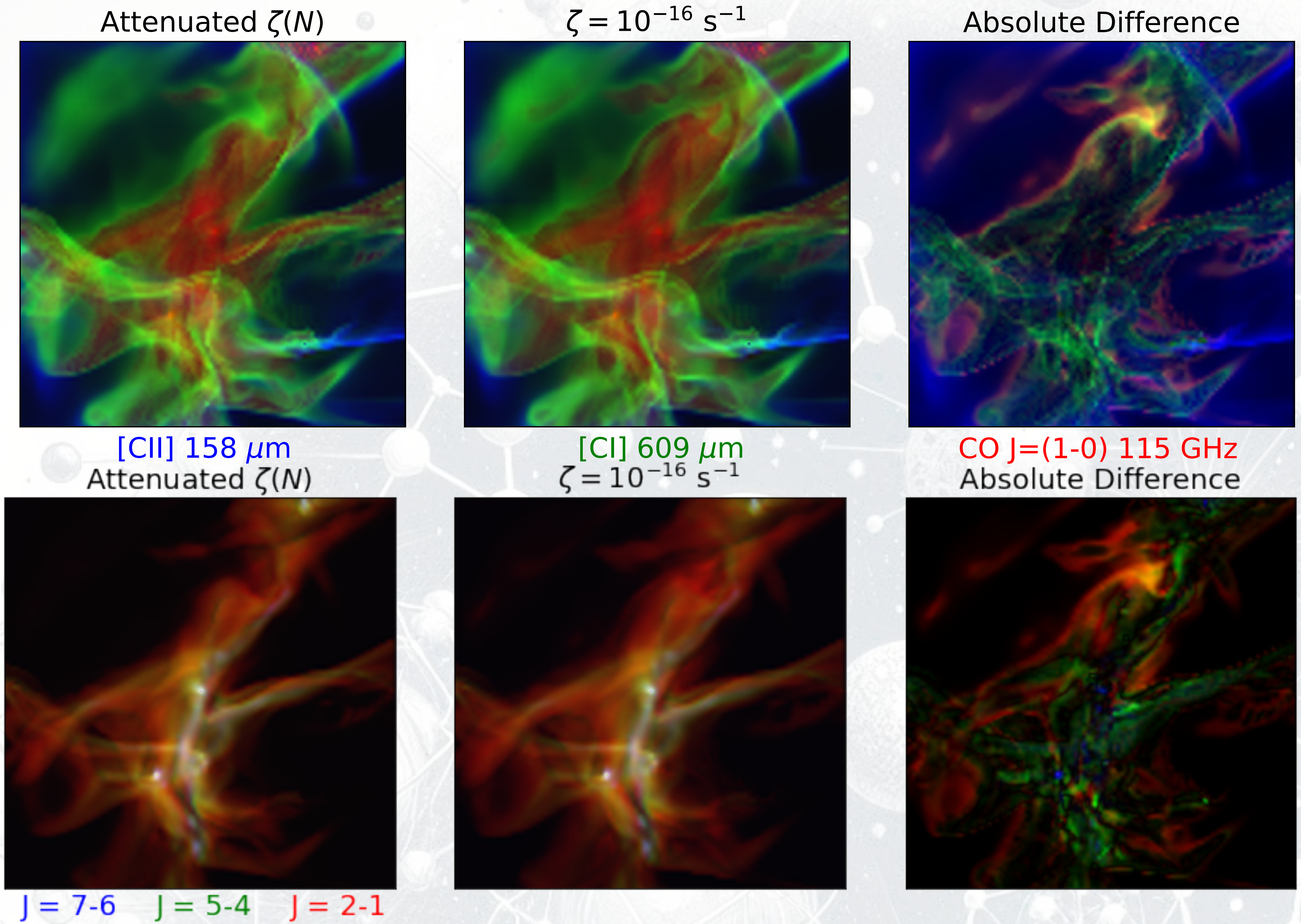
# Astrochemical models with 3D CR physics

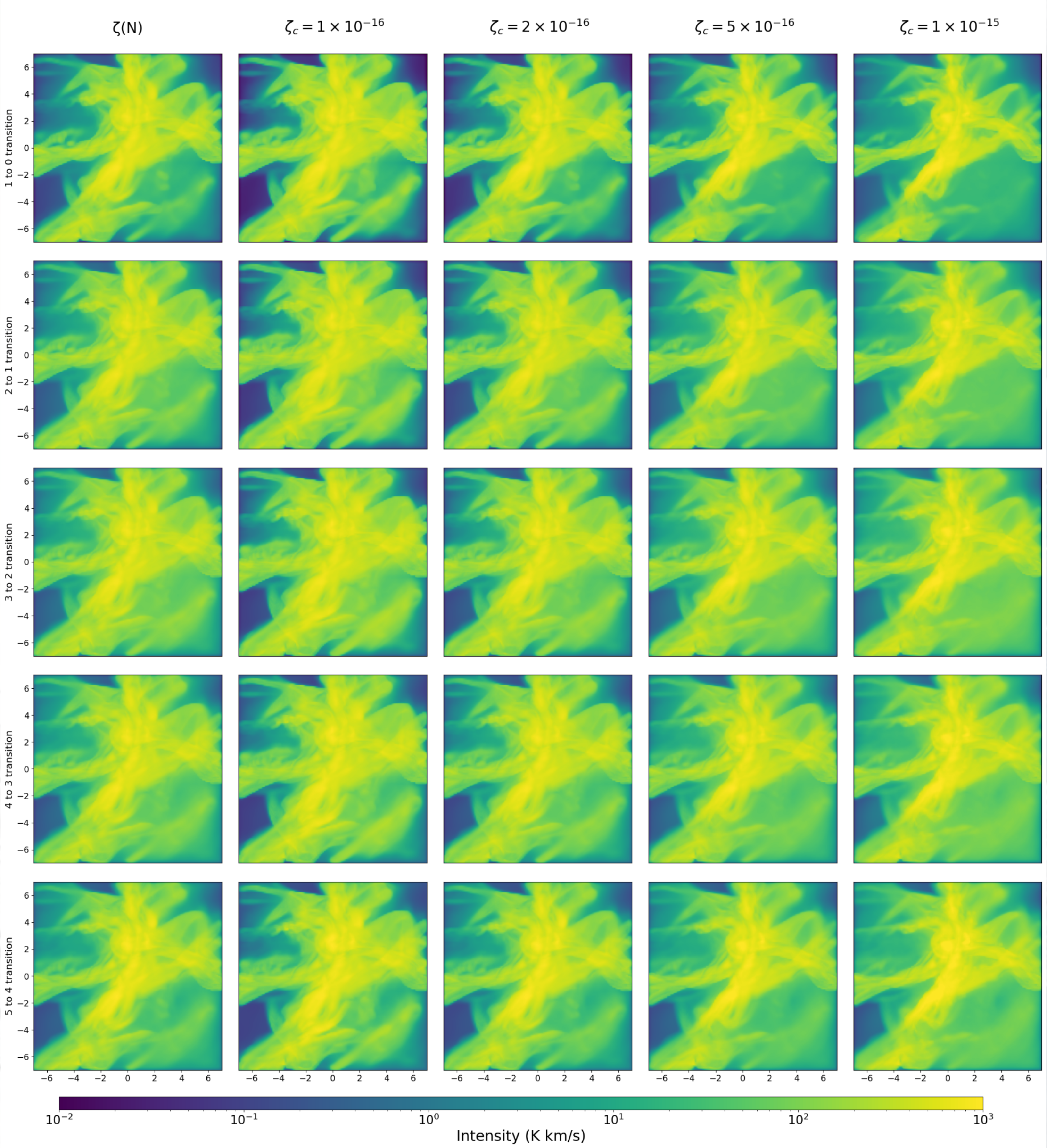


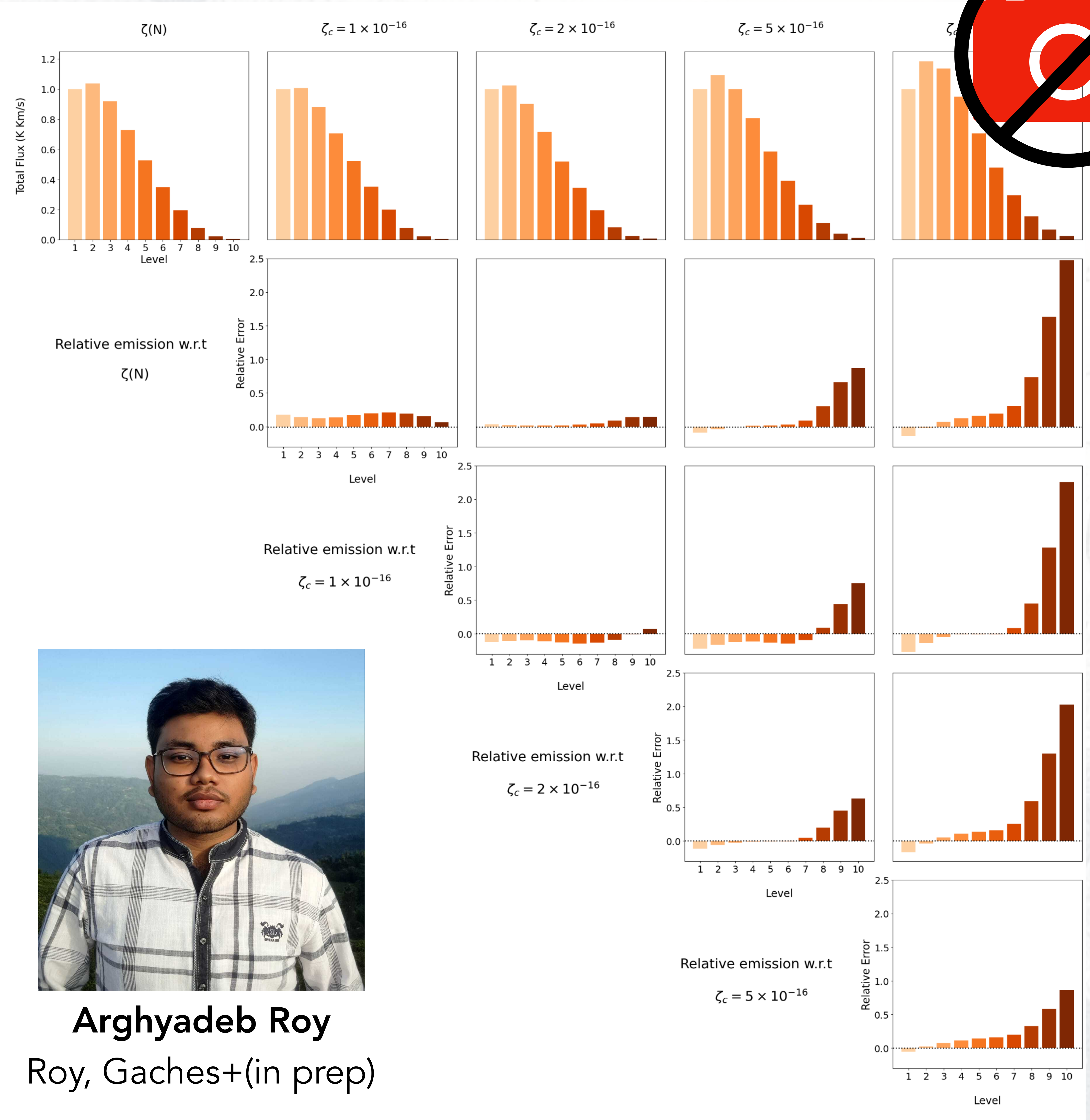

**Gaches**+2022a

**Impact of CR physics on observables:**
There are distinct observable differences between cloud models. Noticeable for [CII], [CI] and high-J CO due to dense gas temperatures.

# Astrochemical models with 3D CR physics

**Preliminary**



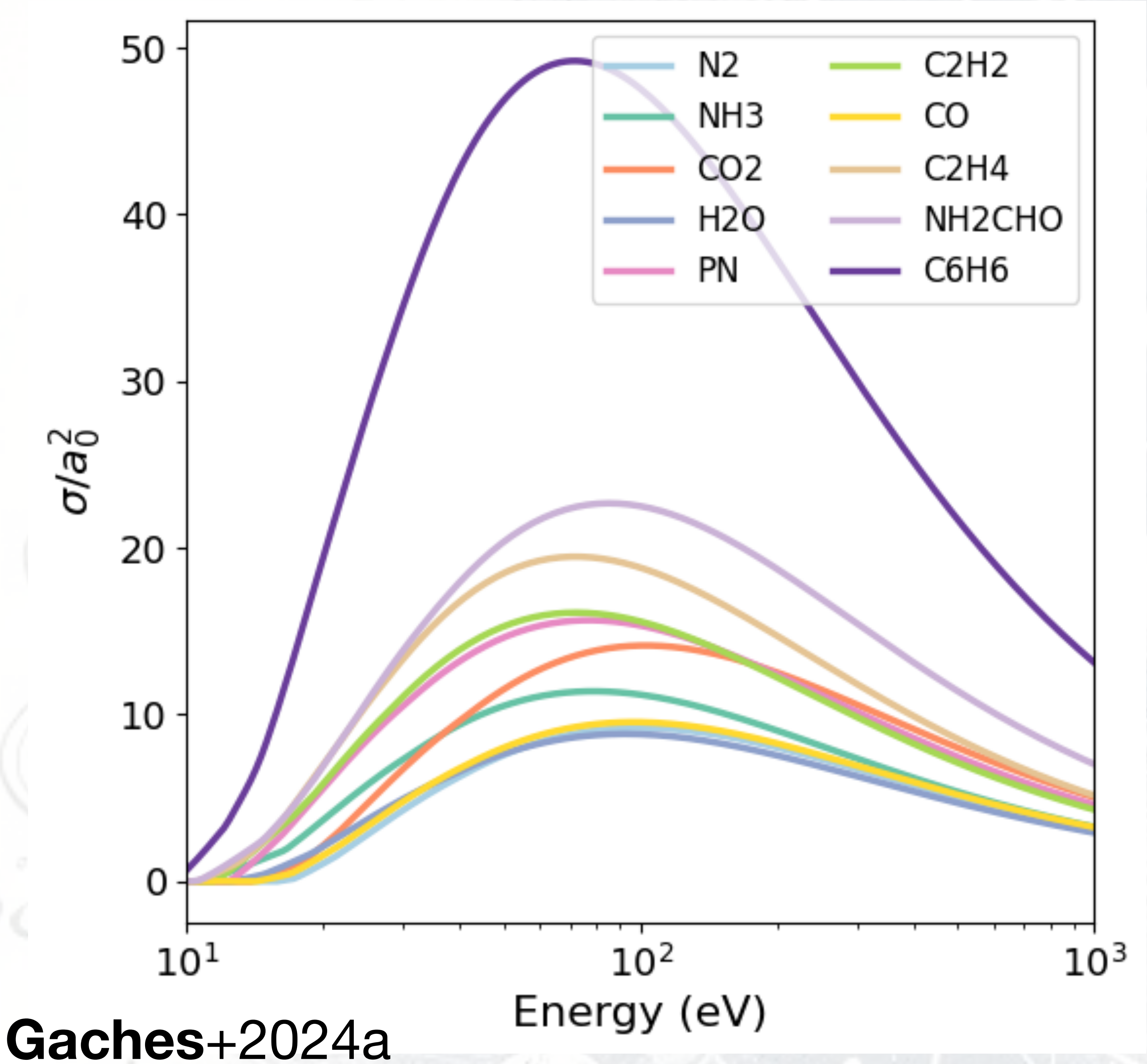




**Arghyadeb Roy**

Roy, Gaches+(in prep)

# The **A**strochemistry **L**ow-energy **e**lectron **C**ross-**s**ection (ALECS) Database

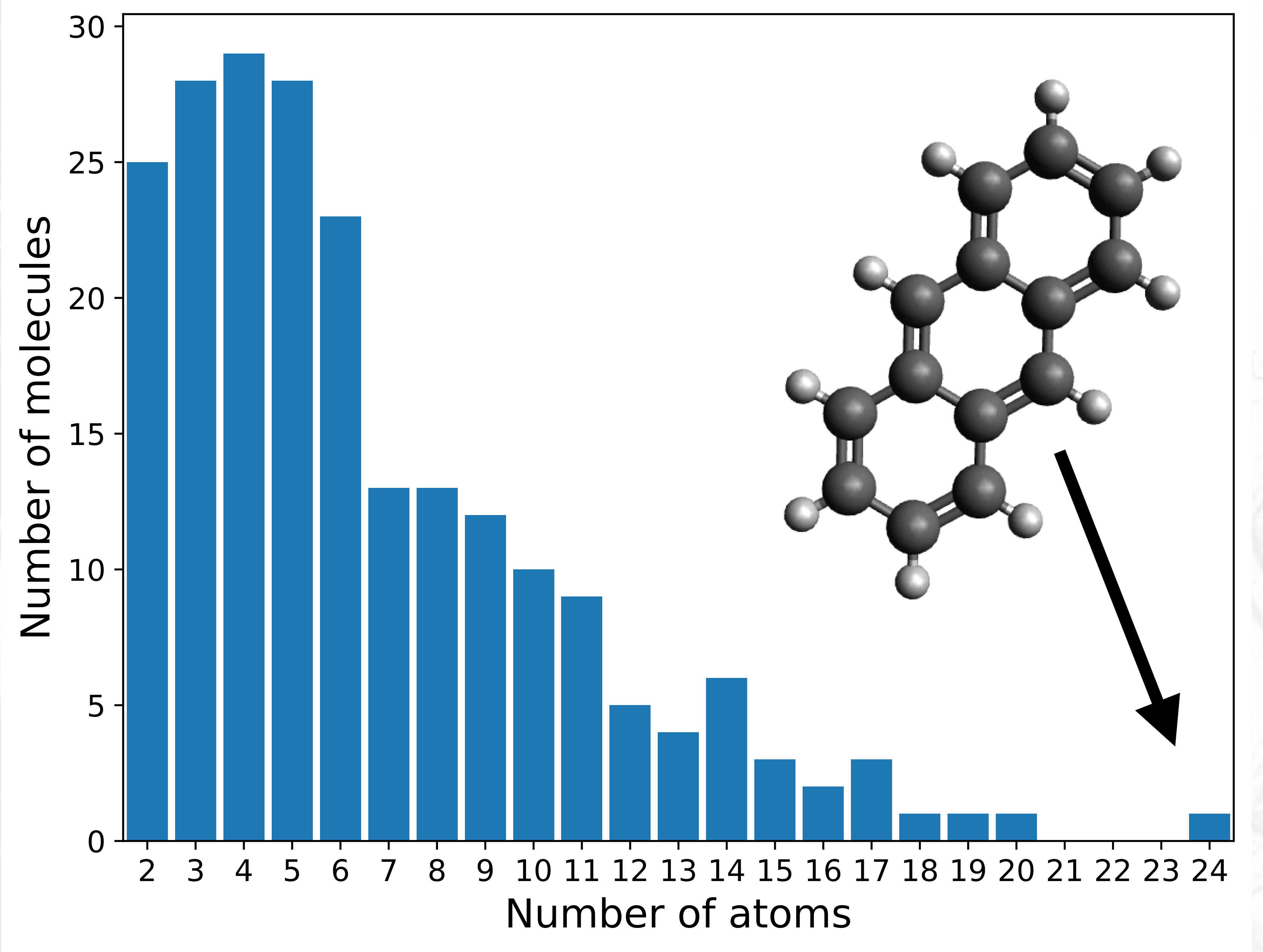
GitHub.com/AstroBrandt/ALeCS



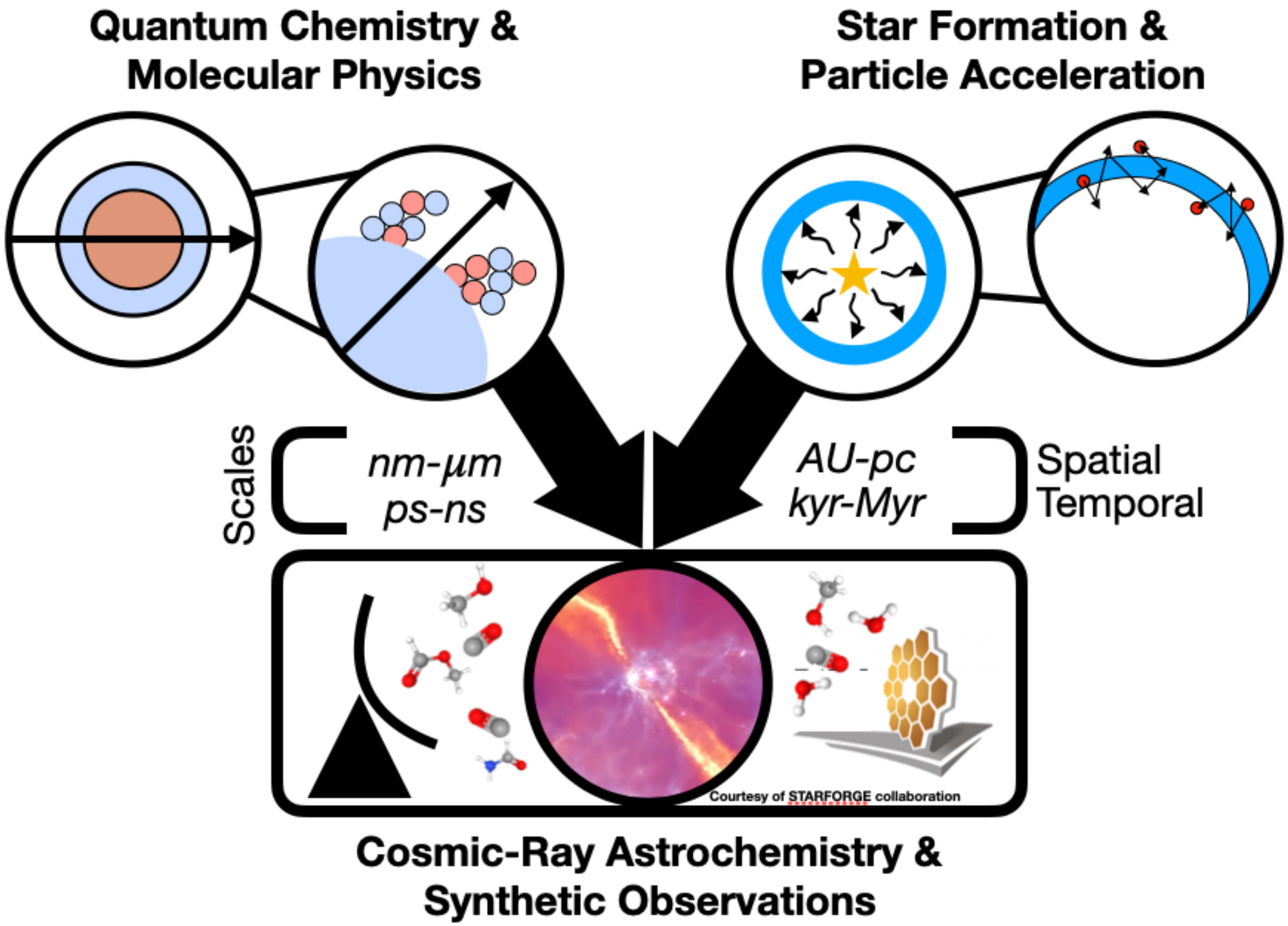

**Gaches**+2024a

**Initial release**

- >200 molecules, optimised geometry and structure. HF, MP2 and CCSD(T) level calculations
- Single ionization cross sections and rates, KIDA & UMIST formats



# Cosmic Ray Astrochemistry: Multi- and Inter-disciplinary



# Conclusions

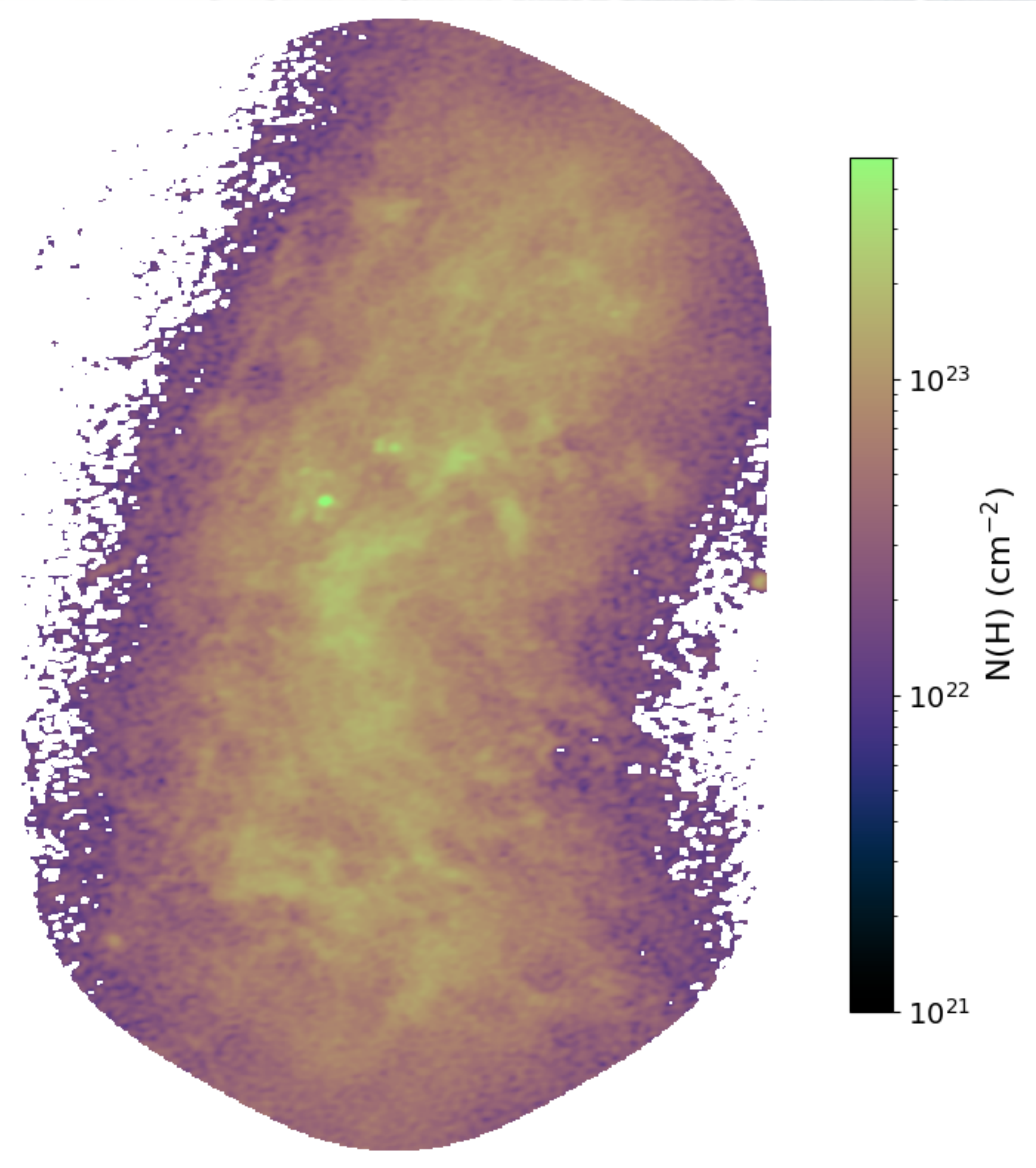
- Observations highlight the *need for more complete models* with cosmic rays.
- Laboratory studies have demonstrated that *energetic particle irradiation can stimulate complex organic chemistry* in astrophysical icy grains.
- There is currently a *substantial gap* in such modeling efforts to include sophisticated treatments of cosmic rays, but new efforts are underway and show promise.
- The thermo-chemistry of dense molecular gas *informs on the spectrum and physics of low-energy cosmic rays* (<1 GeV), which are unobservable to gamma-ray facilities.
- Cosmic-ray chemistry natively *requires collaboration between astronomers, physicists and chemists*, unifying the atomic to astrophysical scales.

If time allows, delve into the CMZ

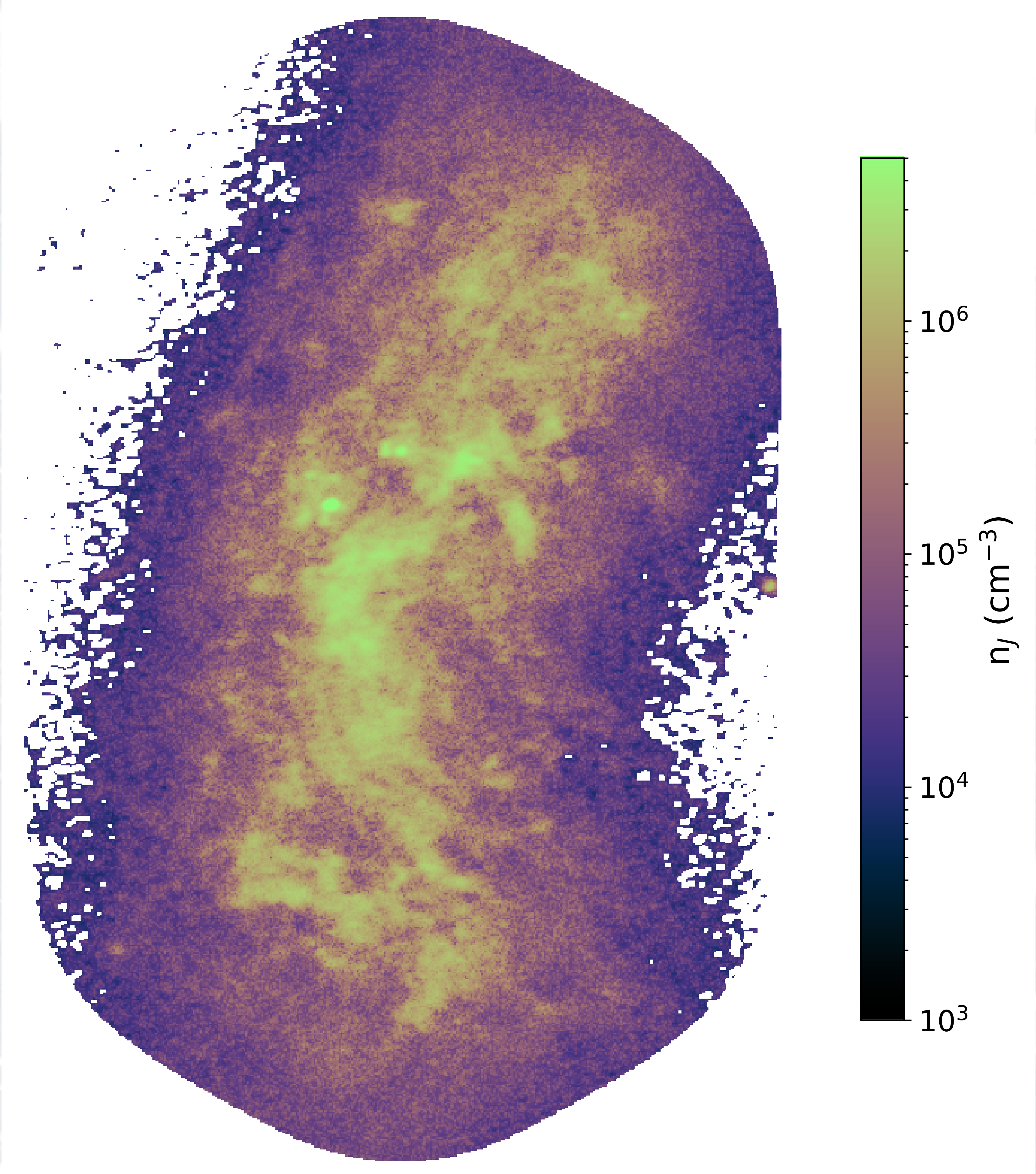
# Impact on organic chemistry - Modelling the Brick

**Preliminary**

Hydrogen column density from Rathborne+2014




Density estimation via Gaches+2024, subm.

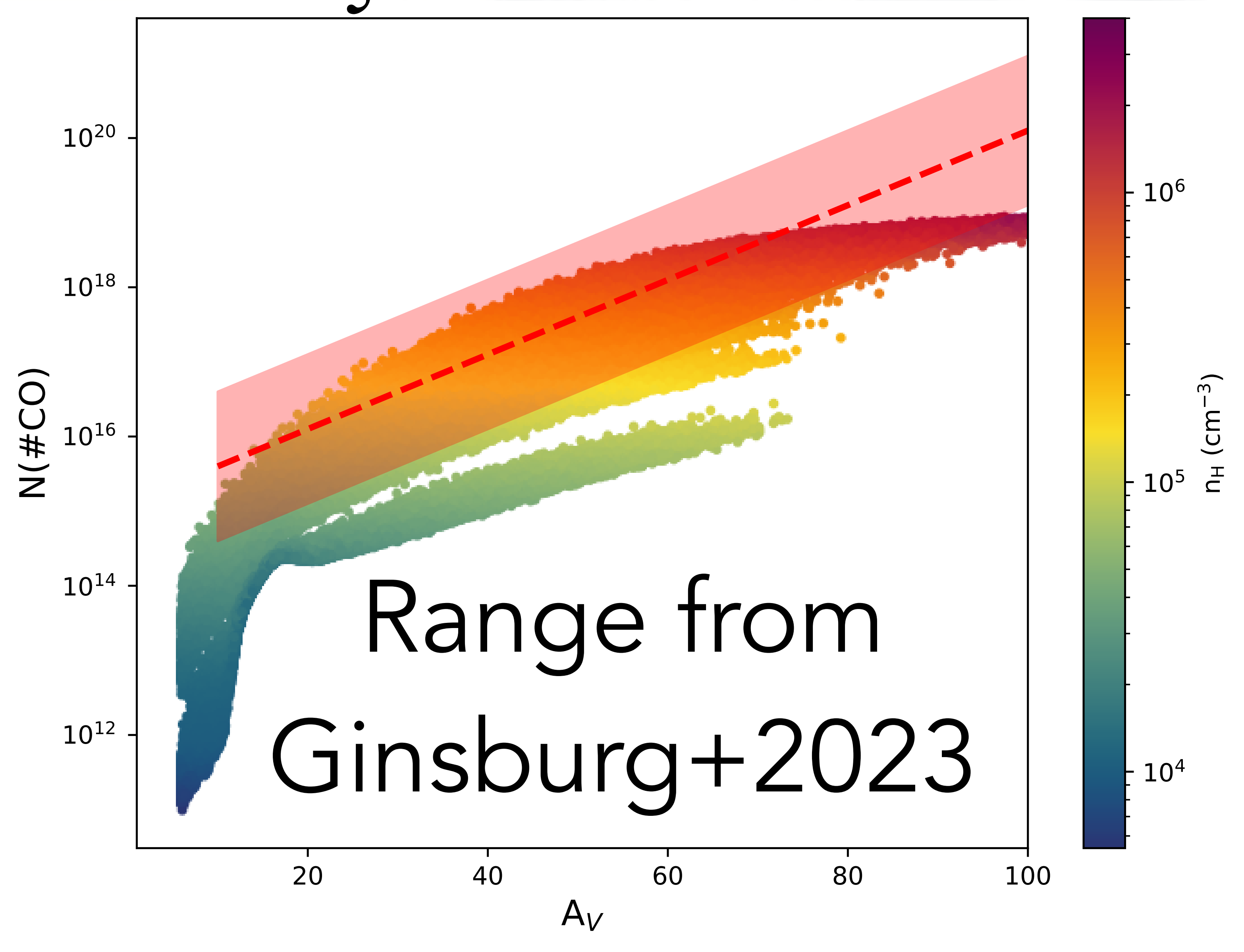


# Impact on ice chemistry - Modelling the Brick

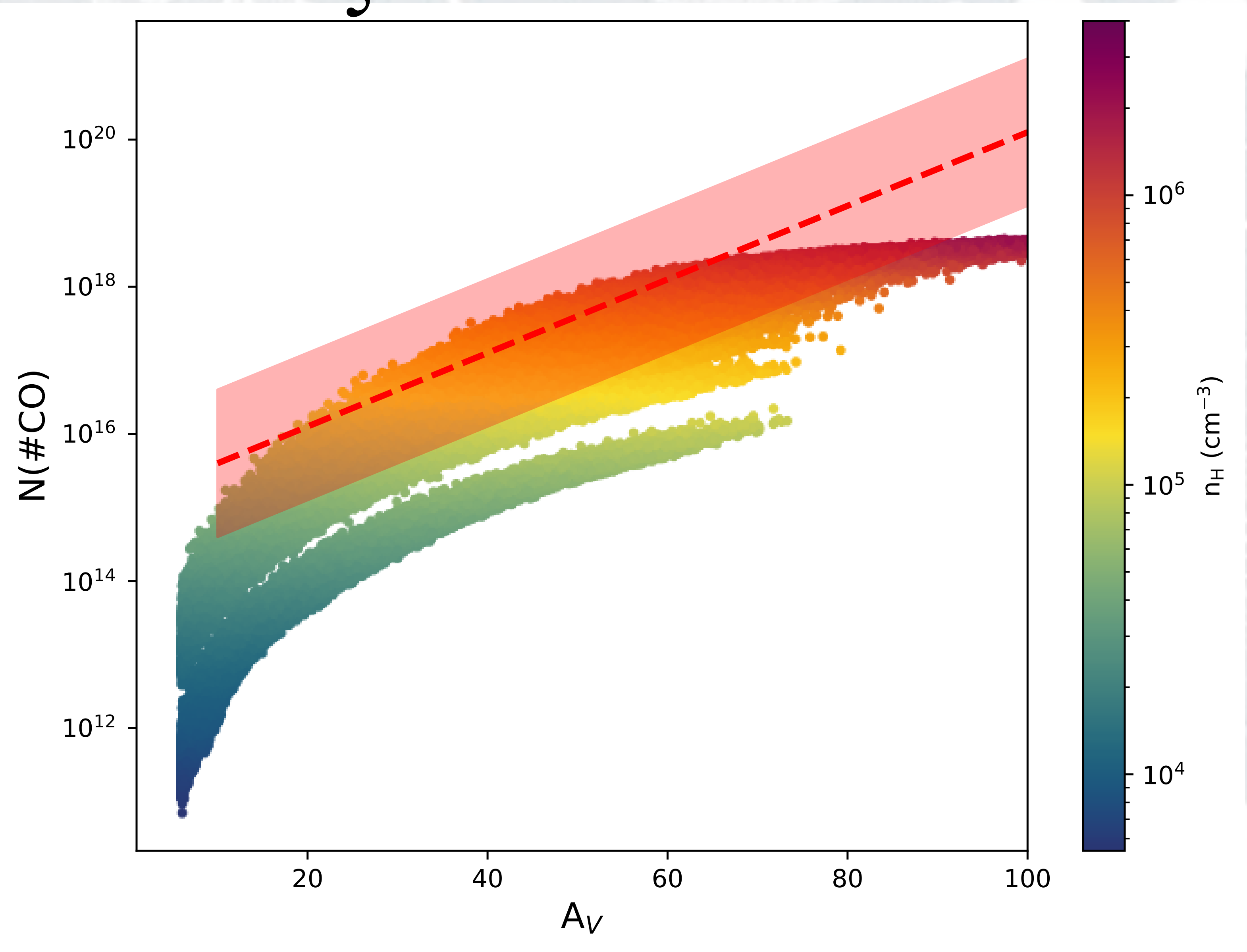
**Preliminary**

The amount of carbon monoxide ice in a cloud is sensitive to the CRIR through **spallation and thermal processes**

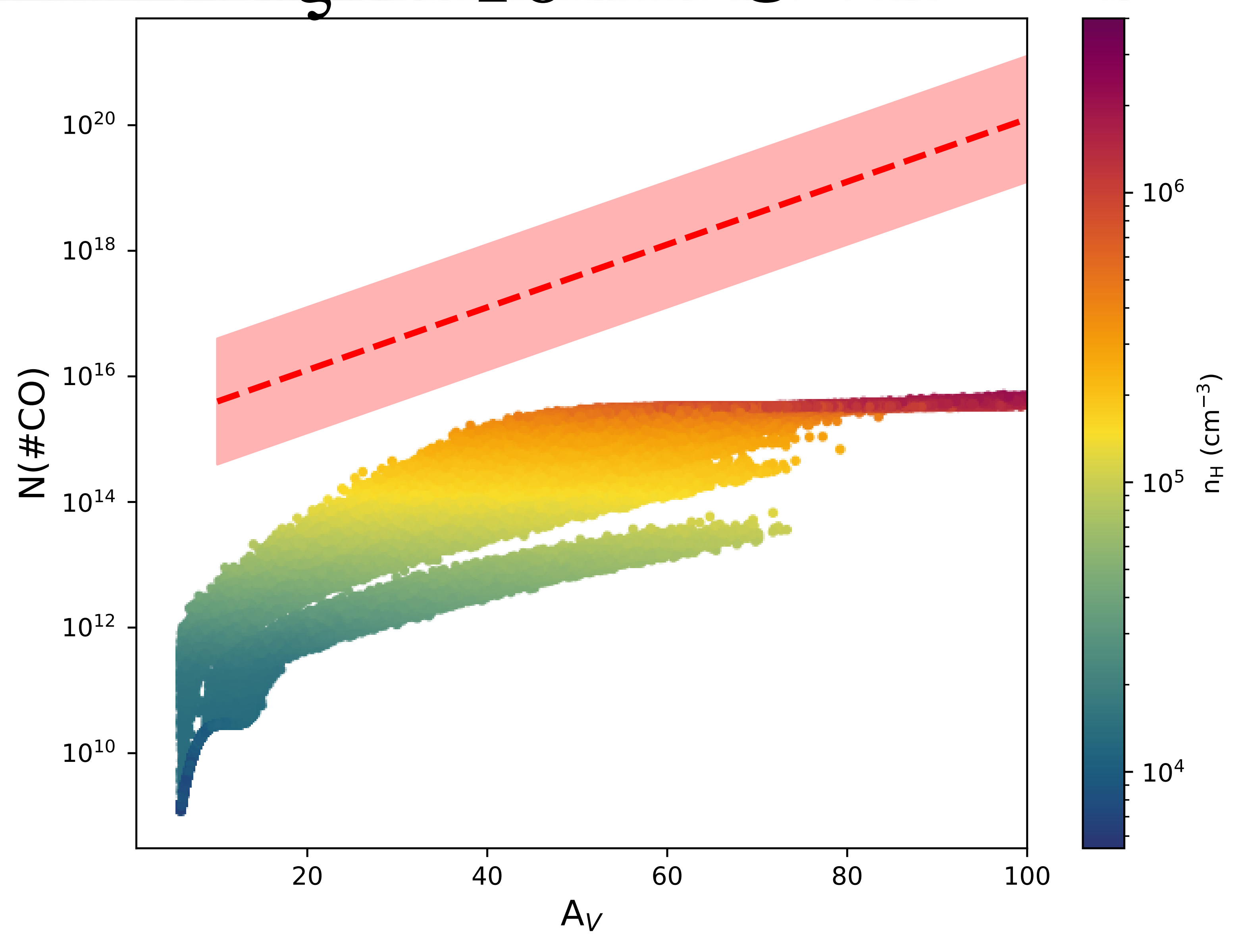
$\zeta = 10^{-16}\ \mathrm{s}^{-1}$




$\zeta = 10^{-15}\ \mathrm{s}^{-1}$



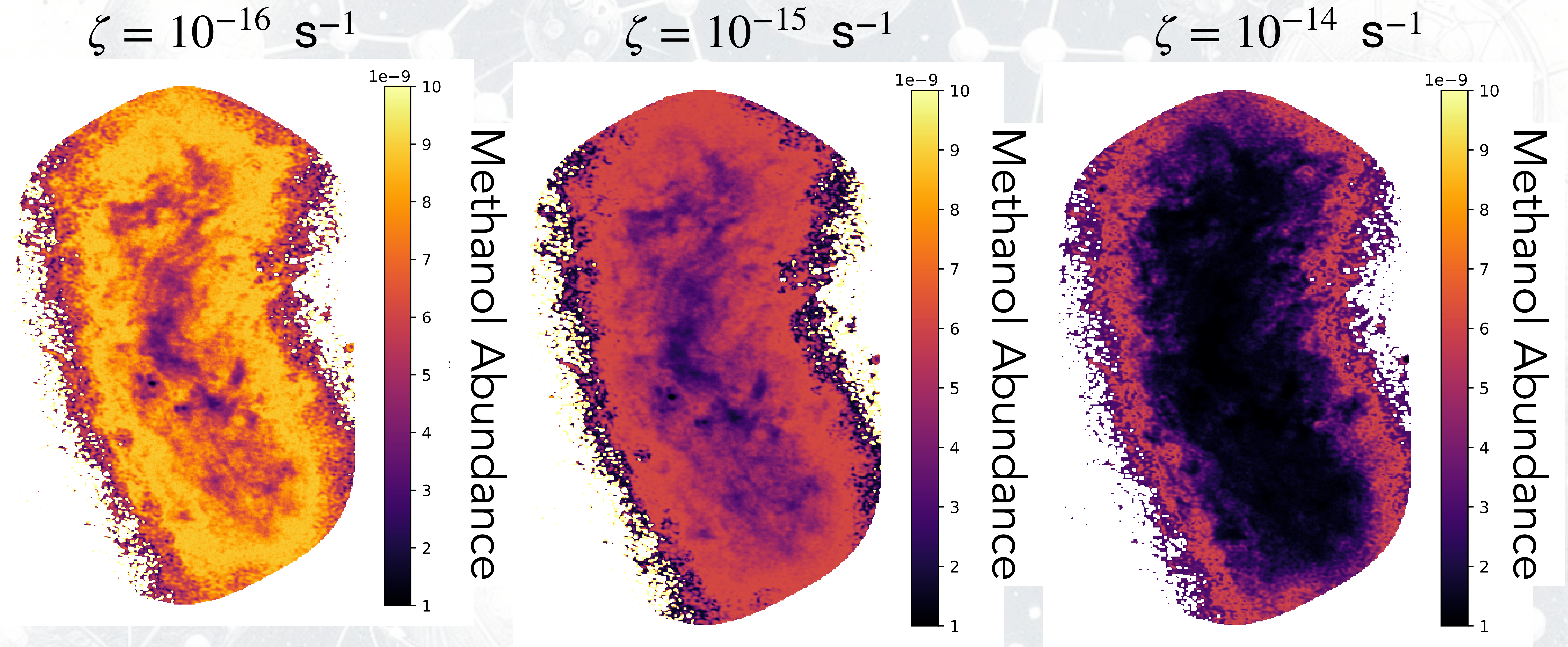

$\zeta = 10^{-14}\ \mathrm{s}^{-1}$



# Impact on organic chemistry - Modelling the Brick

**Preliminary**

While warmer temperatures can favor organic chemistry, higher CR fluxes **inhibit ice growth and dissociate molecules, reducing chemical complexity**



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