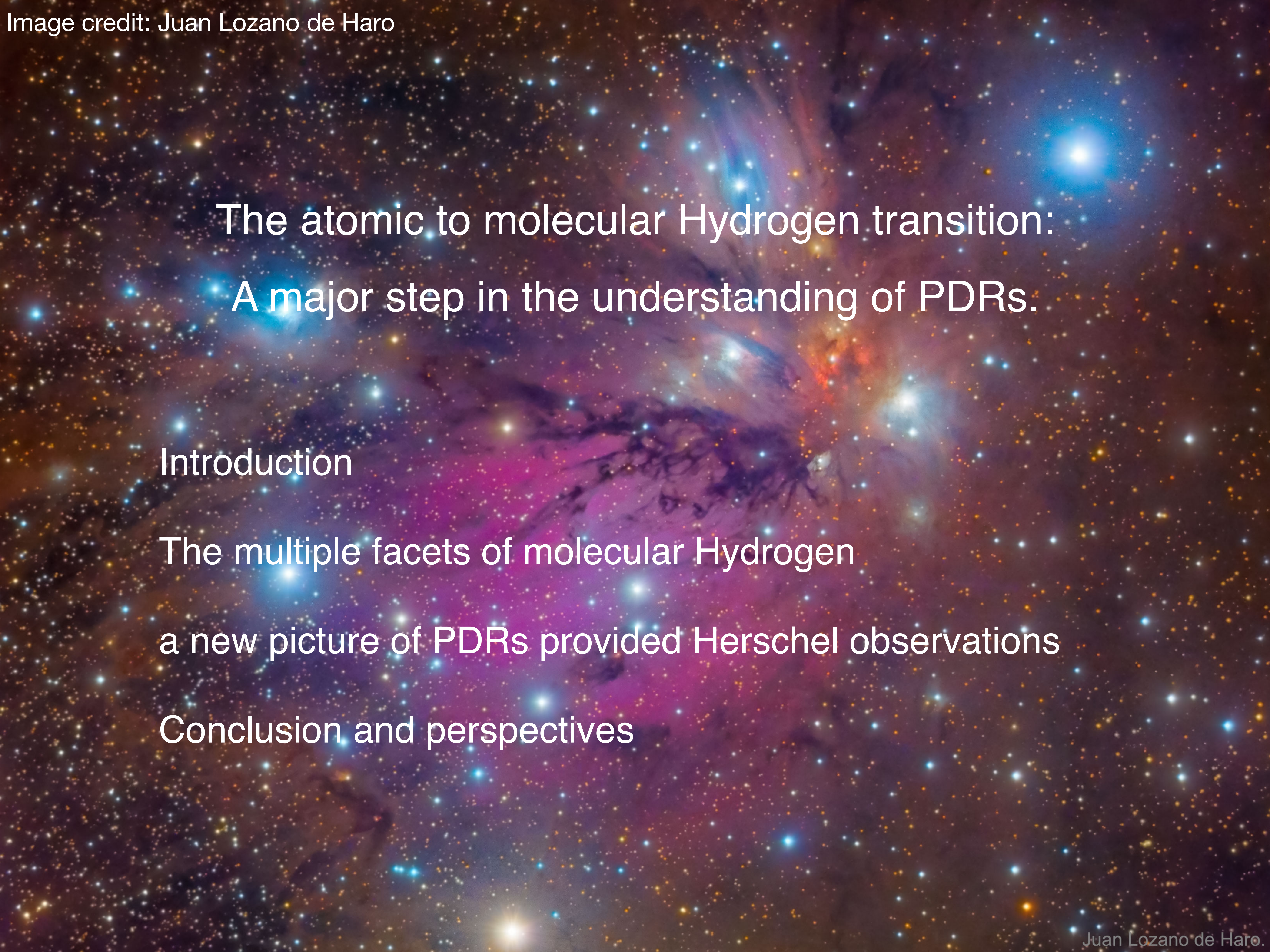
Image credit: Juan Lozano de Haro



# The atomic to molecular Hydrogen transition:

## A major step in the understanding of PDRs.

Introduction

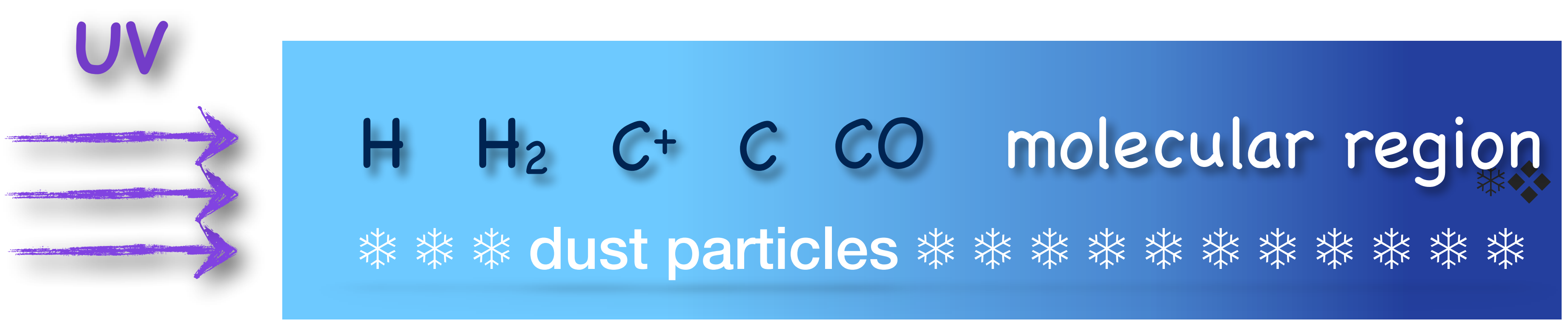
The multiple facets of molecular Hydrogen

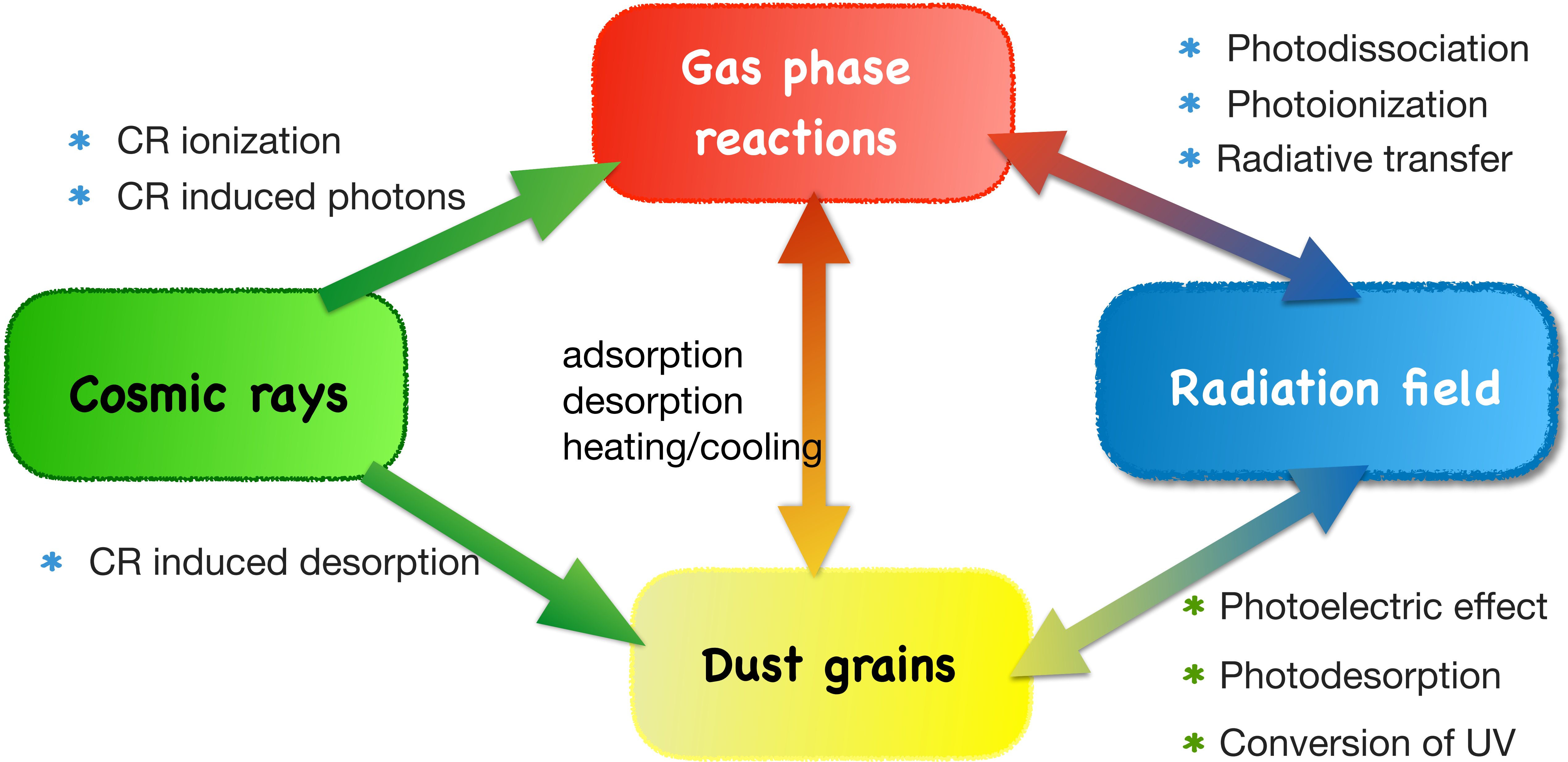
a new picture of PDRs provided Herschel observations

Conclusion and perspectives

Juan Lozano de Haro.

# Photon Dominated Regions (PDRs)




**Gas phase reactions**

**Cosmic rays**

**Radiation field**

**Dust grains**

- CR ionization
- CR induced photons

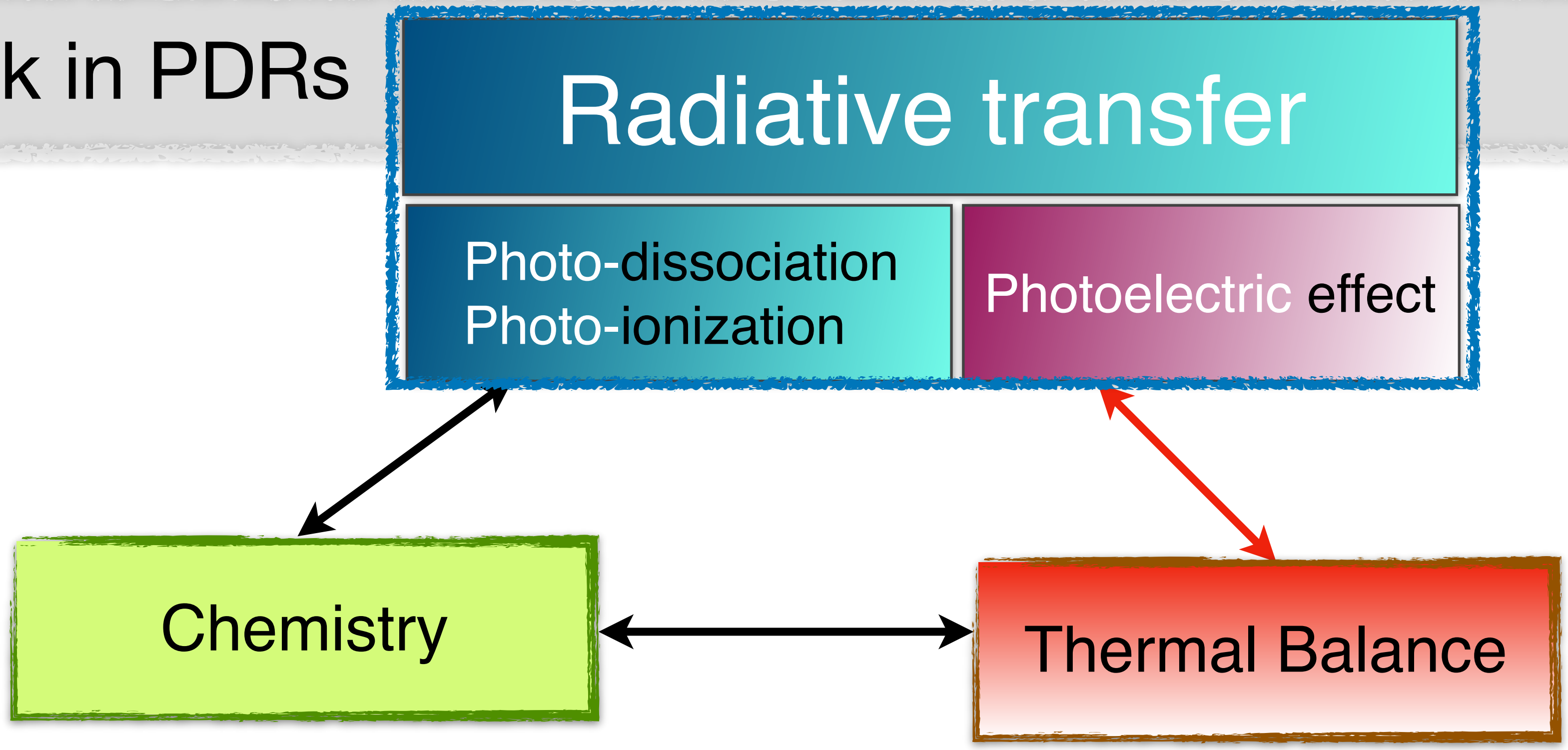
- Photodissociation
- Photoionization
- Radiative transfer

adsorption
desorption
heating/cooling

- CR induced desorption

- Photoelectric effect
- Photodesorption
- Conversion of UV to IR photons

# The physical processes at work in PDRs



## Radiative transfer

UV induced photo processes (gas + dust) continuum + lines

Radiation energy density as a function of $\lambda$

☛ Compute photorates and photoelectric effects

IR - submm - mm : discrete transitions

## Thermal balance : $\Delta G = H - C = 0$

Heating: photoelectric effect, collisional de-excitation of pumped $H_2$, cosmic rays, chemical formation through exothermic reactions

Cooling: radiative emission following collisional excitation

kinetic energy => radiative energy

Solve the detailed balance (collisional excitation, radiative emission/pumping)

endothermic chemical reactions

Gas-grain coupling

## Chemistry : $\frac{d[X]}{dt} = F - D[X] = 0$

Gas phase: reaction rate coefficients are radiation field and temperature dependent

Dust and gas/solid interface: at least for $H_2$ formation

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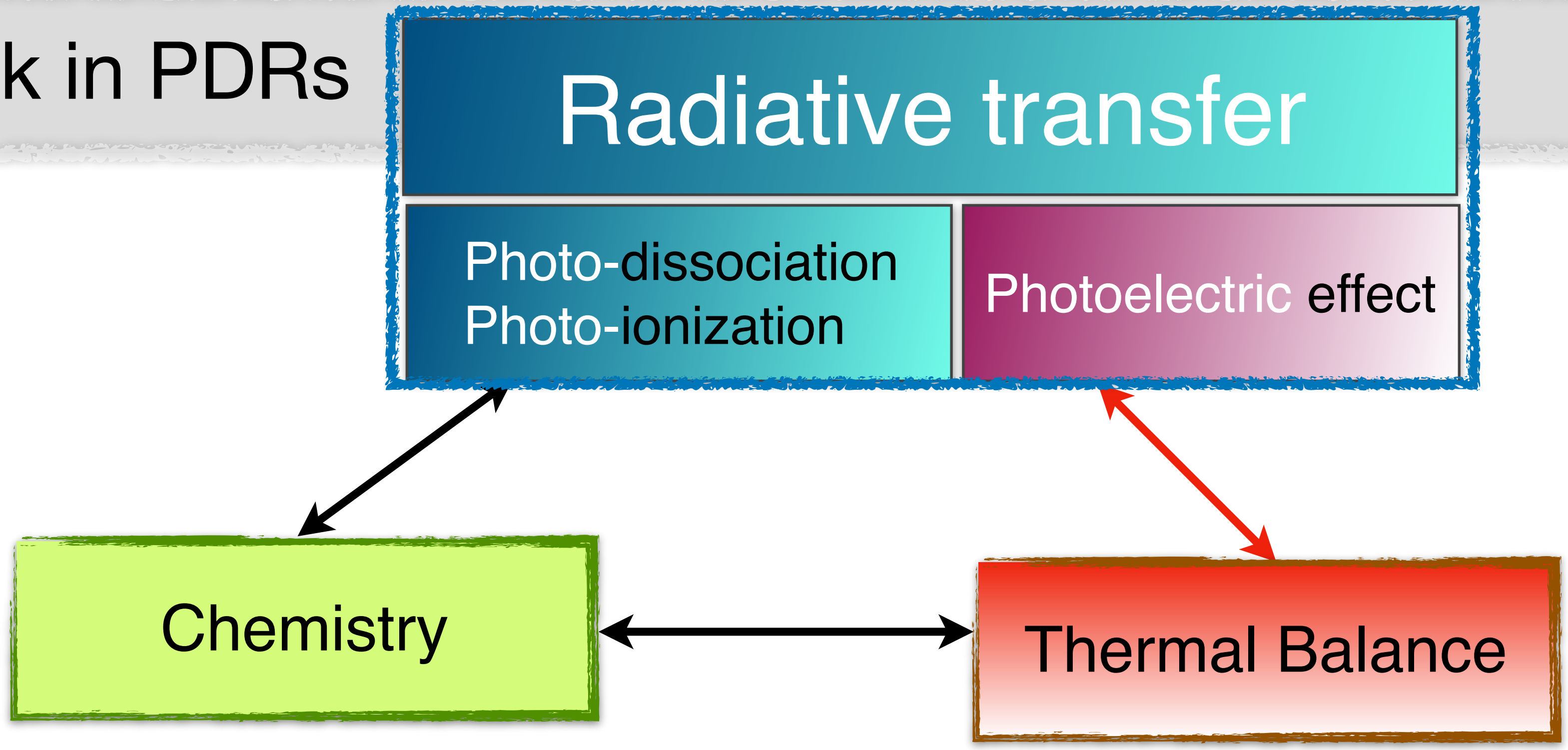

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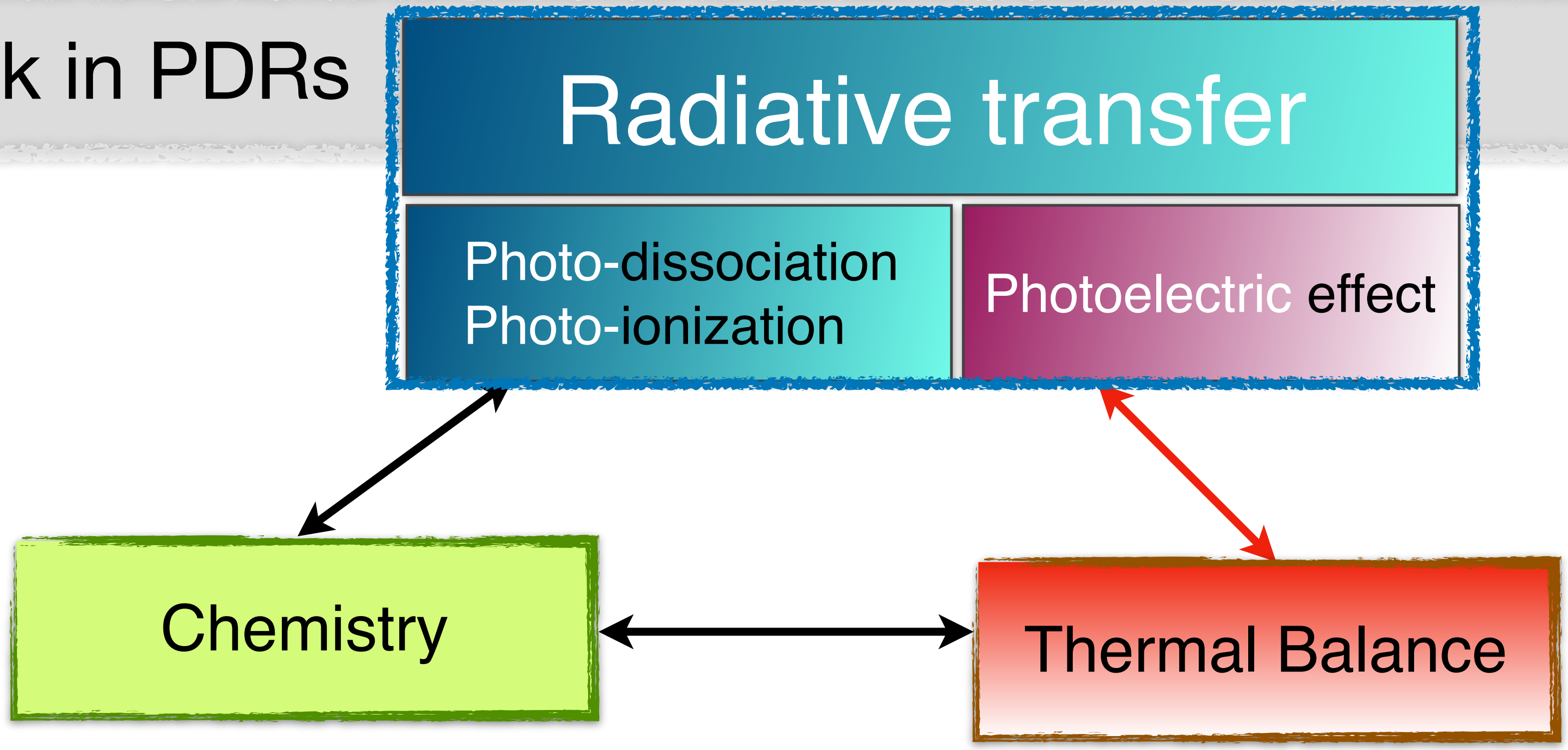
Radiative transfer

Photo-dissociation
Photo-ionization

Photoelectric effect

Chemistry

Thermal Balance

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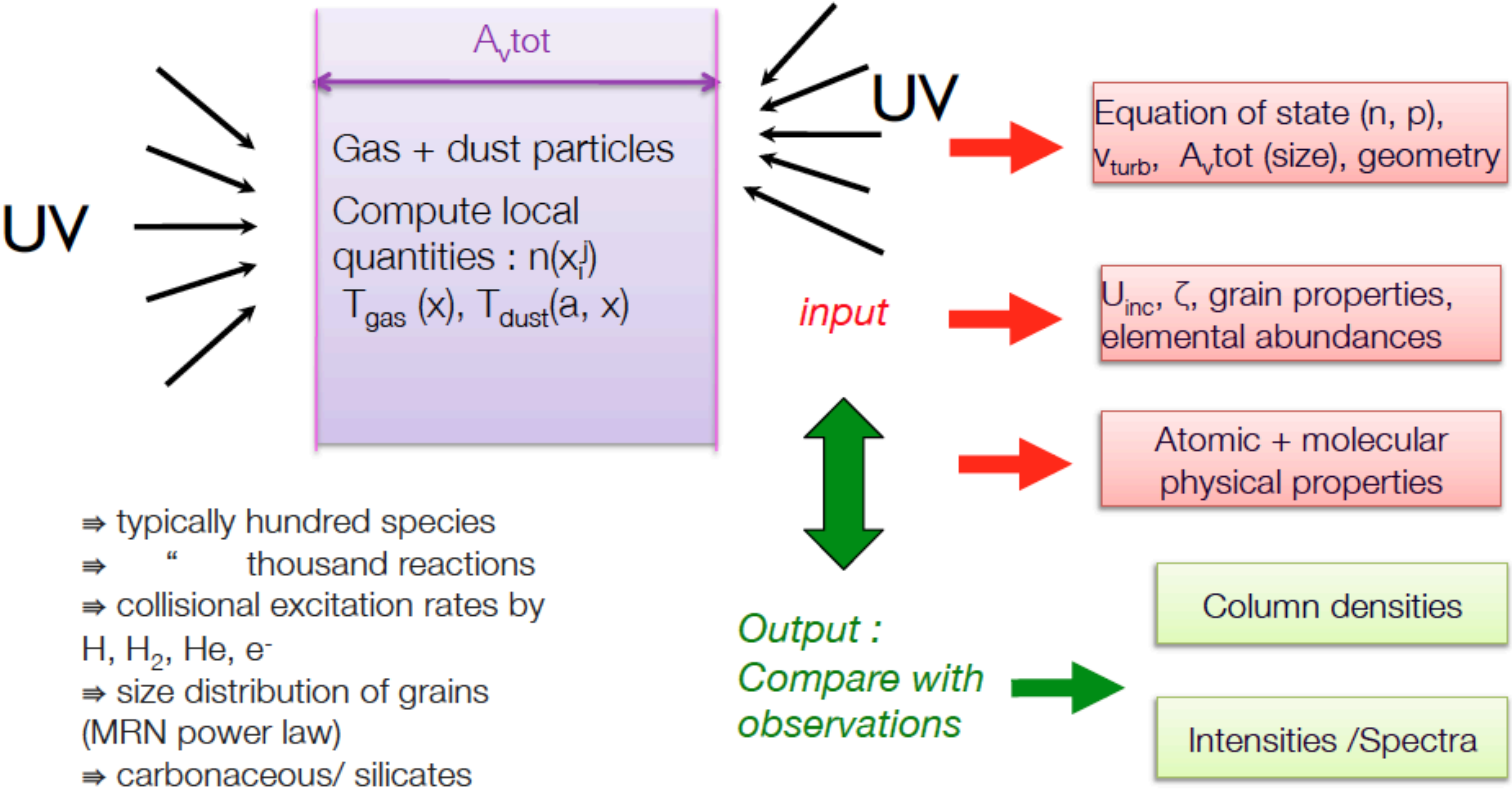
# Inputs /outputs



$A_v$tot

Gas + dust particles

Compute local quantities : $n(x_i^j)$ $T_{gas}(x)$, $T_{dust}(a, x)$

UV

UV

*input*

Equation of state (n, p), $v_{turb}$, $A_v$tot (size), geometry

$U_{inc}$, $\zeta$, grain properties, elemental abundances

Atomic + molecular physical properties

*Output : Compare with observations*

Column densities

Intensities /Spectra

⇒ typically hundred species

⇒ “ thousand reactions

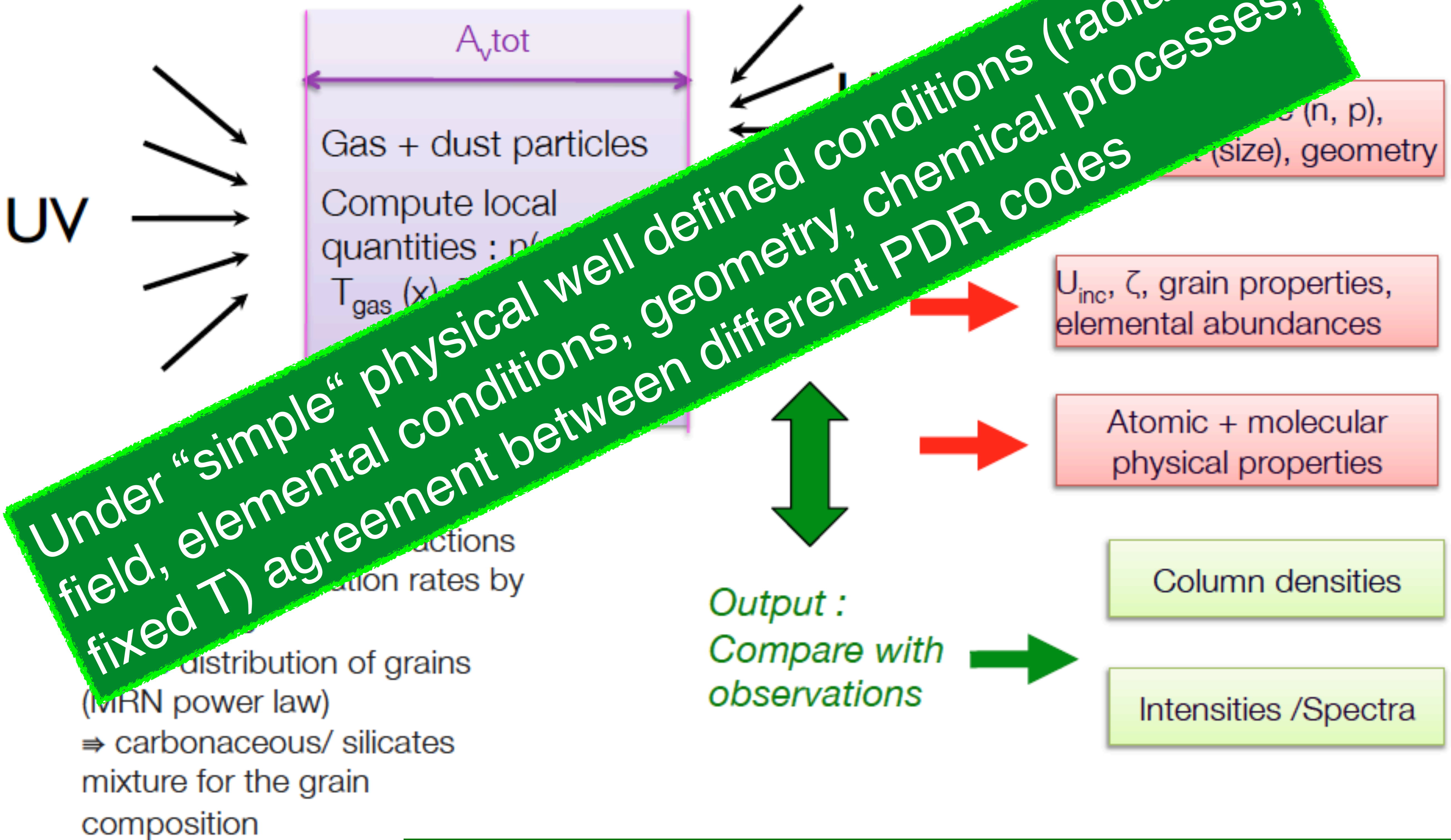
⇒ collisional excitation rates by H, $H_2$, He, $e^-$

⇒ size distribution of grains (MRN power law)

⇒ carbonaceous/ silicates mixture for the grain composition

The Meudon PDR code @ http://ism.obspm.fr

# Inputs /outputs



UV

$A_v$tot

Gas + dust particles

Compute local quantities : n(
$T_{gas}$ (x)

…(n, p),
…(size), geometry

$U_{inc}$, ζ, grain properties, elemental abundances

Atomic + molecular physical properties

…actions
…ation rates by
…distribution of grains
(MRN power law)
⇒ carbonaceous/ silicates mixture for the grain composition

*Output : Compare with observations*

Column densities

Intensities /Spectra

Under “simple“ physical well defined conditions (radiation field, elemental conditions, geometry, chemical processes, fixed T) agreement between different PDR codes

Benchmark exercise : Röllig et al. 2007, A&A 467, 187

# Physics of $H_2$ + photons with hv < 13.6eV

## Spontaneous radiative dissociation:

Solomon process mentioned in Field et al. ARAA 4, 207, 1966 : discrete absorption followed by spontaneous radiative emission into the continuum of X ground electronic state of $H_2$, as well as by infrared radiative cascades within the ground X state

- **efficient shielding**
- **v“, J“ dependence**
- **coupling with excitation and chemistry**

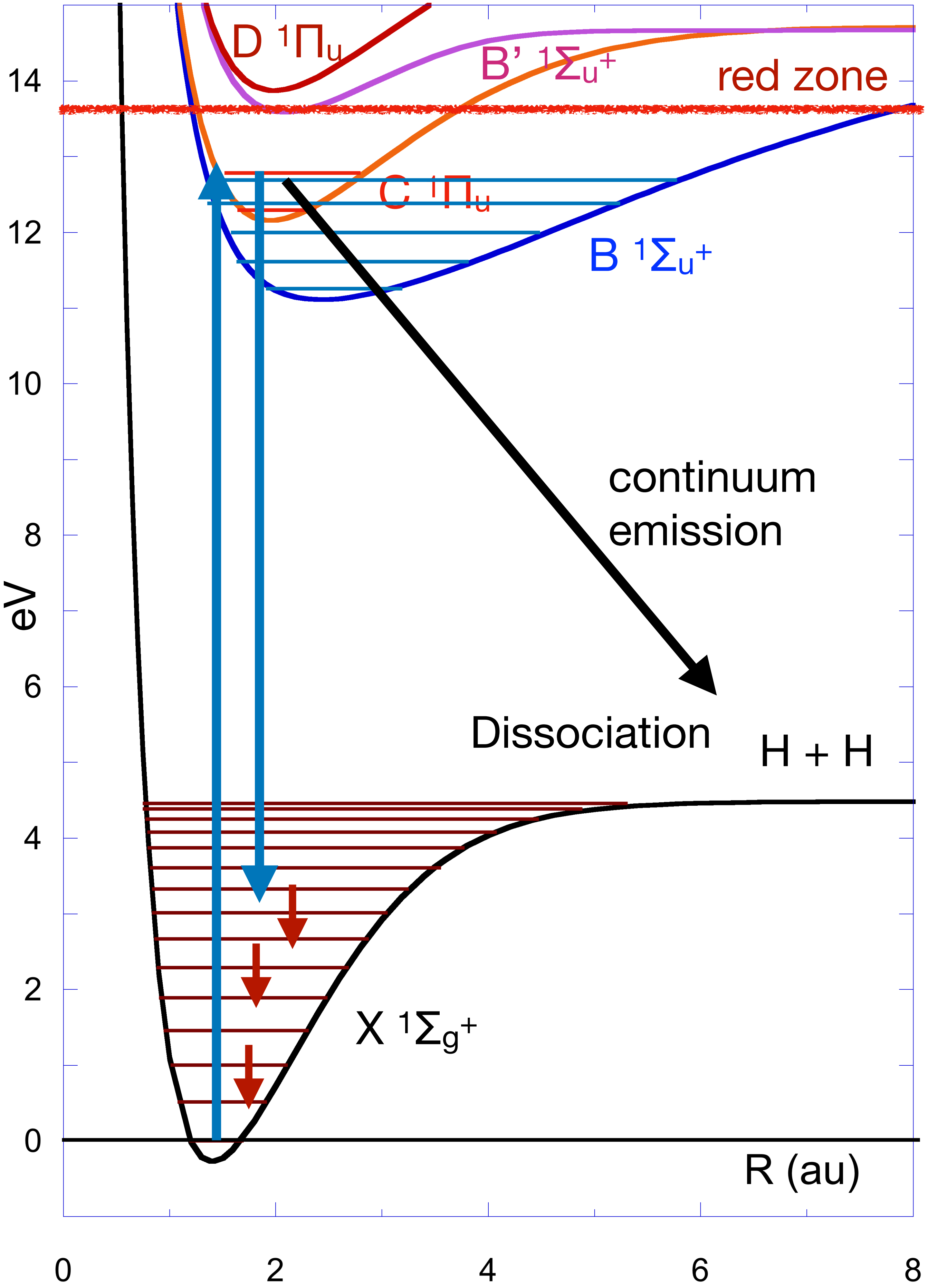
## Lyman / Werner UV transitions

a few experimental investigations (Dabrowski 1984, Launay+Roncin 1994, Ubachs group) on transition positions.

extensive theoretical studies including non adiabatic coupling between B, C, B’,D leading to intensity perturbations (Ford et al. 1975, Abgrall + Roueff 1993, 1994, 2000, 2009, 2015)

## Radiative transitions within X ground state:

few IR studies (Bragg 1982, Campargue group) theoretical QE transition emission probabilities by Wolniewicz et al. 1998, ApJS 115, 293



# Full infrared spectrum of $H_2$

Electric quadrupole ($\Delta J = 0, \pm 2$) + magnetic dipole ($\Delta J = 0$) transitions available within X $^1\Sigma^+$ ground electronic state
(Pachucki + Komasa 2011, PRA 83, 032501)
(Roueff et al 2019, A&A, in press)

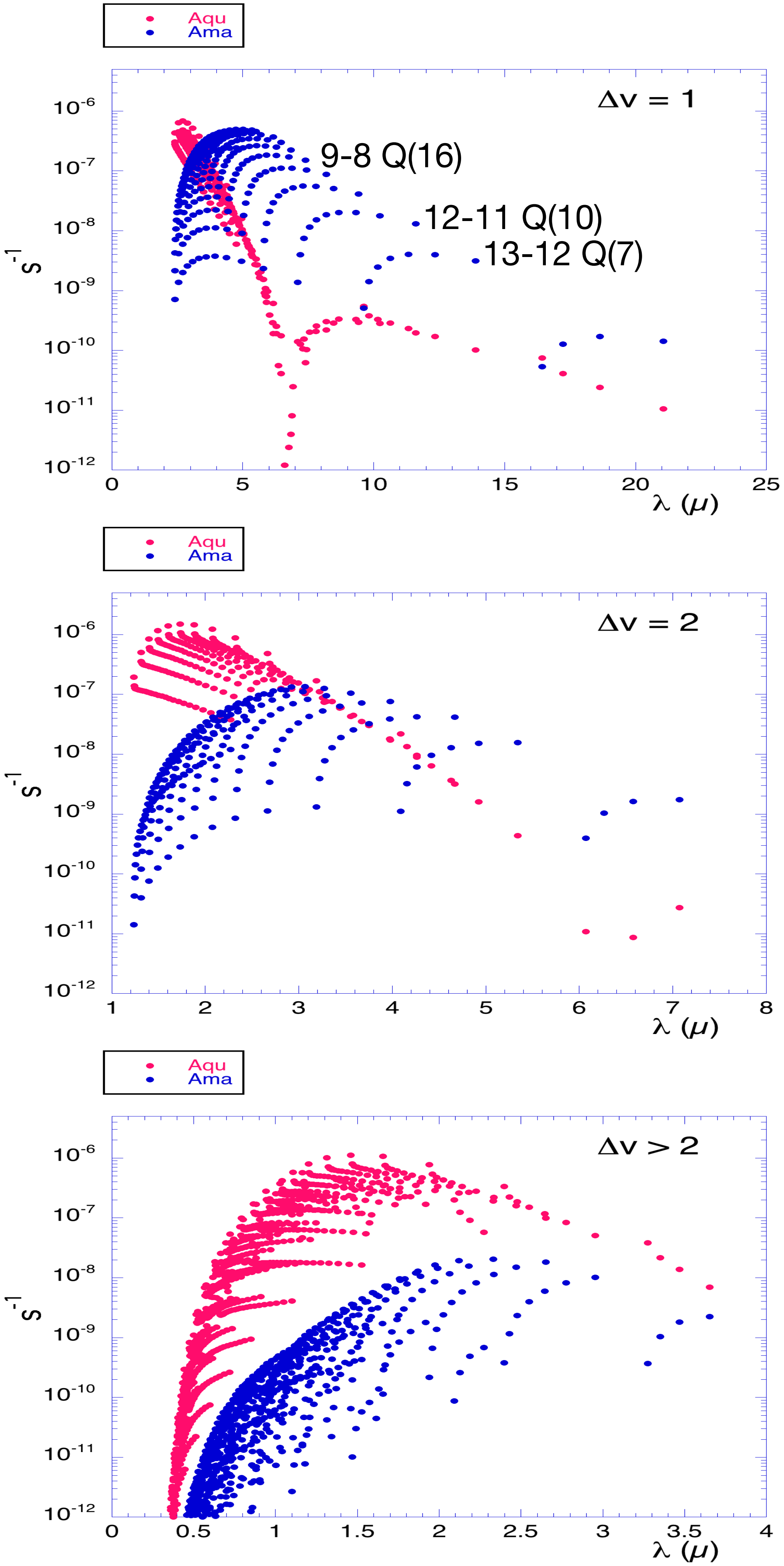
302 bound levels (with v=14, J=4)

4711 transitions

$10^{-3}$ to $10^{-4}$ $cm^{-1}$ wavenumber accuracy which translates to $\approx 10^{-7} - 10^{-8}$ μ for the wavelengths (Pachucki et al. submitted to PRA).

$\Delta v=1$, excited J transitions have larger MD emission probabilities than EQ values.

being included in Meudon PDR code
to be updated for future JWST searches



# modelling of interstellar $H_2$

## Statistical equilibrium of v, J levels within X

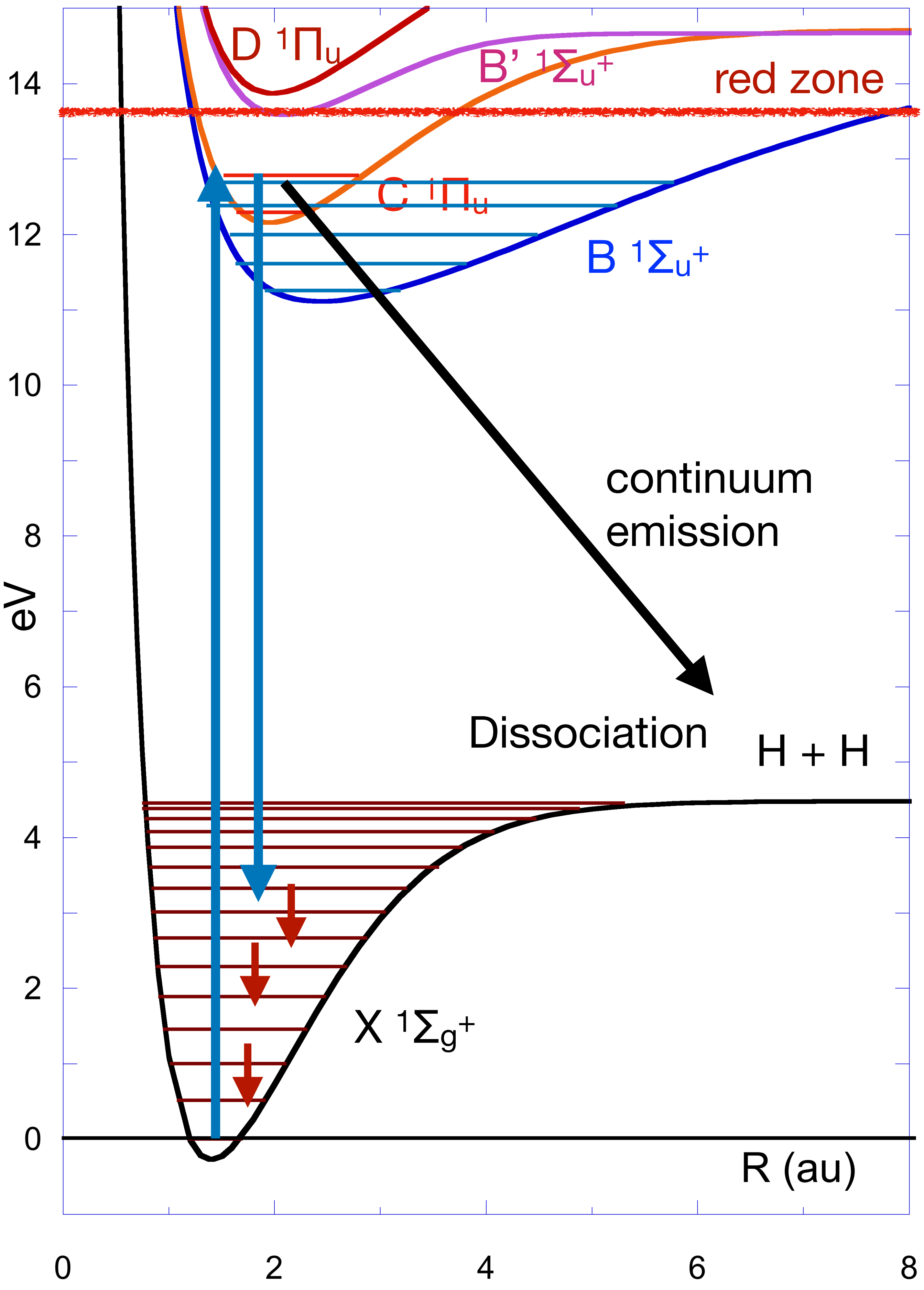
- collisions with H, He, $H^+$, e, $H_2$, …
- radiative cascades
- v, J dependent chemistry (gas phase + surface)

## UV pumping (radiative transfer)

- Line self-shielding + dust shielding

## Coupling to cooling / heating

- Formation from H + H on grain surfaces releases ~ 4.5eV to be shared between $H_2$ internal, kinetic and grain energies
- Collisions with H, He, .. may lead to cooling if $A_{v'J'->v'',J''} > k^{H}_{v'J'->v'',J''}$ n(H) + $k^{He}_{v'J'->v'',J''}$ n(He) + … where kinetic energy from excitation collisions is transferred into radiative energy or heating if collisional desexcitation > radiative quenching



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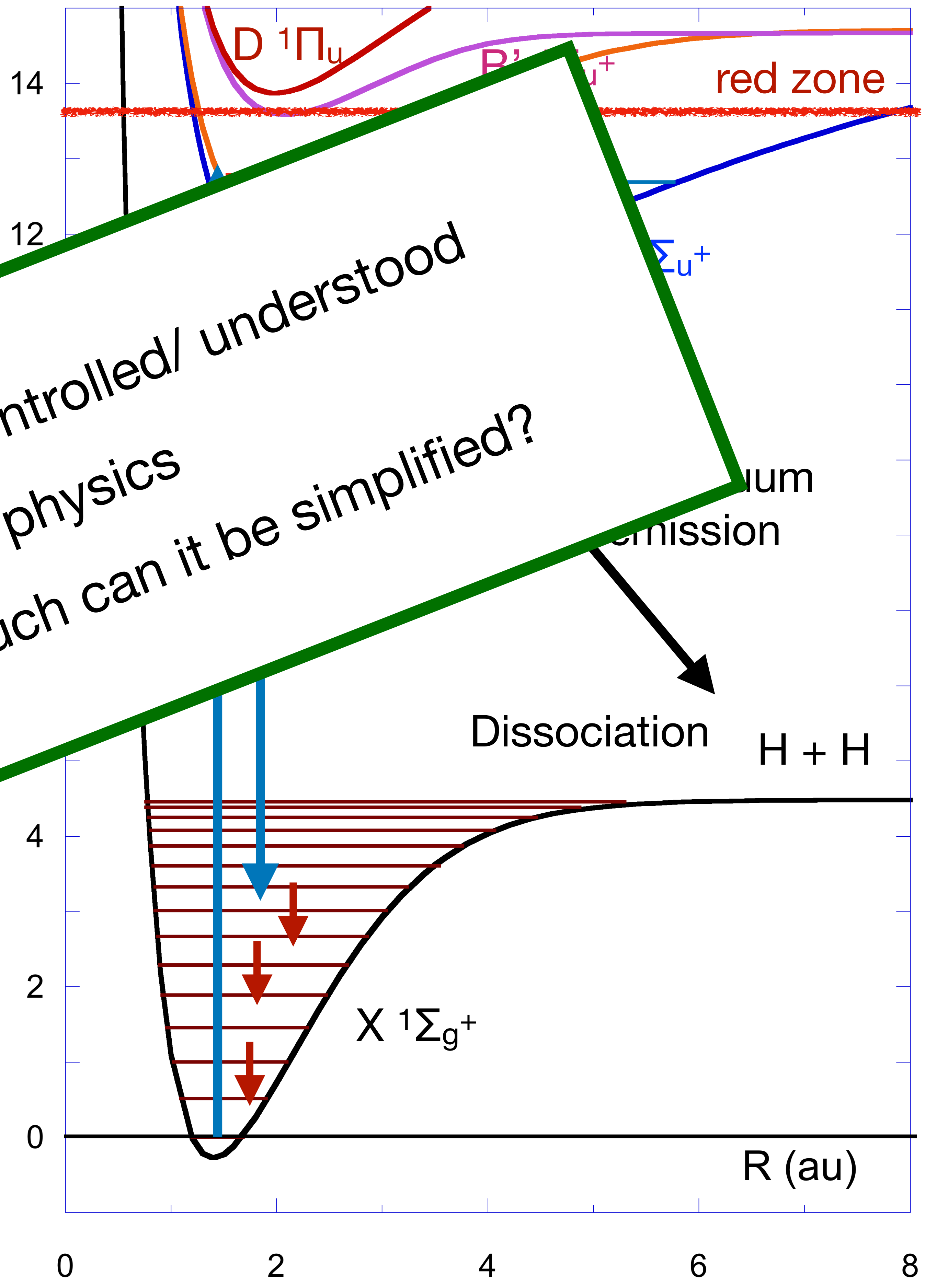
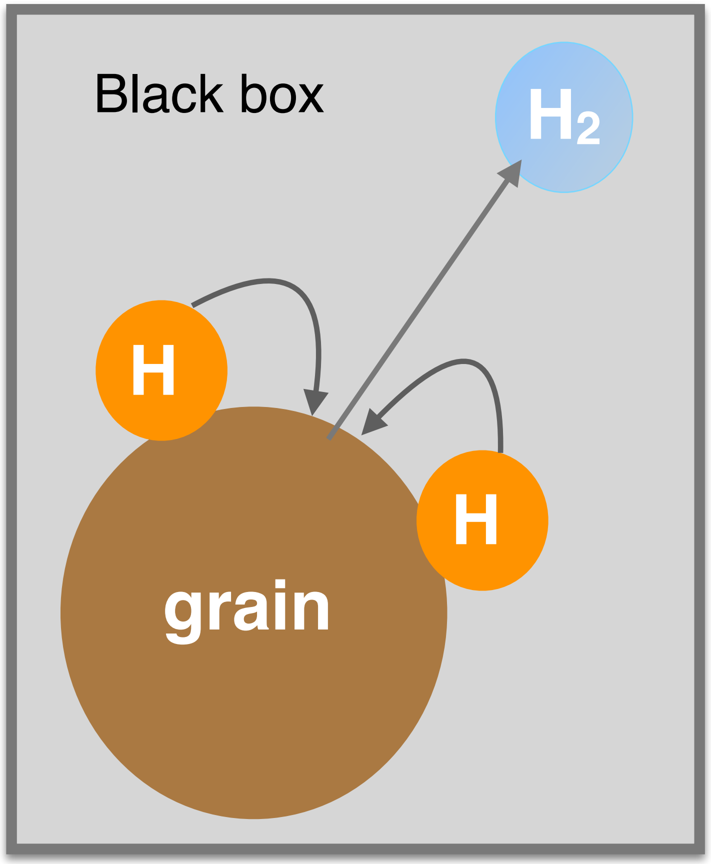
not fully controlled/ understood

Complex physics

How much can it be simplified?



# Formation of $H_2$ on grain surfaces



$$\frac{dn(\mathrm{H_2})}{dt} = \frac{1}{2} R_{\mathrm{H}} n(\mathrm{H})$$

$$R_{\mathrm{H}} = s < \sigma n_d > \bar{v}_{\mathrm{H}}$$

$< \sigma n_d >$ is the mean cross section of dust grains per unit volume

Assuming identical spherical dust grains of radius a

$$< \sigma n_d > = \frac{3}{4} \times \frac{1.4 m_{\mathrm{H}} G}{\rho_d} \times \frac{1}{a} \times n_{\mathrm{H}}$$

With G : dust to gas mass ratio ≈ $10^{-2}$

$\rho_d$ : volumic mass of dust ≈ 3 g cm$^{-3}$

a = 0.1 µm

$$R_{\mathrm{H}} = 1.6 \times 10^{-16} \times s(T_d, T_K) \times \sqrt{\frac{T_K}{300}}$$

≈ Tielens & Hollenbach 1985, ApJ 291: 722

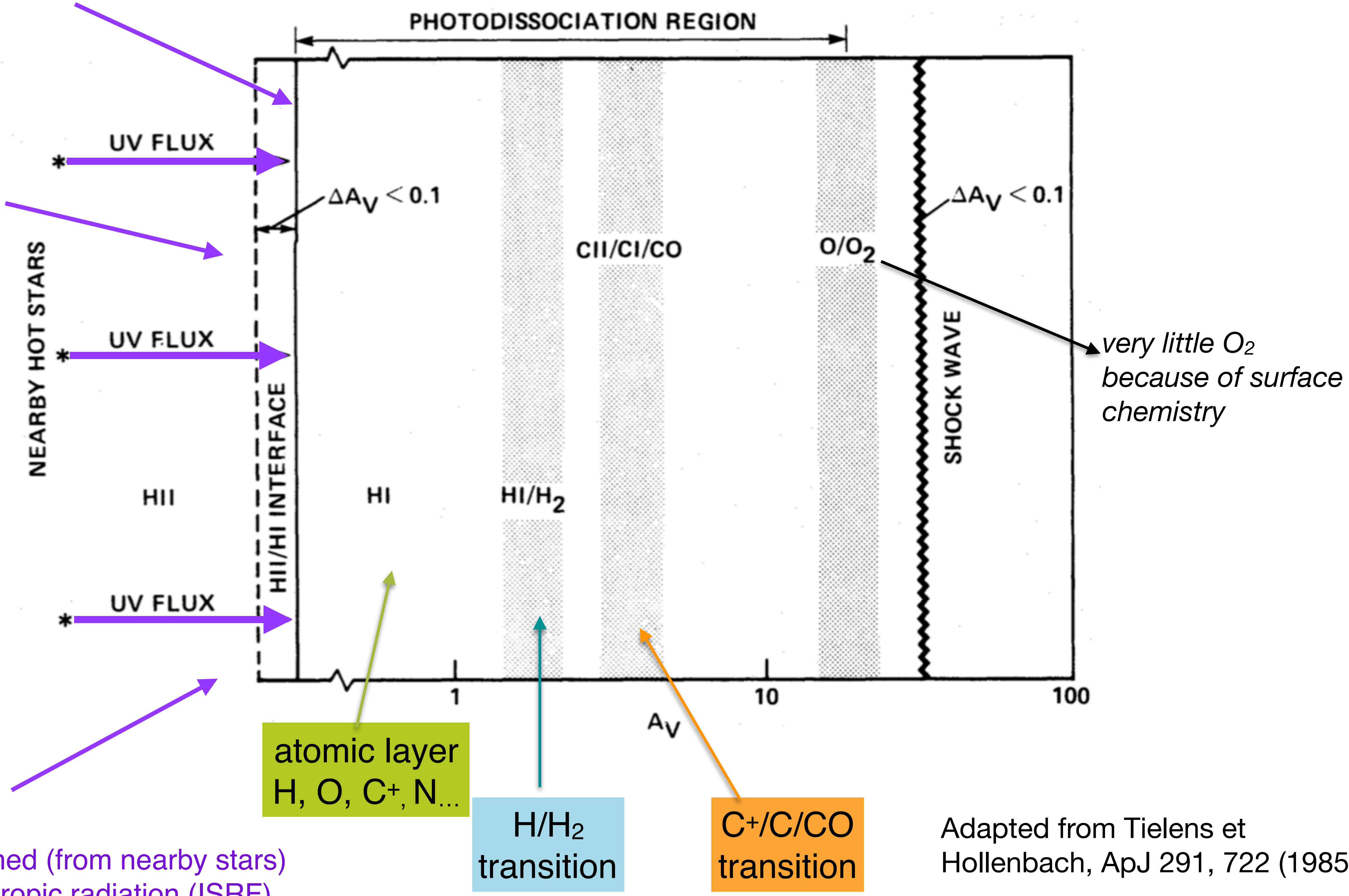
$s$ = sticking coefficient ≤ 1, depends on $T_d$ and $T_K$ (Hollenbach & McKee 1979)

With the Mathis et al. (1977) dust grain size power law distribution ≈ $a^{-3.5}$,

$$< \sigma n_d > = \frac{3}{4} \times \frac{1.4 m_{\mathrm{H}} G}{\rho_d} \times \frac{1}{\sqrt{a_{min} \cdot a_{max}}} \times n_{\mathrm{H}} \longrightarrow R_{\mathrm{H}} = 4.8 \times 10^{-16} \times s(T_d, T_K) \times \sqrt{\frac{T_K}{300}}$$

with $a_{min}$ = 3 nm, $a_{max}$ = 0.3 µ

# The chemical phases of Photodissociation regions



*very little $O_2$ because of surface chemistry*

atomic layer
H, O, $C^+$, N…

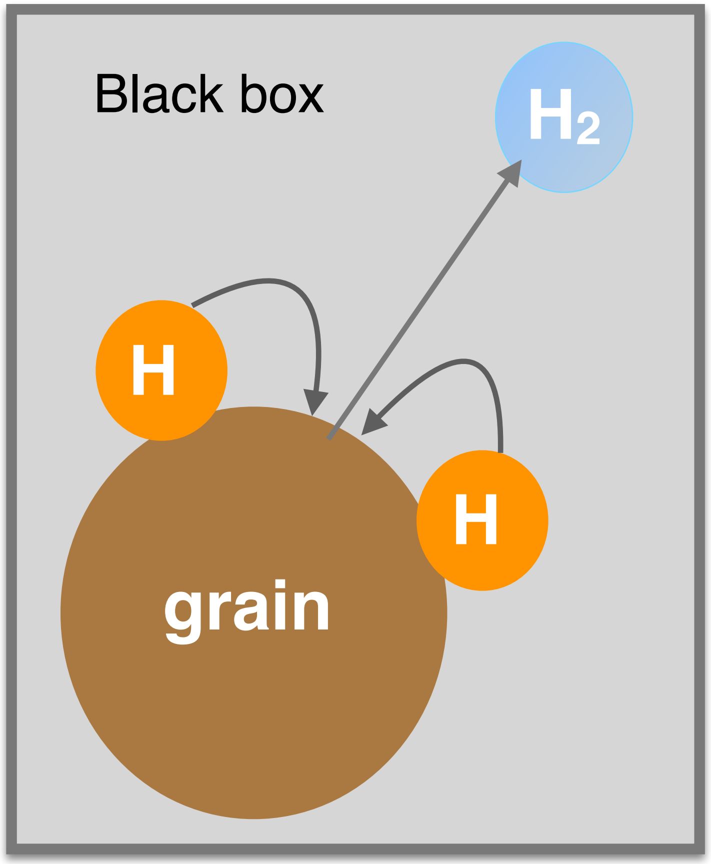
$H/H_2$ transition

$C^+/C/CO$ transition

Beamed (from nearby stars) + isotropic radiation (ISRF)

Adapted from Tielens et Hollenbach, ApJ 291, 722 (1985)

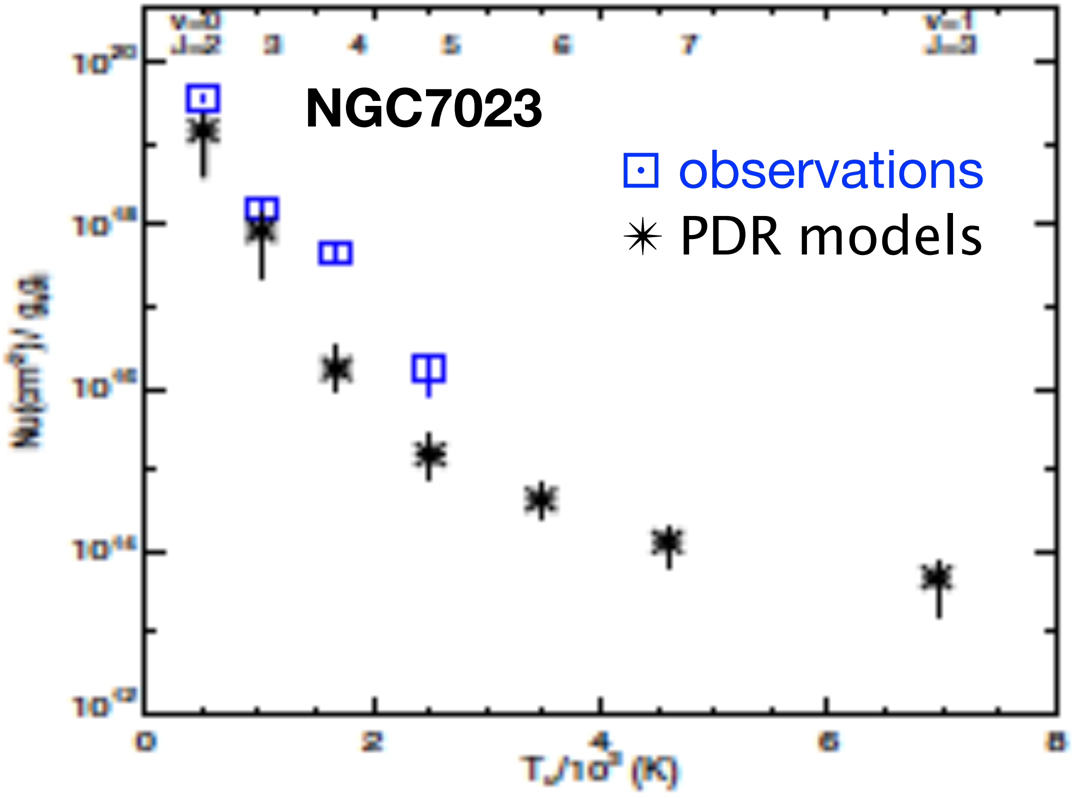
# Formation of $H_2$ on grain surfaces



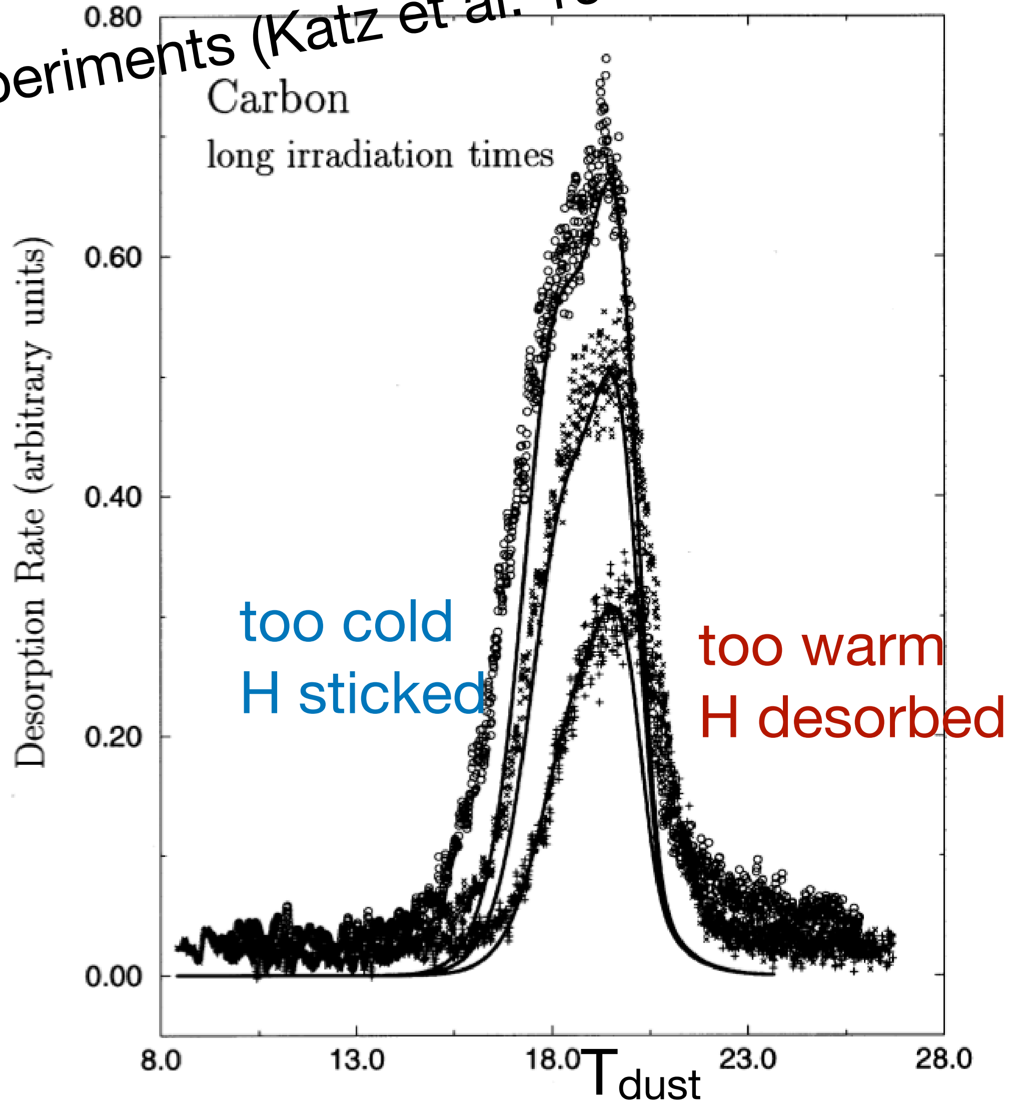
Allows to explain observations of H and $H_2$ in diffuse interstellar neutral gas

- Copernicus (Jura 1975)
- FUSE (Gry et al. 2002)

$H_2$ formation rate of a few $10^{-17}$ $cm^3$ $s^{-1}$ : too low to explain pure rotational $H_2$ transitions in PDRs with Spitzer (Habart et al. 2011, A&A 527, A122)



Laboratory experiments (Katz et al. 1999, ApJ 522, 305)



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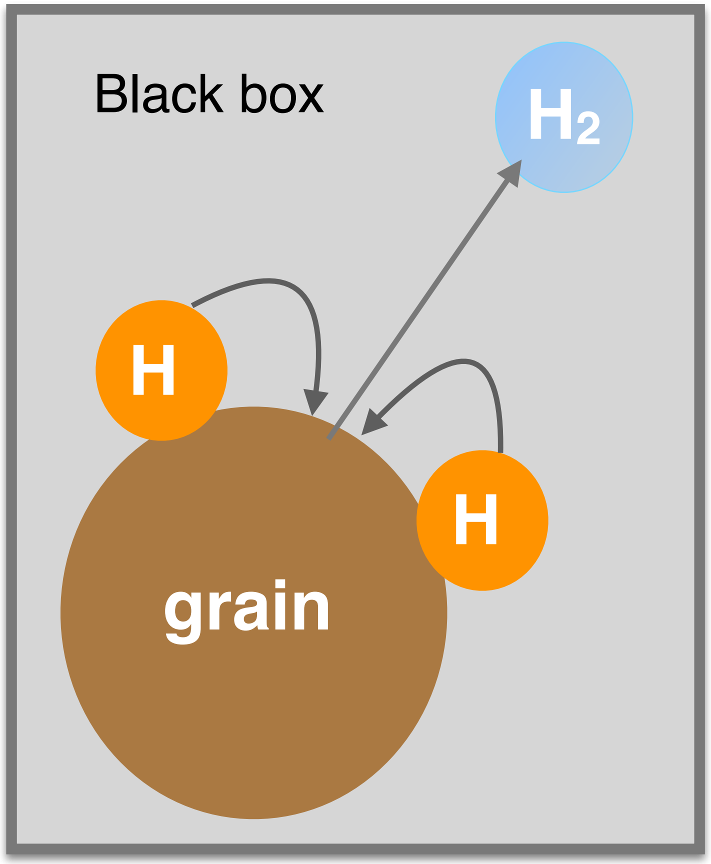

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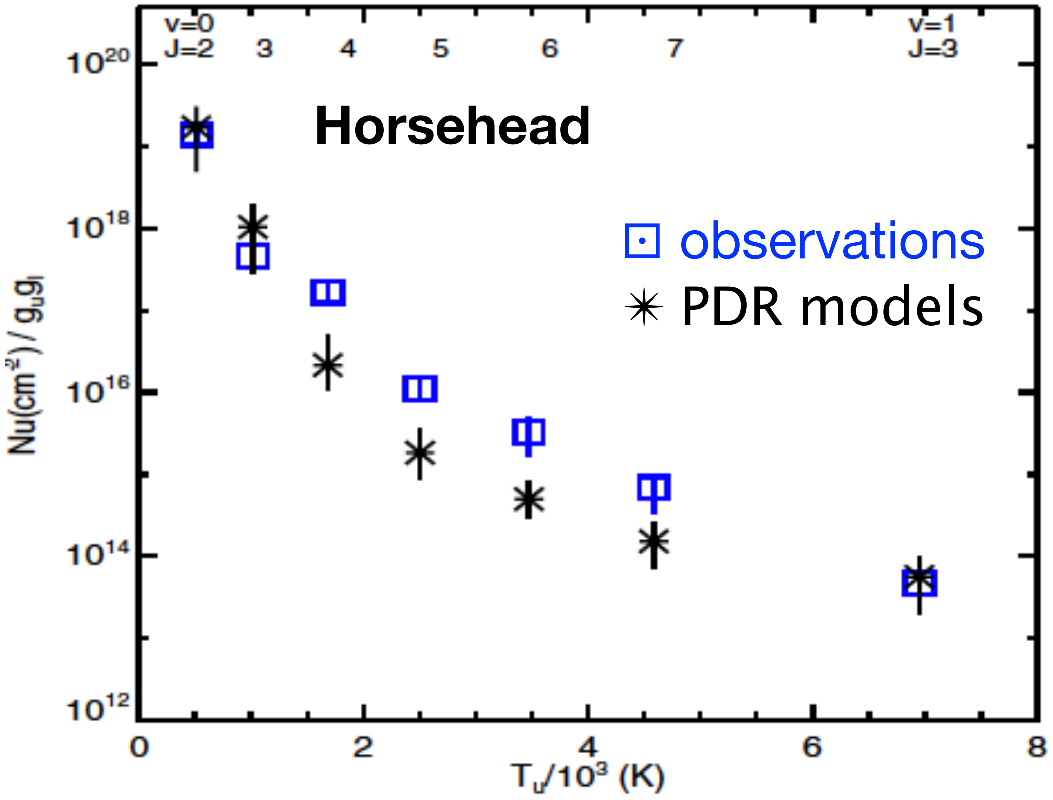

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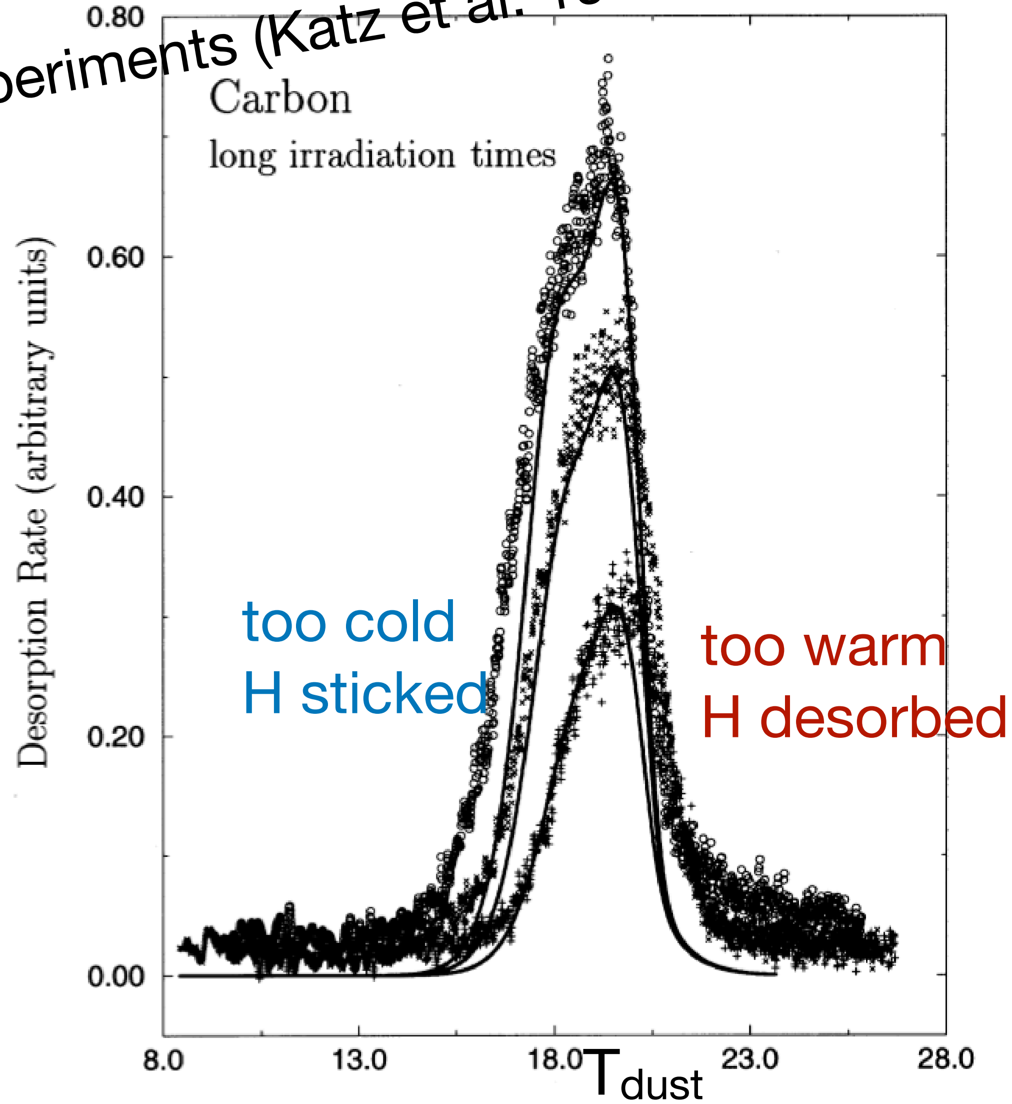
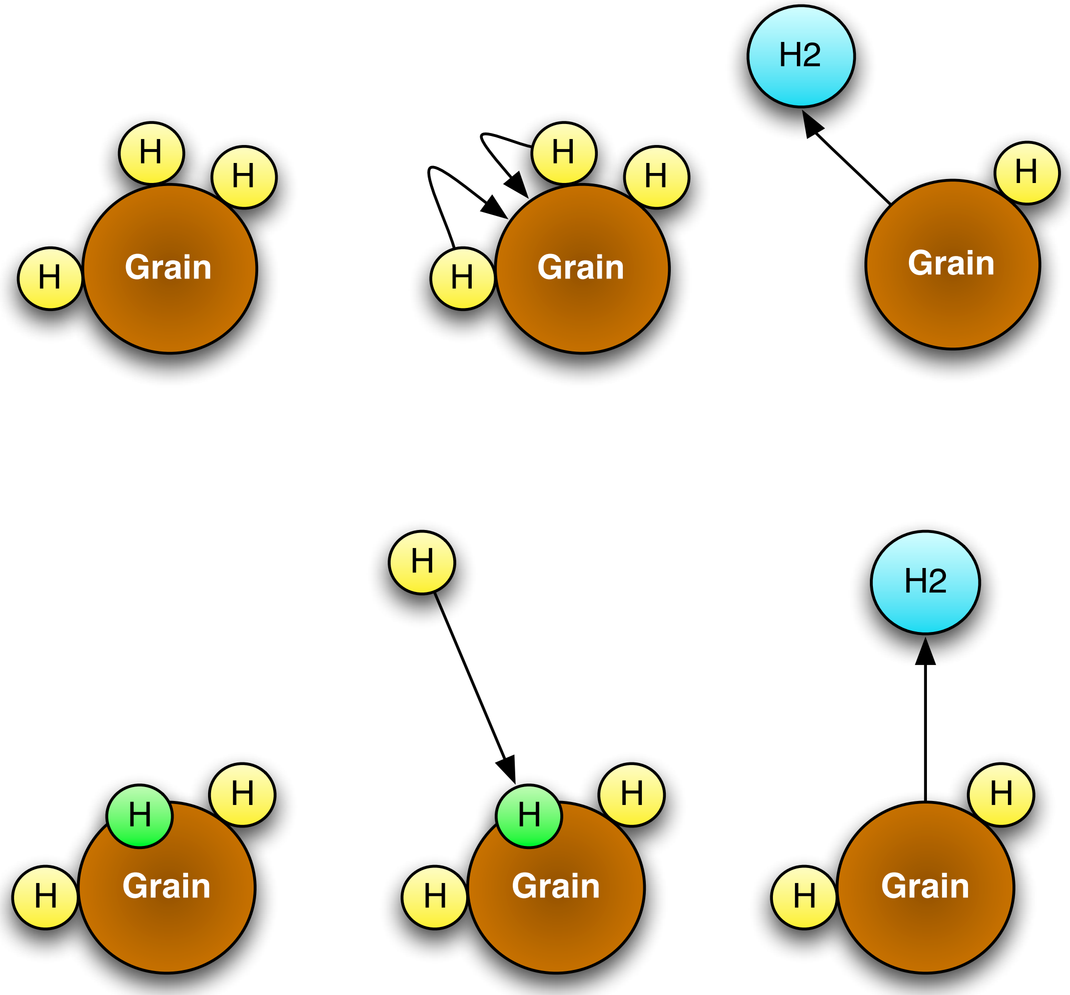


too cold
H sticked

too warm
H desorbed

# Formation of $H_2$ on grain surfaces

more detailed description required



**Langmuir-Hinshelwood / Physisorption**

✦ binding energy ≈ 658 K

✦ diffusion energy ≈ 510 K

⟶ Formation of $H_2$ is efficient only in a narrow range of dust temperatures

**Eley-Rideal / Chemisorption**

✦ binding energy: several thousands K efficient at the edge of PDRs

Cazaux & Tielens, ApJ575, L29, 2002

# Formation of $H_2$ on grain surfaces

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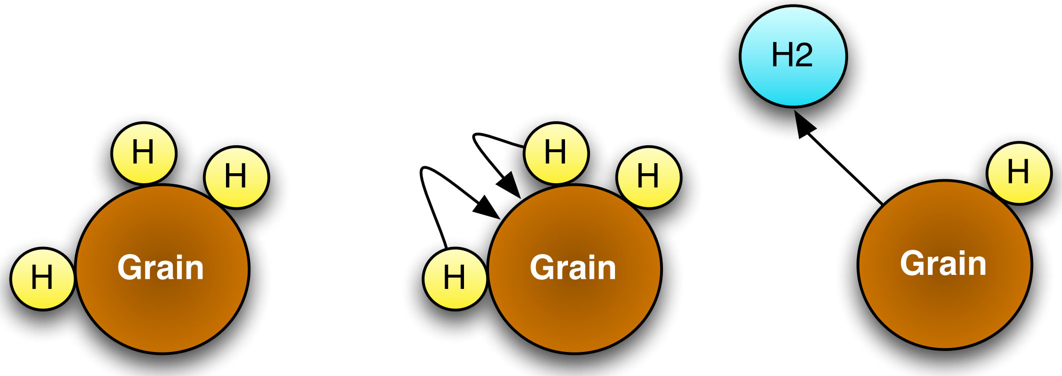
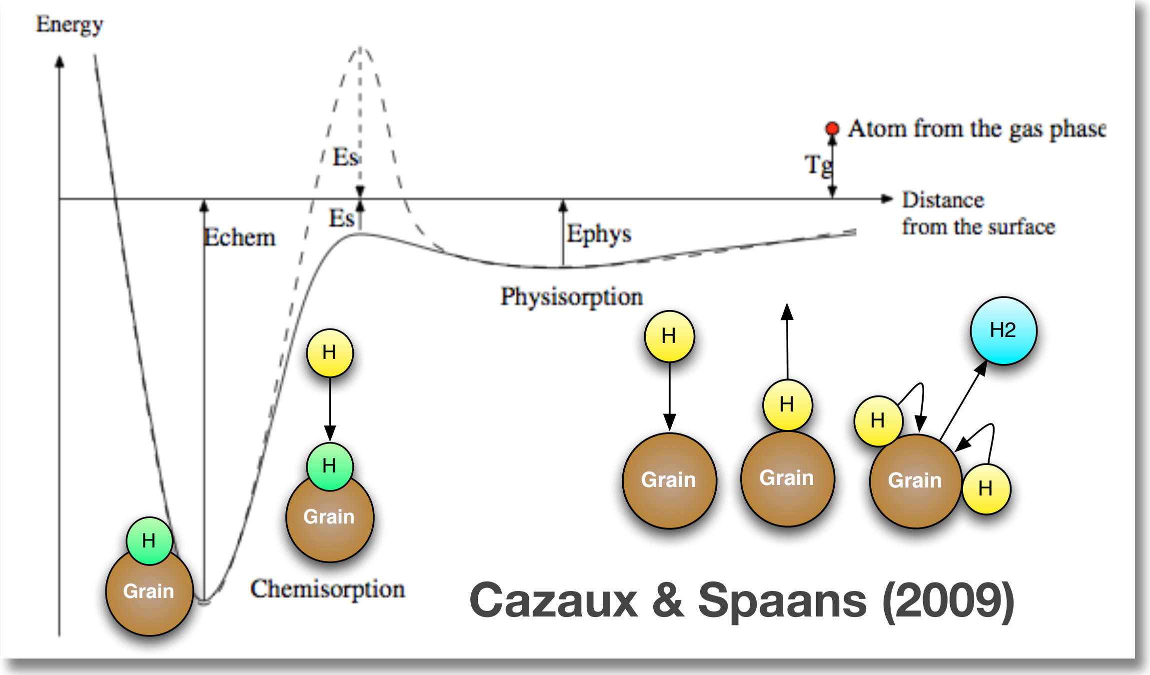




Cazaux & Spaans (2009)

**Langmuir-Hinshelwood / Physisorption**

✦ binding energy ≈ 658 K

✦ diffusion energy ≈ 510 K

⟶ role of temperature fluctuations on small grains help (Bron et al. 2014, A&A 569, A100)

**Eley-Rideal / Chemisorption**

✦ binding energy: several thousands K efficient at the edge of PDRs

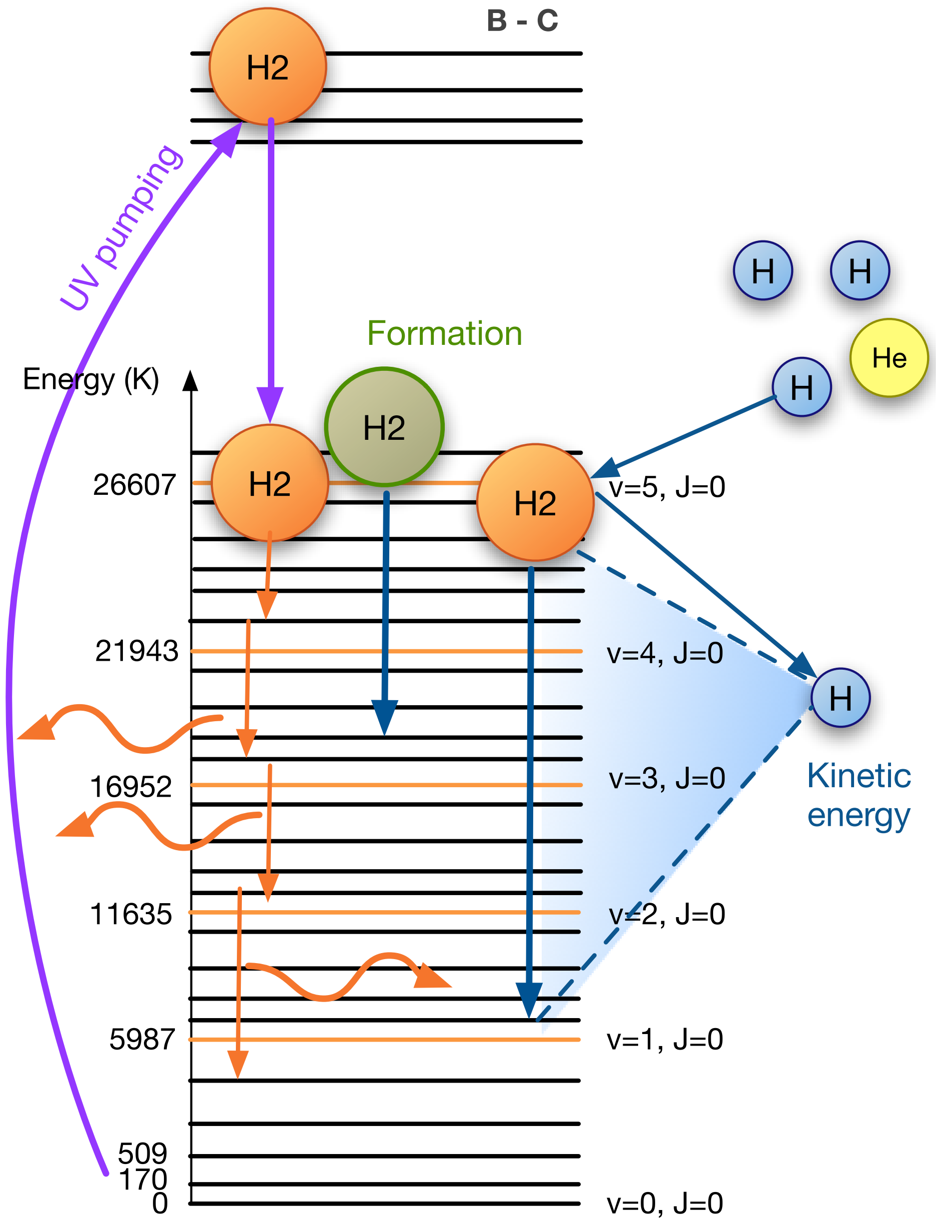
chemisorption threshold : 300 K (to reach a chemisorption site)

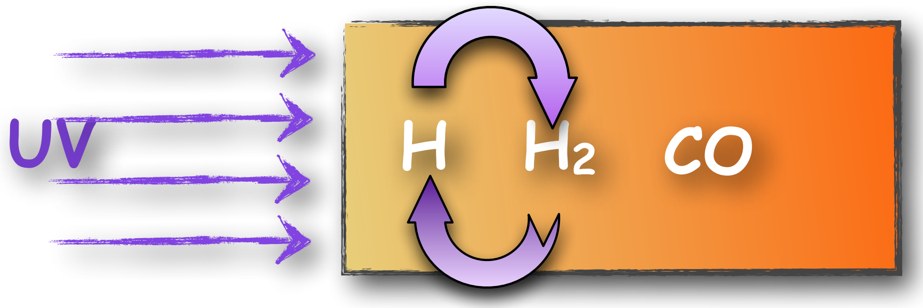
The efficiency of the **LH** mechanism depends on **grain** temperatures

The efficiency of the **ER** mechanism depends on the **gas temperature**

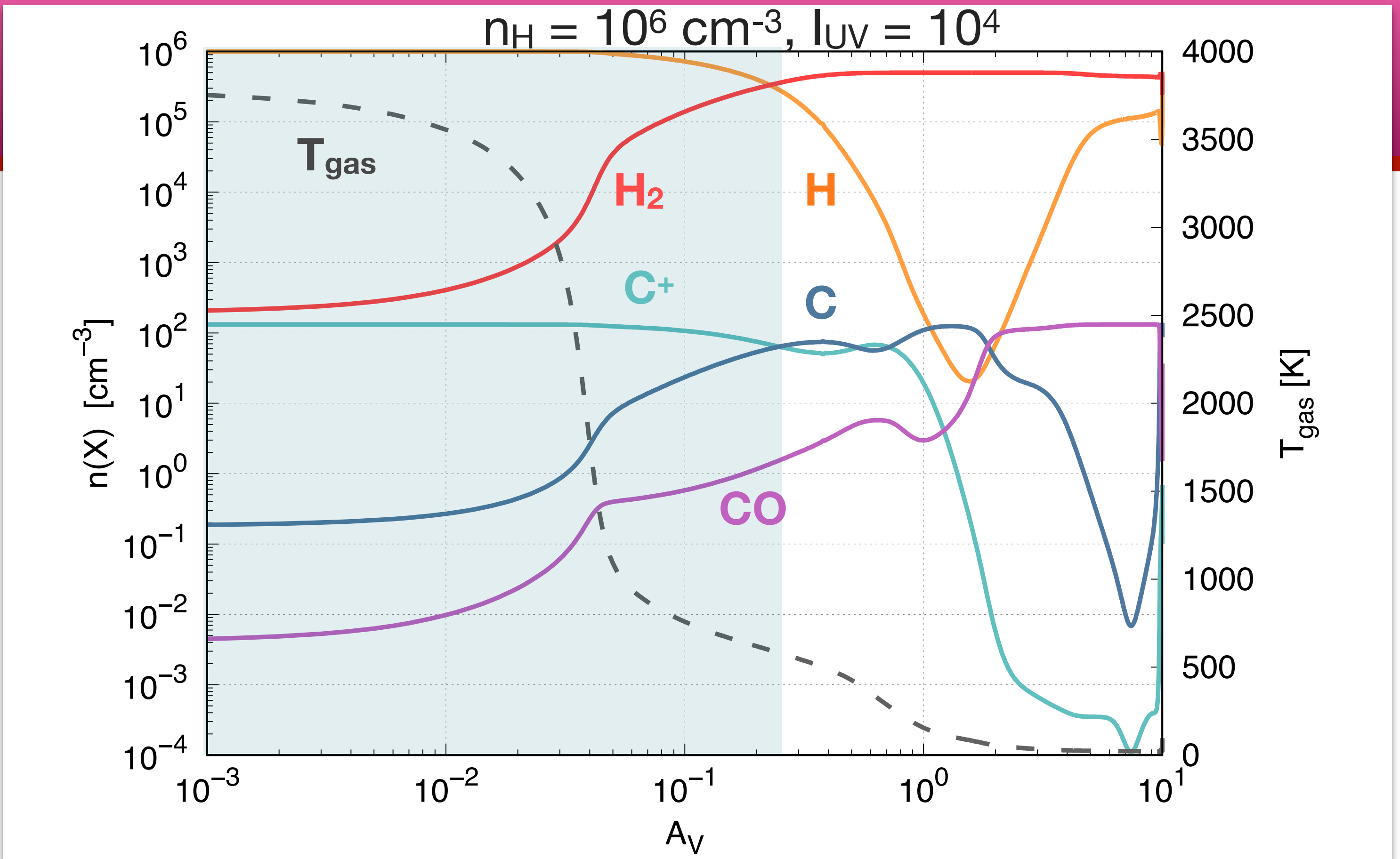
when $H_2$ heats the gas ➔ positive loop to form $H_2$ and heat the gas

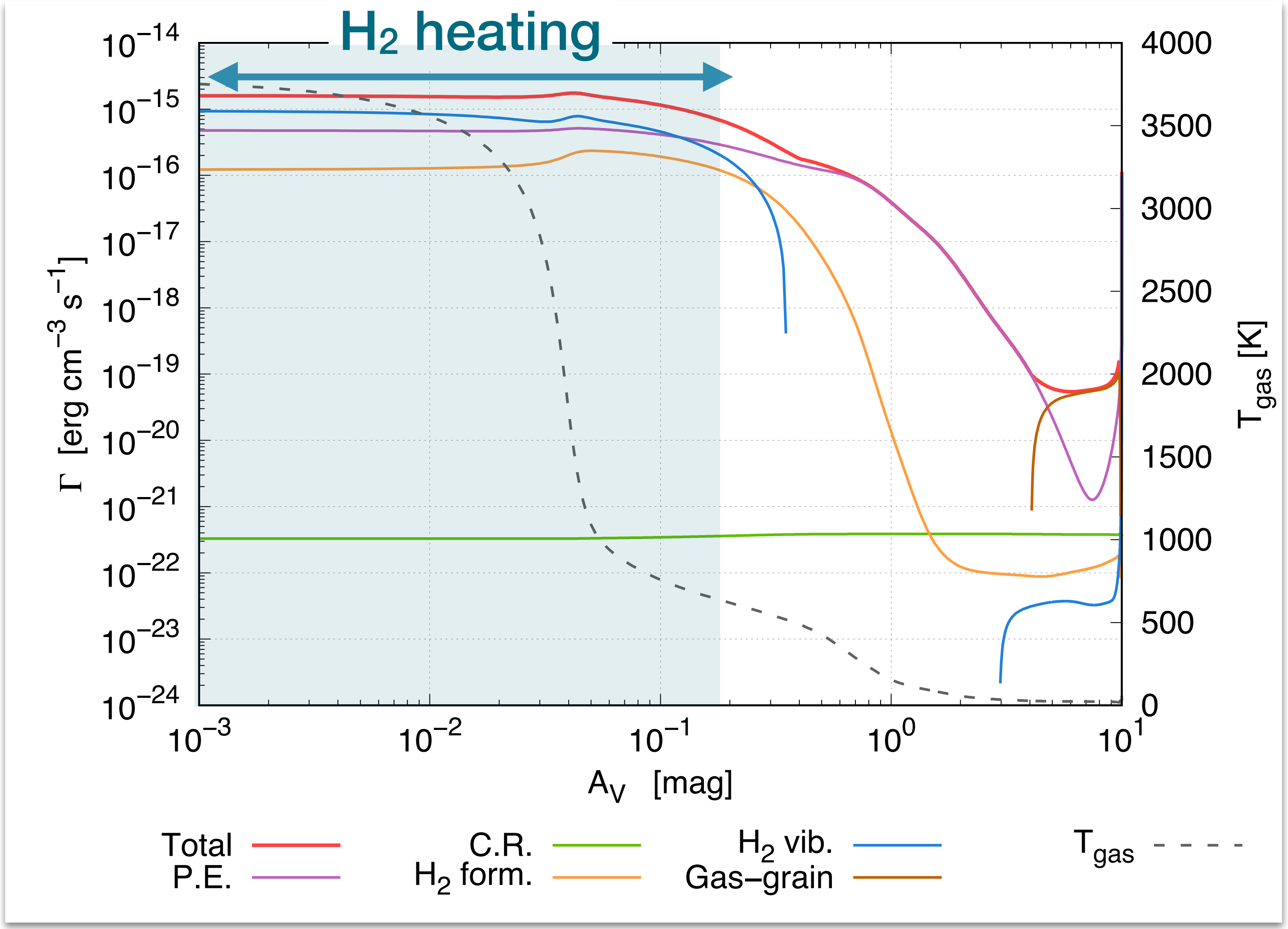
# Heating by $H_2$





For high densities, $H_2$ may convert UV photon energy into kinetic energy



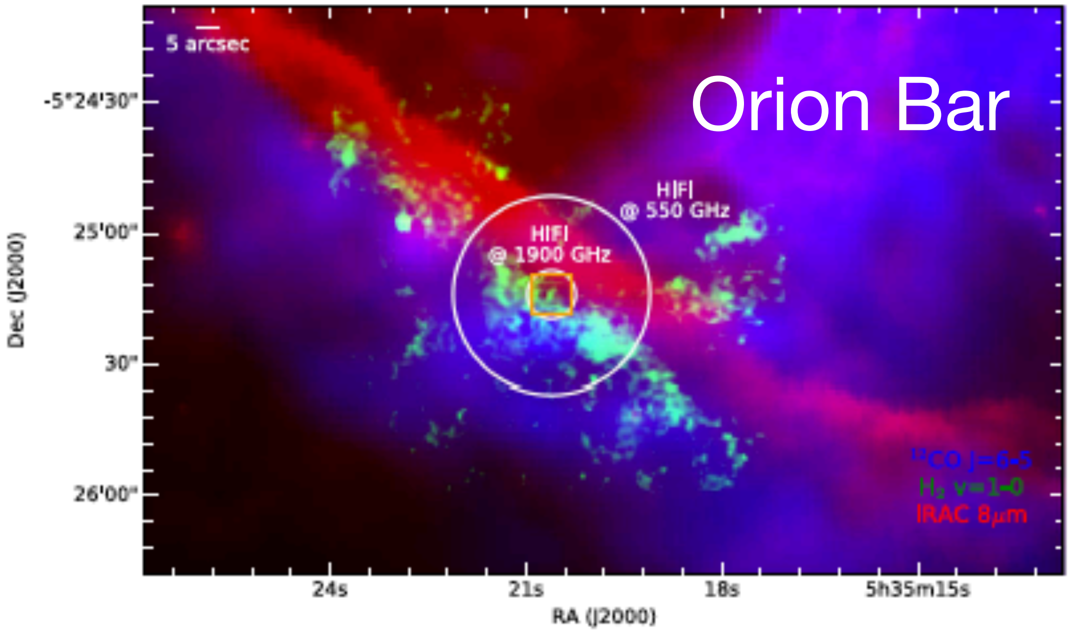


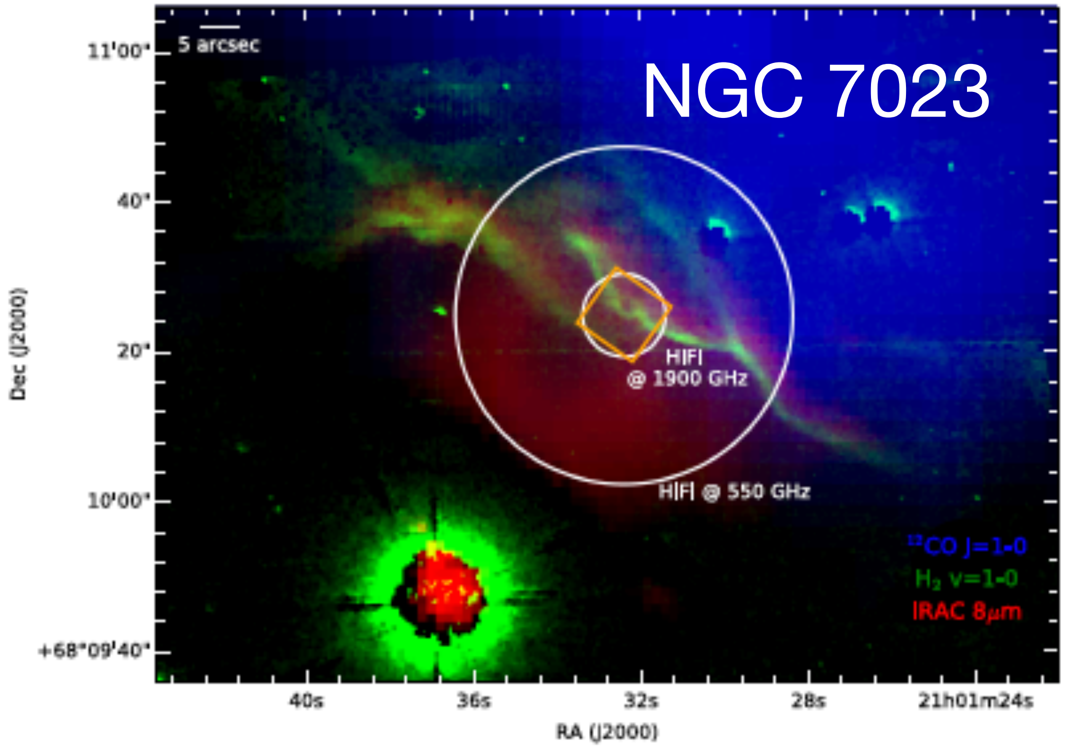
# Two archetypal PDRs

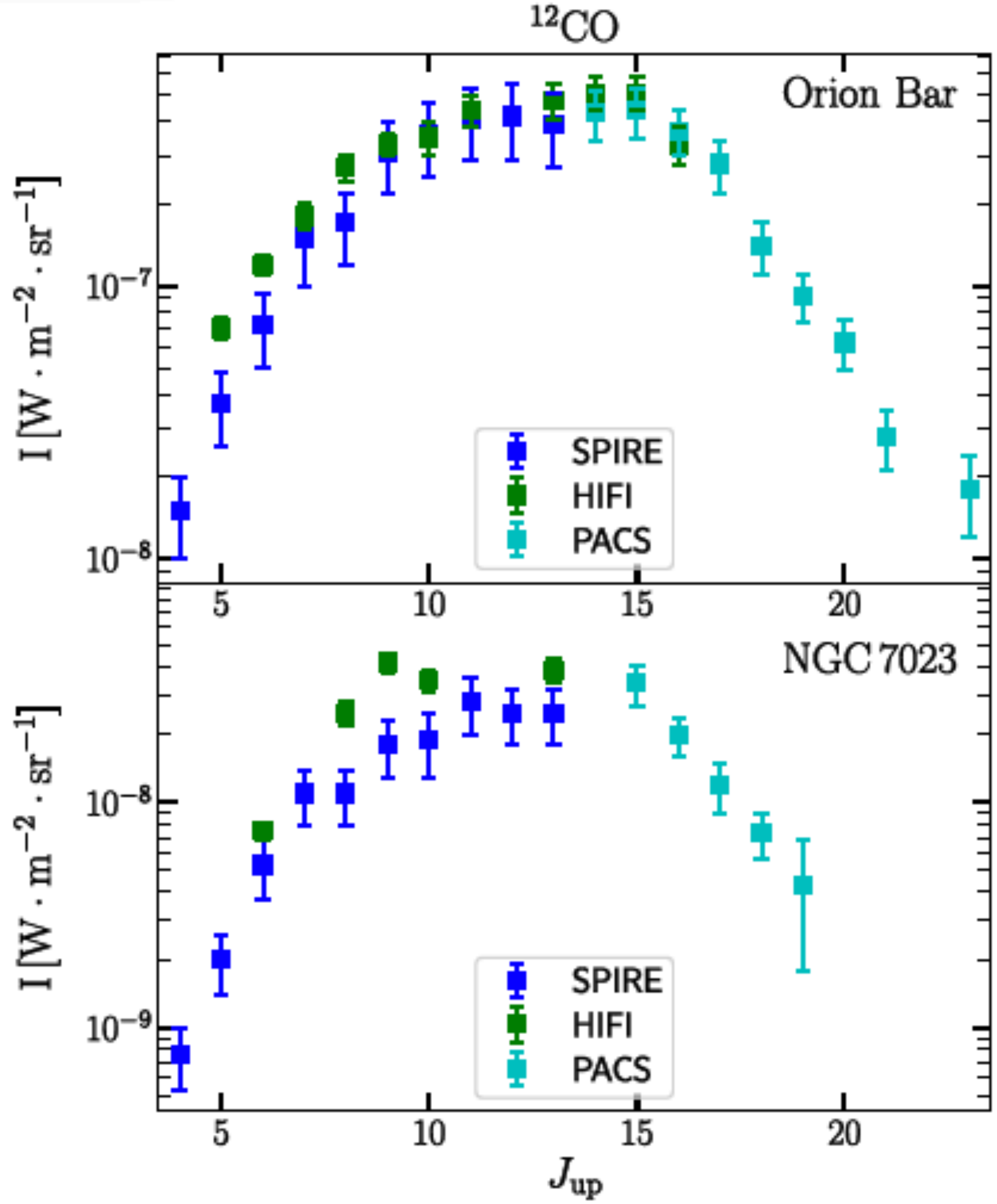
Joblin et al., 2018, A&A 615, A129, 2018

Herschel GTKPs observations of two nearby, bright galactic PDRs :

Orion Bar (Hexos, PI T. Bergin), and NGC 7023 NW (WADI, PI V. Ossenkopf-Okada)







Rotationally excited CO

# Two archetypal PDRs

Joblin et al., 2018, A&A 615, A129, 2018

- In addition to HIFI, SPIRE, PACS Herschel data:

  observations from Spitzer, ISO, CFHT, IRAM-PdB, ...

## Observational constraints

Full $^{12}$CO ladders (4-3 to ~ 20-19), $H_2$ ro-vibrational lines,

$^{13}$CO, $CH^+$, $HCO^+$, $C^+$, O, HD

Total: ~ 40 lines

## Astrophysical knowledge

Properties of illuminating stars / clusters is known

➔ UV field intensity is known a priori

NGC 7023 NW: G0 ~ 2600

Orion Bar: G0 ~ $2\times10^4$

Modelling: difficult (impossible) to reproduce CO excitation in constant density models

➔ *isobaric PDR models*

use of a grid of isobaric PDR models

Only 2 free parameters:

- ➡ thermal pressure
- ➡ beam filling/geometrical factor

Allows to consistently satisfy the constraints:

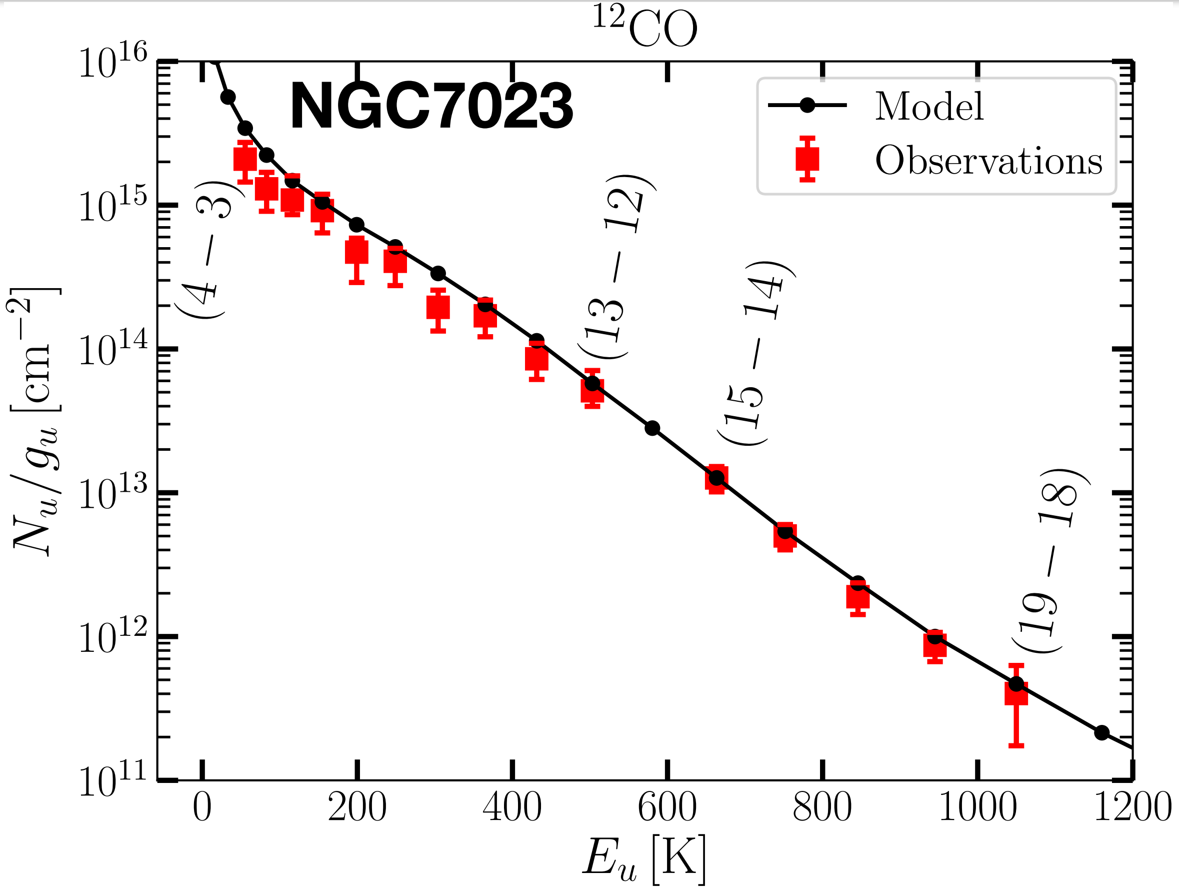
~20 constraints used in the fit
(+6 other successfully reproduced a posteriori)

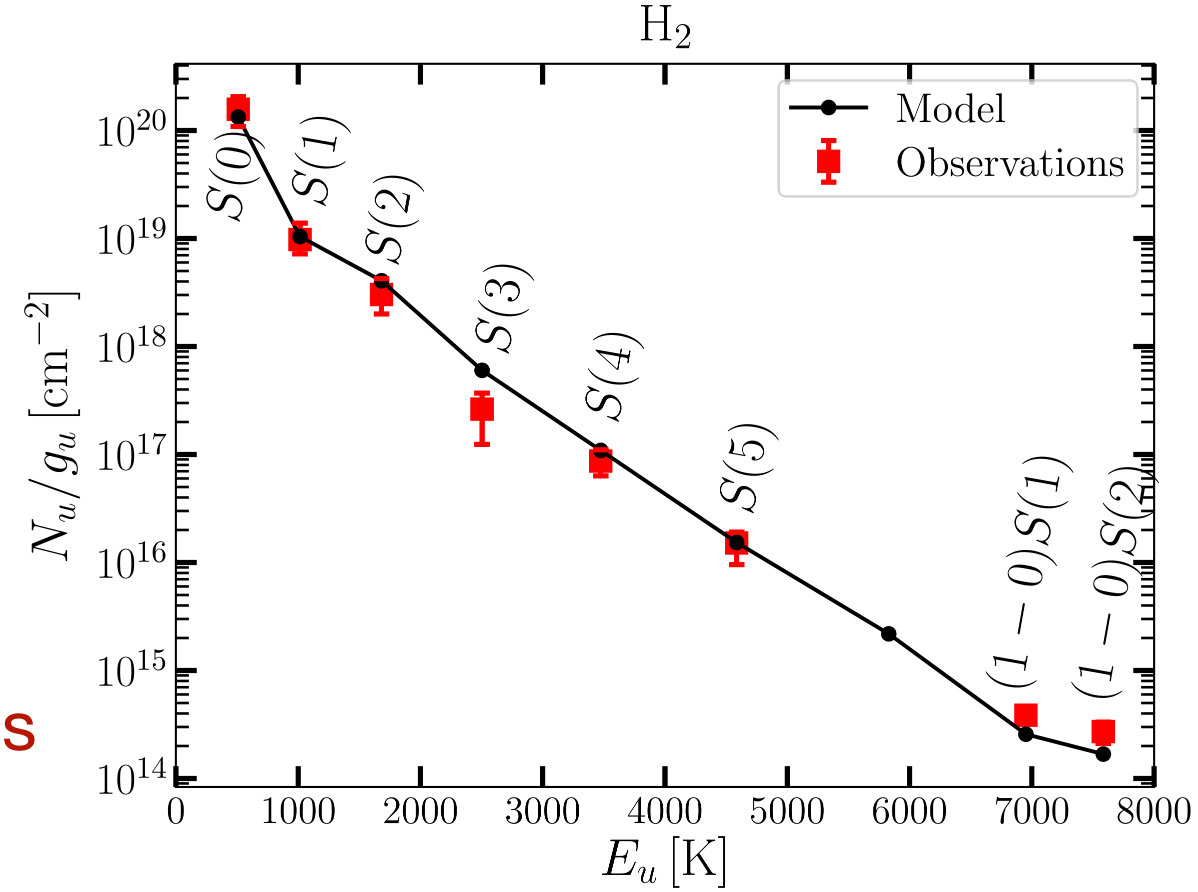
**Excited CO, $H_2$, $CH^+$, HD, $HCO^+$, …**

➡ High thermal pressures ~$10^8$ K cm$^{-3}$

but does not reproduce tracers in the atomic/H II region or deep inside the cloud

➡ Warm compressed layer at the edge of PDRs





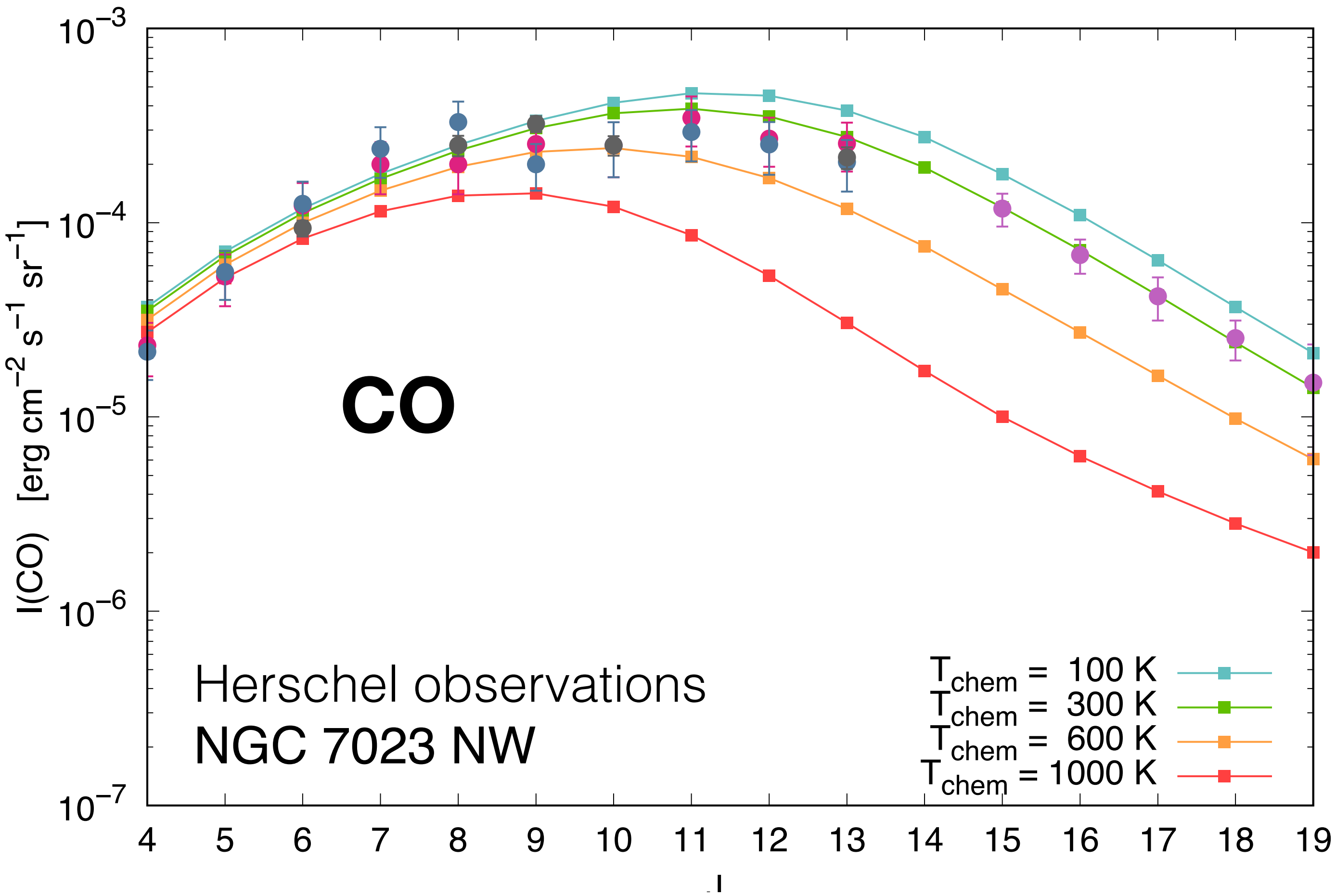
# A new picture of PDRs

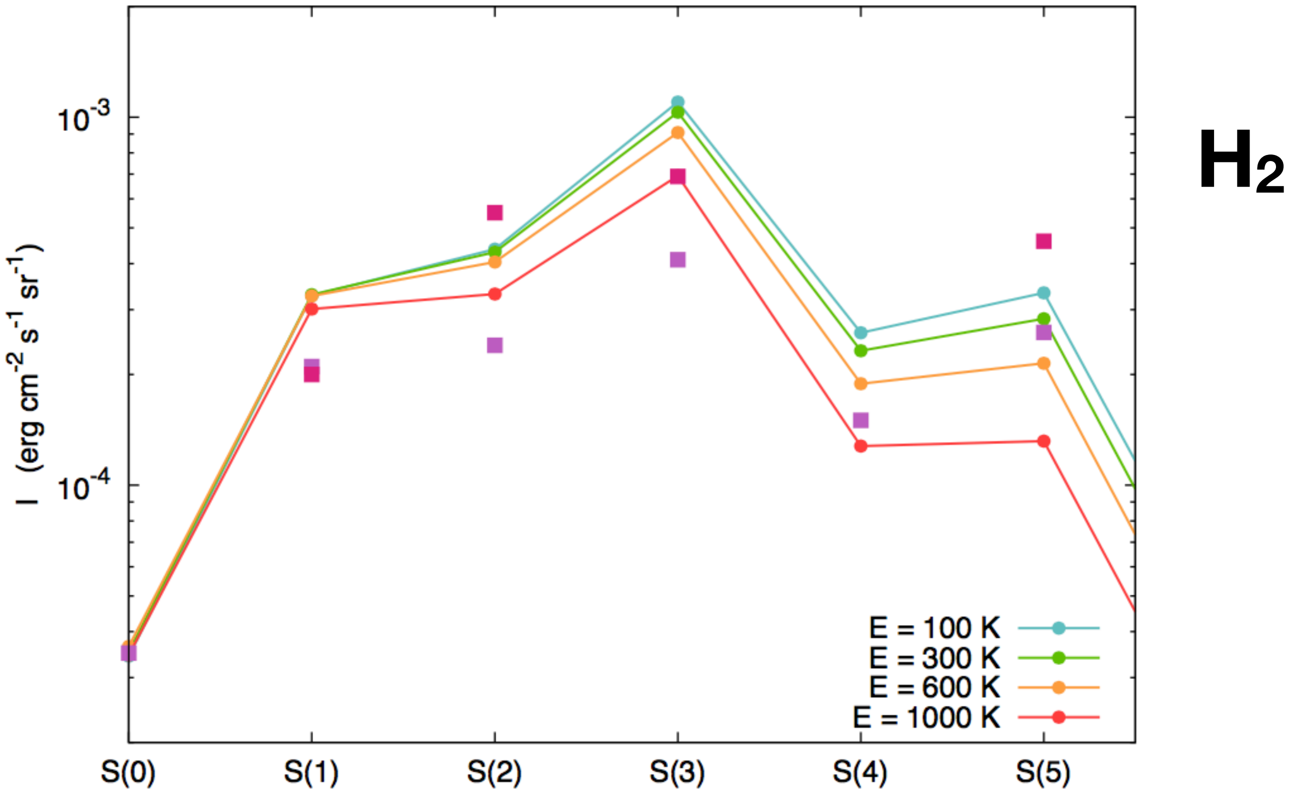
# far-reaching effects of $H_2$ formation

## effect of the chemisorption threshold

Stronger impact on excited CO lines than on $H_2$ lines !

Controls the amount of warm molecular gas (1000-100 K) → new active chemistry





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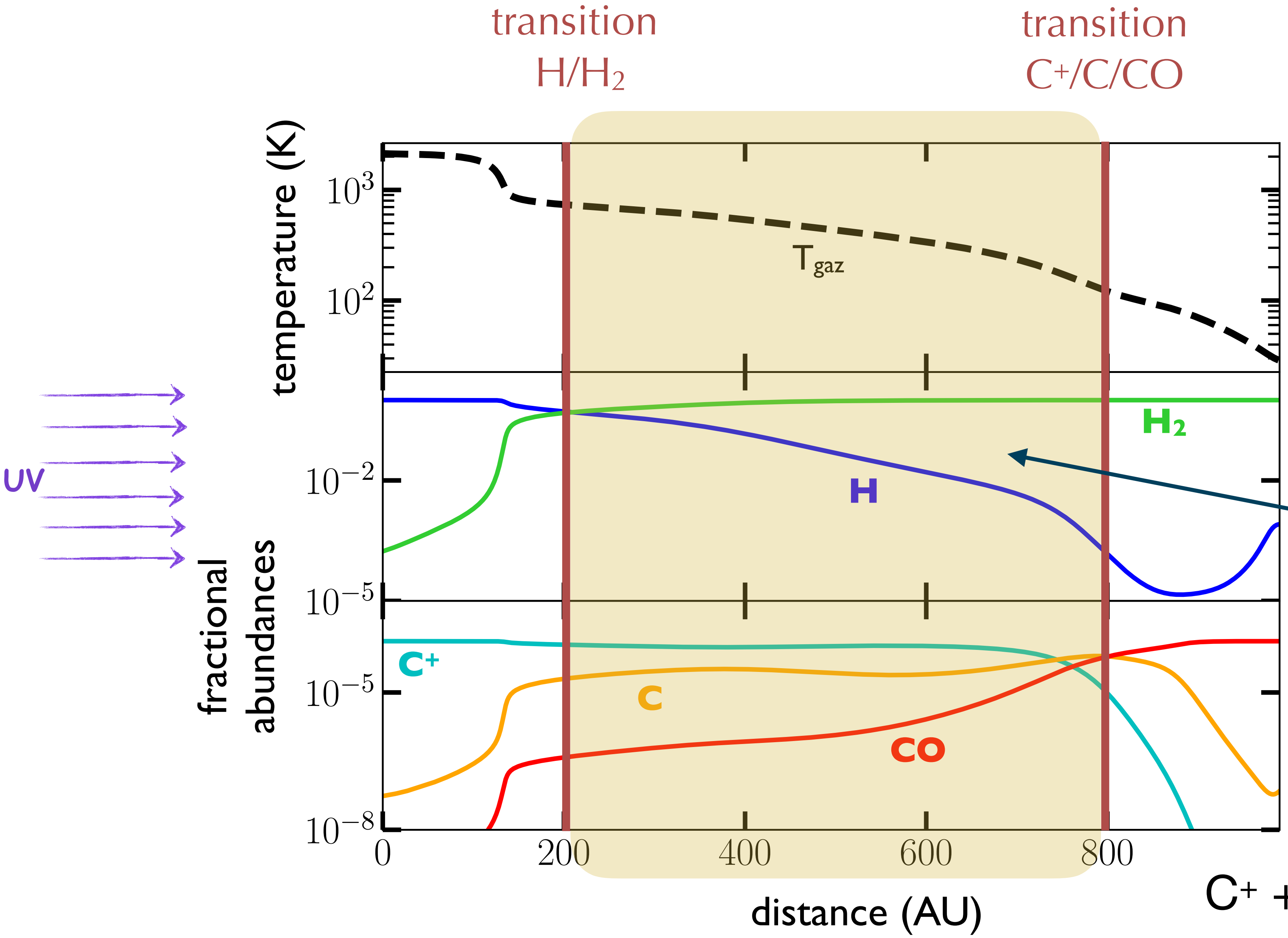


**warm molecular layer**

vibrationnally excited pumped $H_2$

➡ occurrence of endothermic reactions

$C^+ + H_2(v,J) \rightarrow CH^+ + H$ (4640 K)

$S^+ + H_2(v,J) \rightarrow SH^+ + H$ (9860 K)

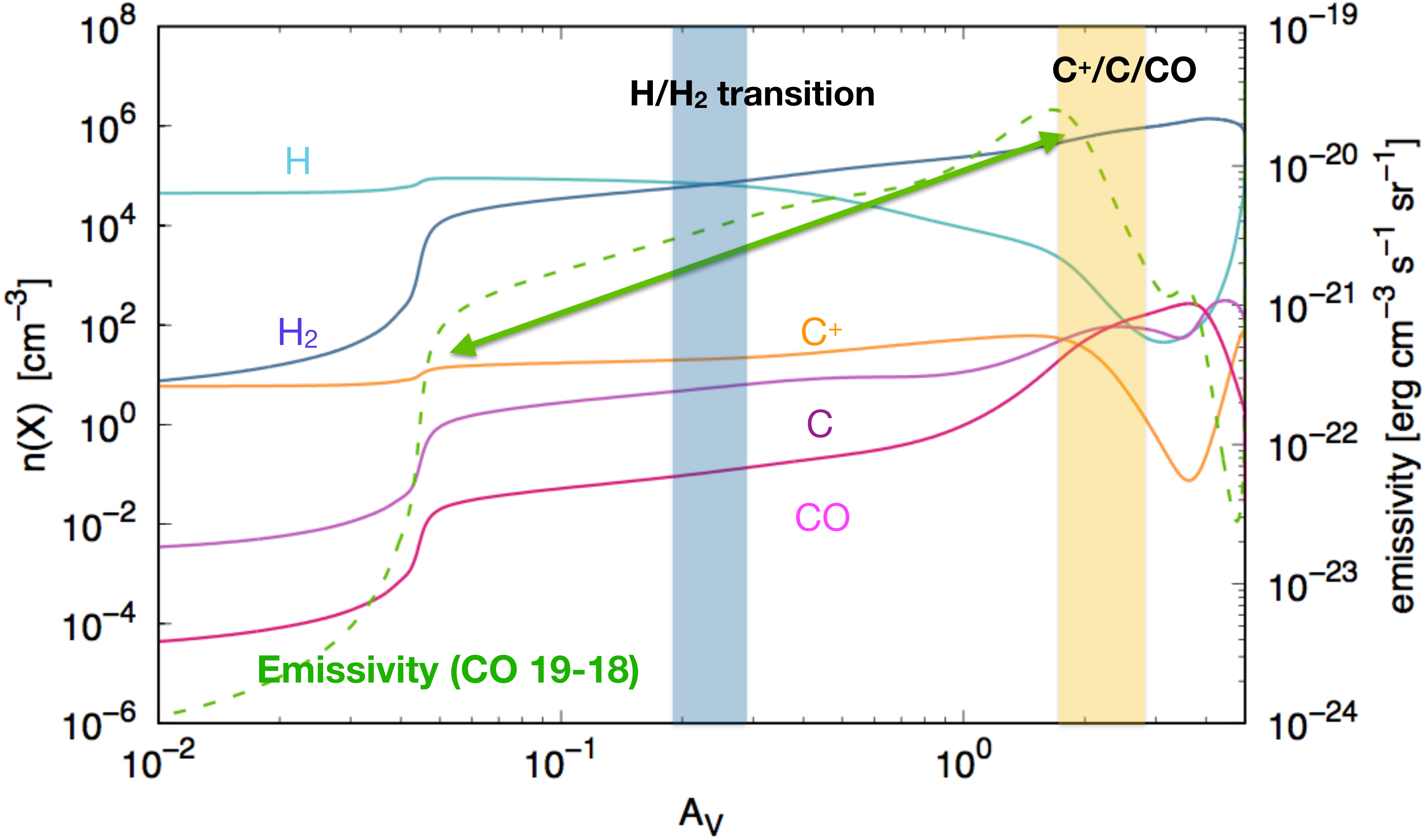
Agundez et al. 2010, ApJ 713, 662,
Zanchet et al. 2013, 2019, A&A626, A103

➡ surmounting activation barriers: $O + H_2(v,J) \rightarrow OH + H$ (3241 K)

$OH + H_2(v,J) \rightarrow H_2O + H$ (1751 K)

# A new picture of PDRs

# far-reaching effects of $H_2$ formation



~ 50% of CO: 19-18 emission comes from a region in front of the C/CO transition

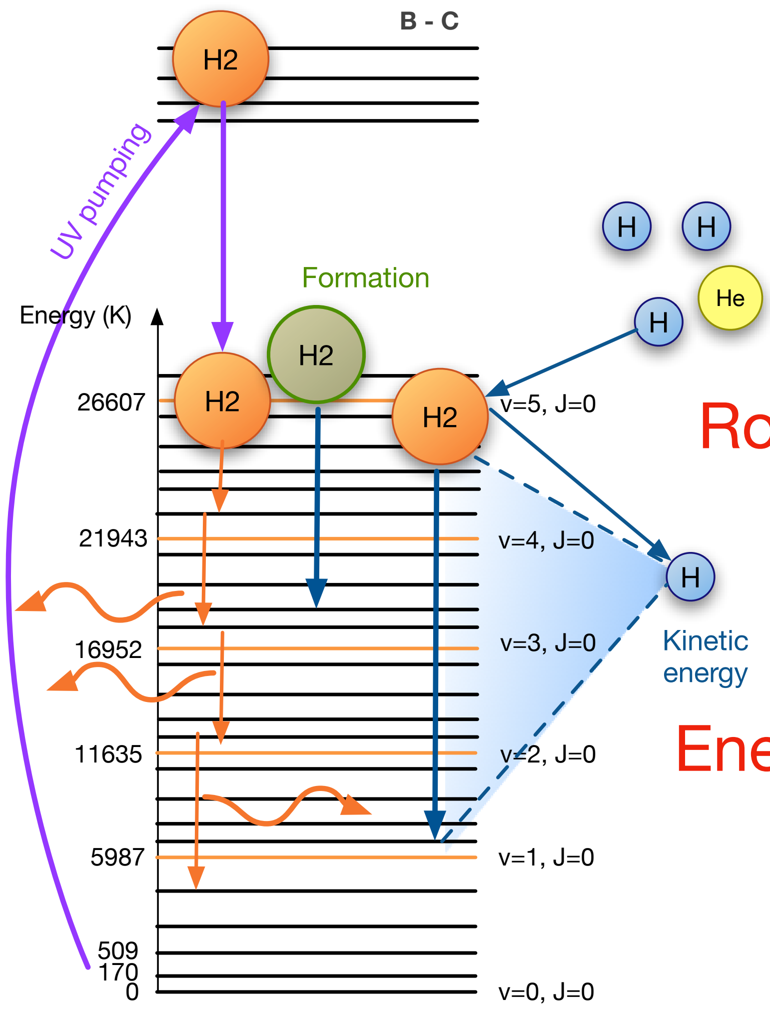
# A new picture of PDRs

## warm chemistry at work at the edge

*Formation of $H_2$ occurs in a region:*

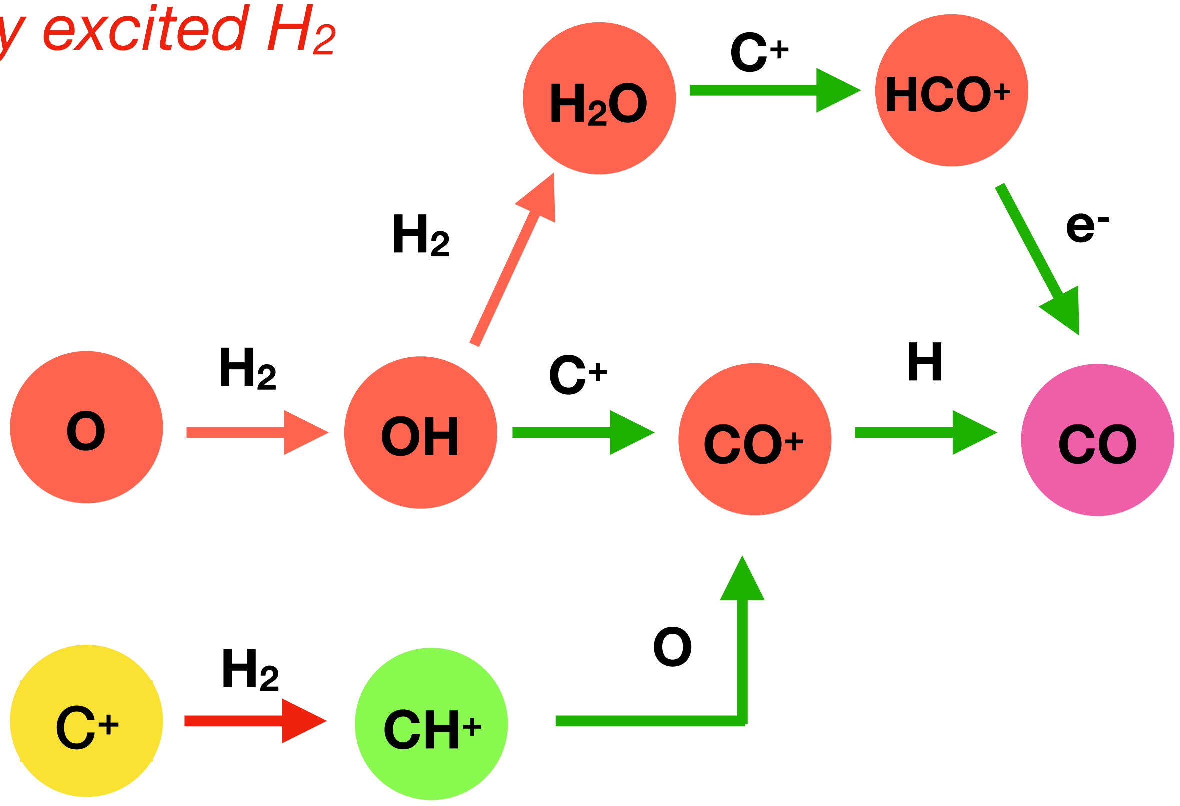
- *high temperature*
- *UV photons (thanks to an efficient formation rate)*

*➔ ro-vibrationally excited $H_2$*



Ro-vibrationally excited $H_2$

Energy stored in $H_2$



$O + H_2(v,J) \rightarrow OH + H$ (**3241** K)

$OH + H_2(v,J) \rightarrow H_2O + H$ (**1751** K)

$C^+ + H_2(v,J) \rightarrow CH^+ + H$ (**4540** K)

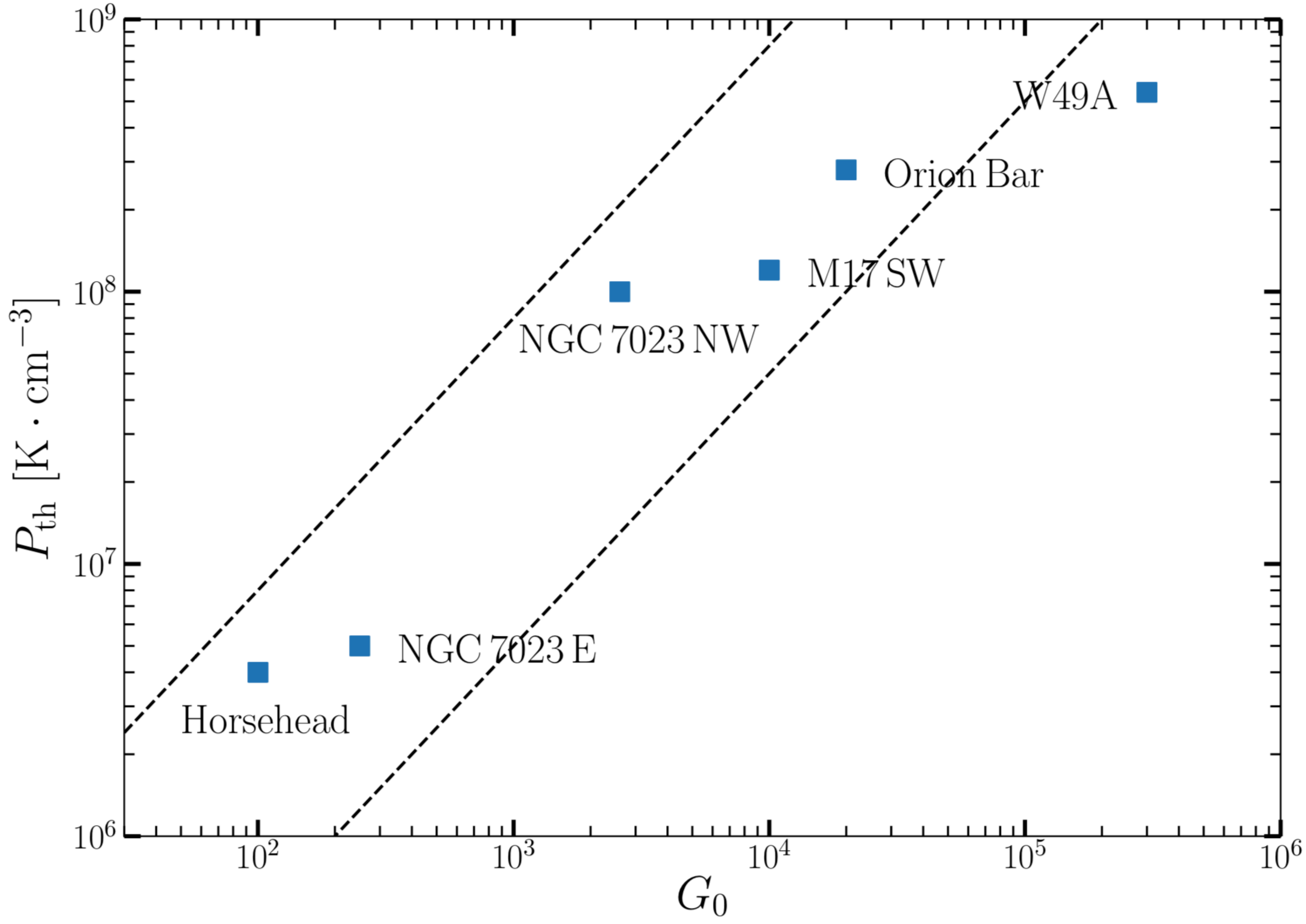
- chemical reaction rate dependent on $H_2(v,J)$: **state-dependent chemistry**
- $H_2$ internal energy used to overcome endothermicity / activation thresholds

**warm chemistry at the edge of PDRs leads to the formation of CO via OH and $CH^+$**

# A new picture of PDRs

# relation between p and UV intensity

Comparison to other PDRs

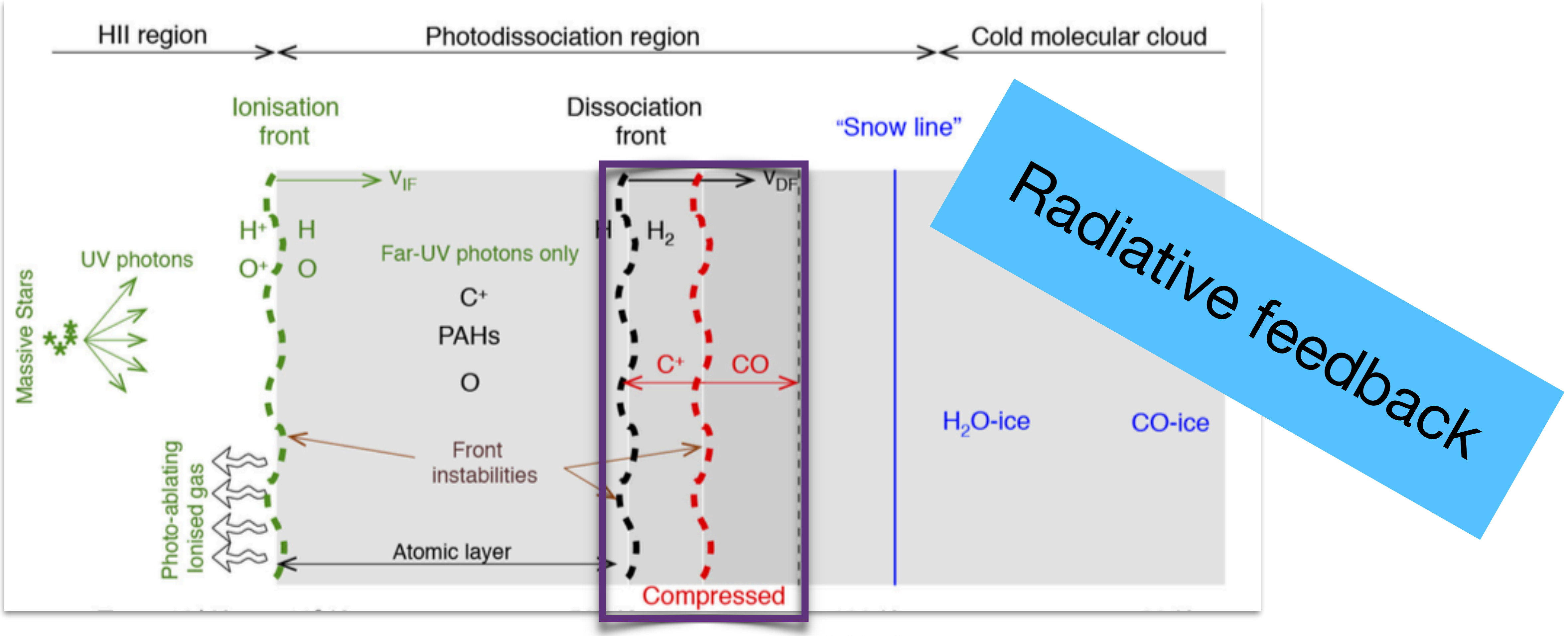


The UV radiation field seems to be responsible for the high pressures at the edge of PDRs

# A new picture of PDRs

## relation between p and UV intensity

Goicoechea et al. (2016, Nature 537, 207)



Radiative feedback

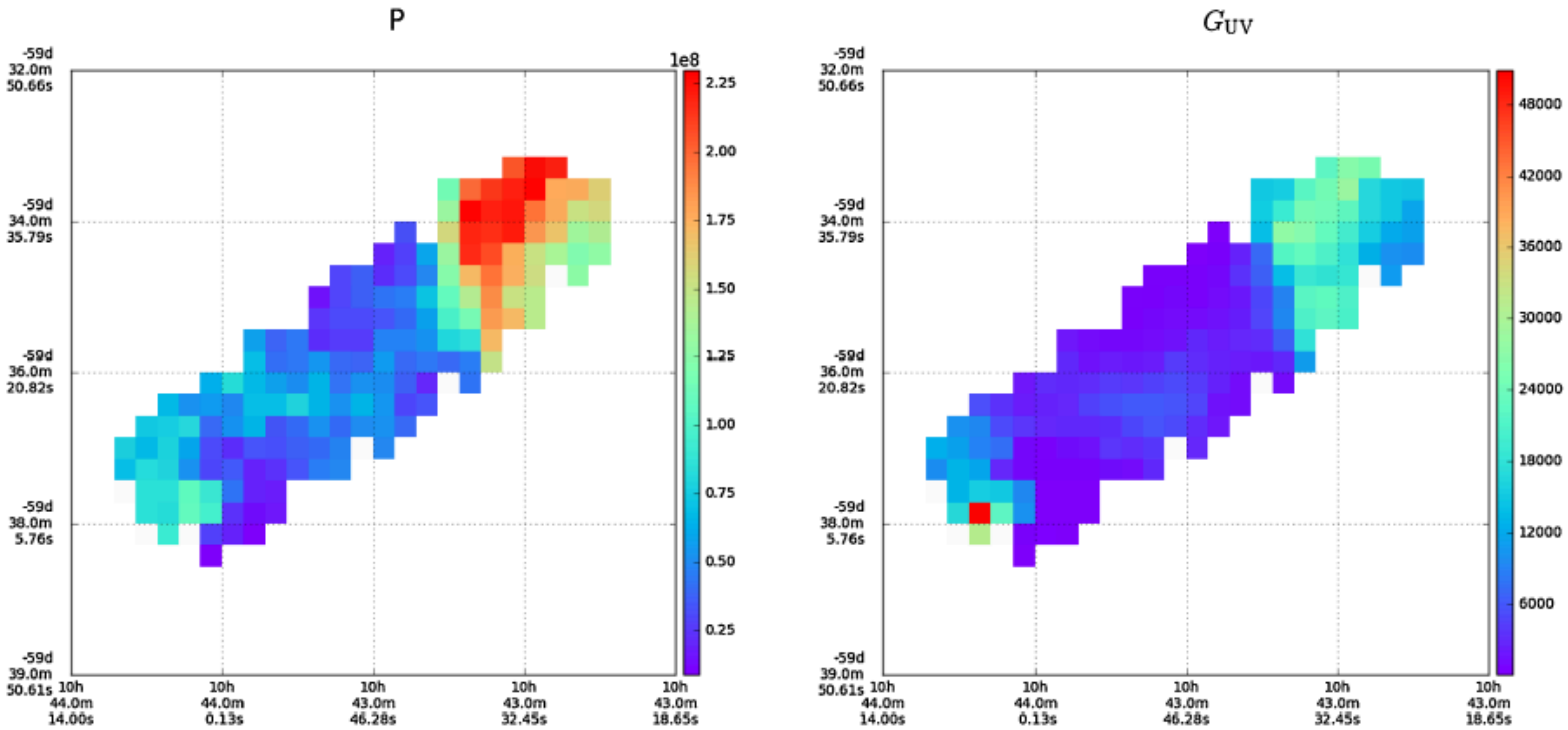
$p < 10^8$ K cm$^{-3}$

UV field → High pressure
$p \sim 10^8$ K cm$^{-3}$

- ➡ UV photons can bring the energy to excite CO in PDRs
- ➡ no need of additional hypothesis (additional heating sources, clumps, ...)
- ➡ the molecular edge of PDRs is characterized by high pressures maintained dynamically

# relation between p and UV intensity

- Link between UV field intensity and gas pressure at the edge of PDRs found in other lines of sight (eg. Trumpler 14 in Carina)

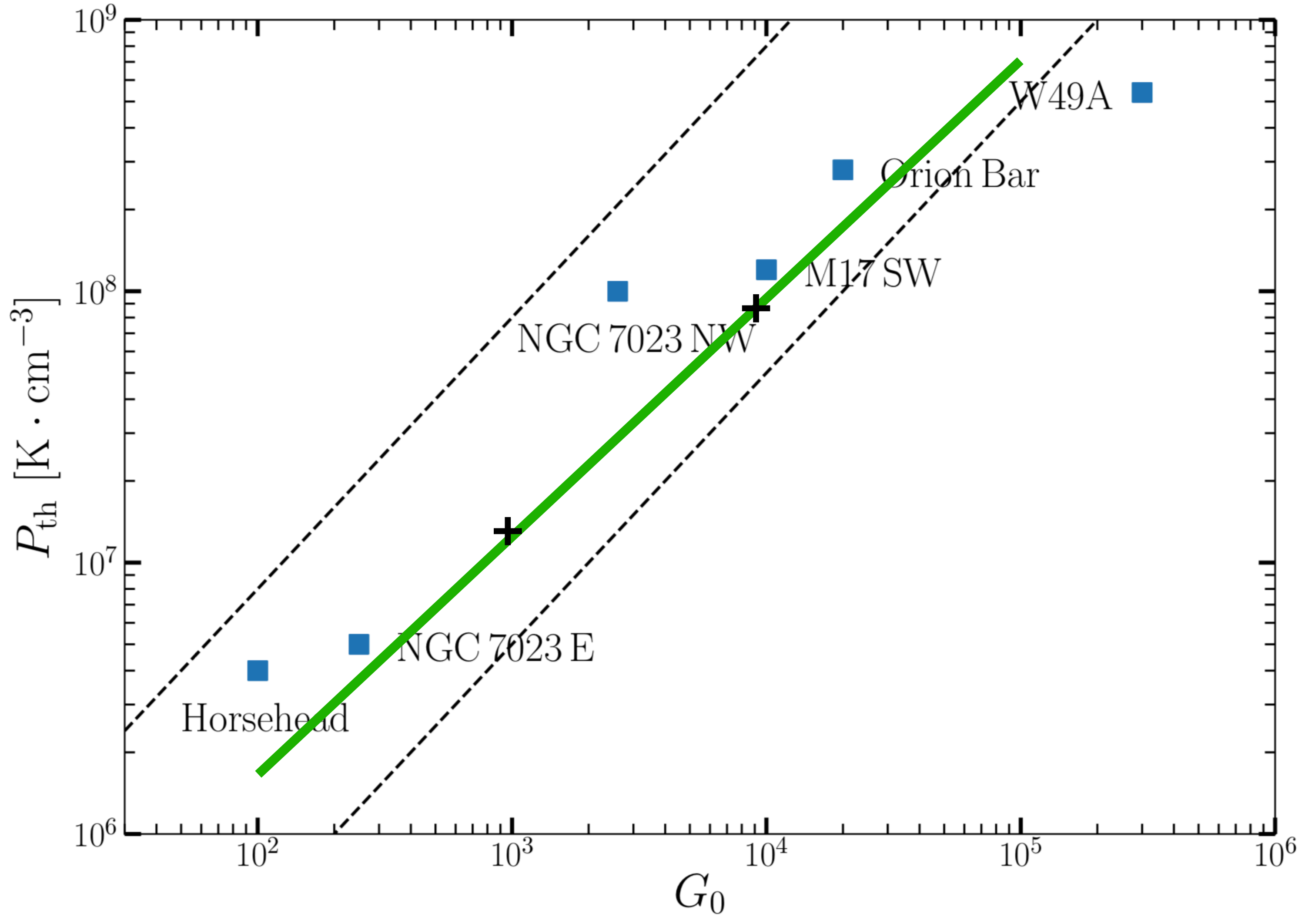


Wu, Bron et al. 2018, A&A 618, A53

# A new picture of PDRs

# relation between p and UV intensity

- Link between UV field intensity and gas pressure at the edge of PDRs found in other lines of sight (eg. Trumpler 14 in Carina)



$p \sim 2.1\ 10^4 \times G_0^{0.9}$ cm$^{-3}$ K

in the range of values found for diffuse translucent regions ($G_0$ ~1) Jenkins & Tripp 2001, ApJS137, 297

Wu, Bron et al. 2018, A&A 618, A53

# Conclusions and perspectives (1)

## Emphasis on $H_2$

- Introduction of detailed $H_2$ formation/excitation/destruction mechanisms

- under high density and high radiation field conditions, radiative energy can be converted into kinetic energy
  - ➡ efficient heating at the edge of PDRs
  - ➡ positive loop to form $H_2$ and heat the gas
  - ➡ $H_2$ state dependent chemistry at work (reactions with $C^+$, $S^+$, O, C, N …)

- Far reaching effects of $H_2$
  - ➡ CO formation channel through $CH^+$ + O, OH + $C^+$
  - ➡ excited CO transitions are emitted before the $C^+$/C/CO transition
  - ➡ no additional hypothesis (clumps, shocks, …) required

- Link between the strength of the impinging radiation field and gas pressure applicable from diffuse/translucent clouds to strong PDRs

# Conclusions and perspectives (2)

## For the future: observations

another promising source: Herschel 36 in the bright Messier 8 face-on PDR (Rachford et al. 2014, ApJ 786, 159, Oka et al. 2013, ApJ 773, 42, Tiwari et al. 2019, A&A 626, A28)

➔ *talk by Tiwari at 16:55 : link to hydrocarbon chemistry*

preparing JWST (spatial resolution ≈ $10^{-3}$ pc in the Orion bar)

allows to resolve the hot layer of PDRs

JWST Early Release Science program: radiative feedback from massive stars (PIs: O. Berné, E. Habart, E. Peeters)

Access to main key processes in PDRs

➡ $H_2$ formation rate

➡ Photo-electric heating & $H_2$ heating rates

➡ warm chemistry

# Conclusions and perspectives (3)

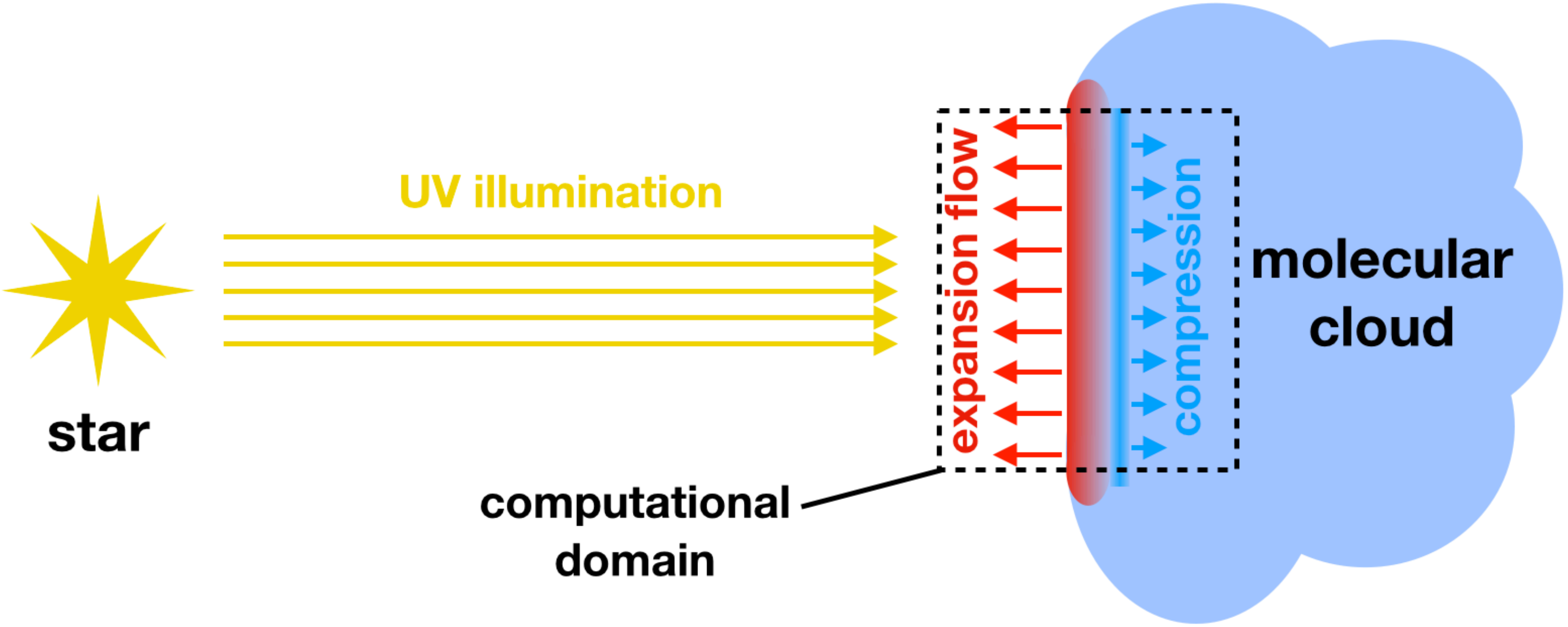
## For the future: modelling efforts

➔ introduce PAHs, photo-desorption and more complex surface chemistry

talks of C. Joblin, P. Bréchignac, F. Dulieu, S. Cazaux, …

➔ new class of models

UV photons can induce compression through photoevaporation



- Extend the studies for small clumps inside HII regions (e.g. Bertoldi & McKee 1990) to the edge of larger scale molecular clouds (Bron et al. 2018, arxiV, Kirsanova & Wiebe 2019, MNRAS 486, 2525)

  ➔ impact on the PDR structure ?

# Conclusions and perspectives (4)

**For the future: debating with Xander on the formation of $H_2$**

Eley-Rideal / Photoinduced polycyclic aromatic hydrocarbon dehydrogenation.
( Castellanos et al. A&A616, A167, 2018)

**and specific thanks to my young colleagues**

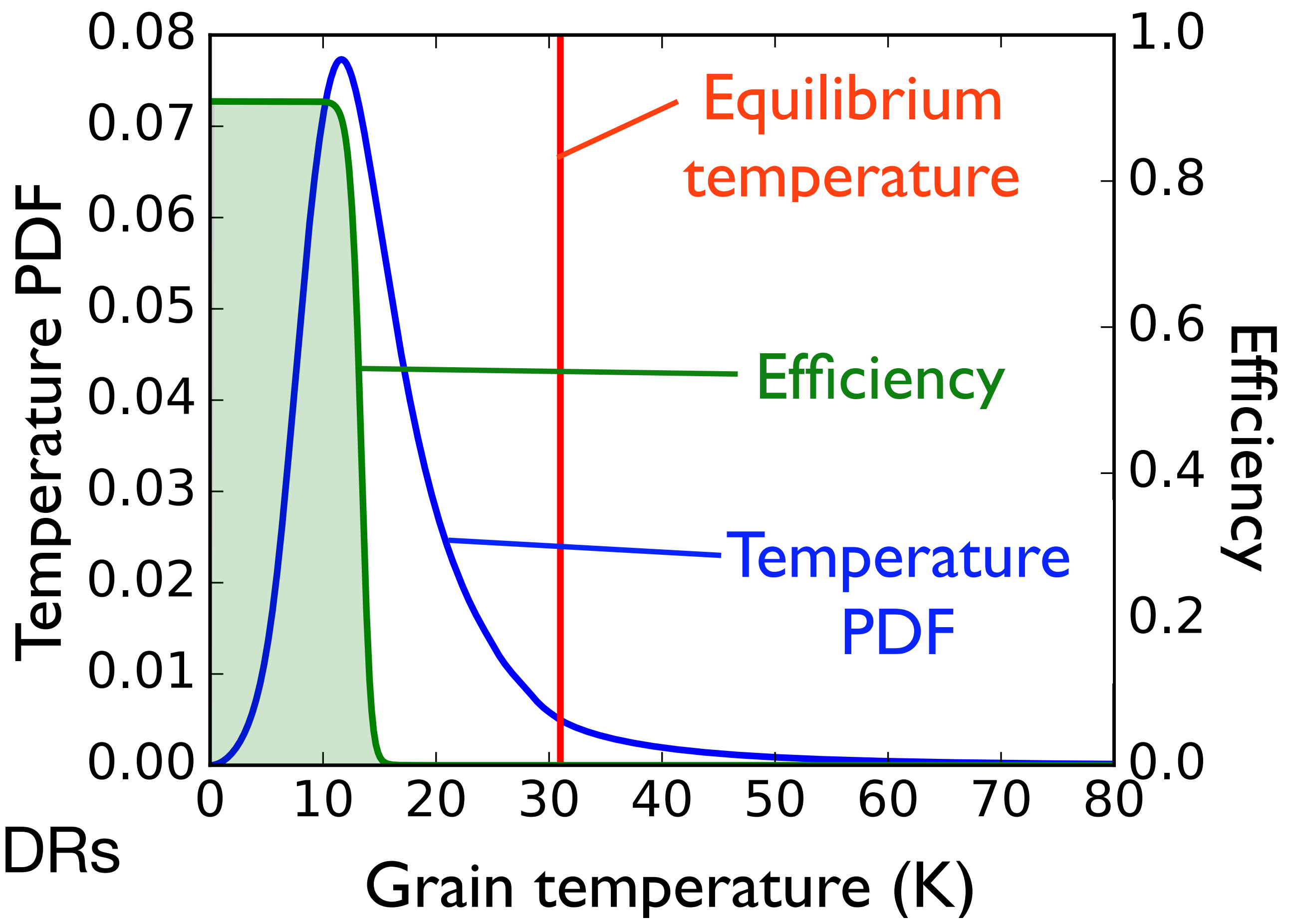
Emeric Bron, Franck Le Petit, Jacques Le Bourlot

# Stochastic processes

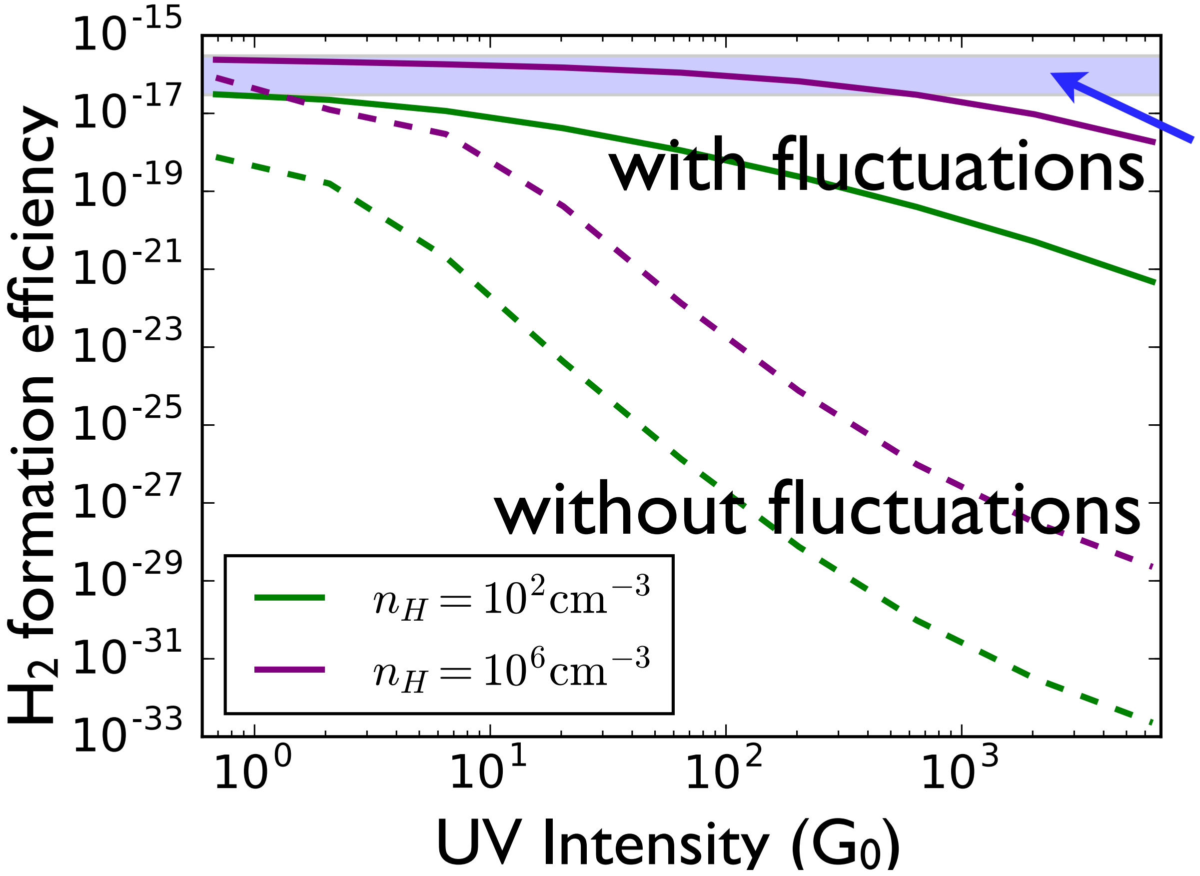
(Bron et al. A&A 2014, 2016)

New formalism to simulate $H_2$ formation

- **Master equation formalism** to consider fluctuations of the dust temperature and of the surface chemical state
- **PDF of dust temperature + populations** of adsorbed species on grains
- **Mean formation rate** coupled to the Meudon PDR code



➔ solve the problem of $H_2$ formation in bright PDRs



Observations ISO/Spitzer (PDRs)

- Efficient formation on small grains
- Grains spend most time being cold
- Langmuir-Hinshelwood alone could be sufficient in most PDRs