Microphysical processes

Simon Glover

The atomic to molecular transition

- Two things that we might mean if we say that a cloud is “molecular”:
    - Dominated by molecular hydrogen (H_2), not atomic H
    - Visible in CO emission
- These two things are not the same!
- Clouds detectable in CO have much more H_2 than H
- But not all clouds dominated by H_2 have significant CO

- Clouds in which $n_{H2} > n_H$ but only a tiny fraction of total C in CO are termed **diffuse molecular clouds**

- These have low visual extinctions (A_V ~ 0.1 — 1), often large residual atomic H fractions

- Clouds with $n_{H2} >> n_{H,}$ large fraction of C in CO are termed **dark (or dense) molecular clouds**

- These have $A_V >> 1$; average values range from 5—10 for local clouds, peak values can exceed 100

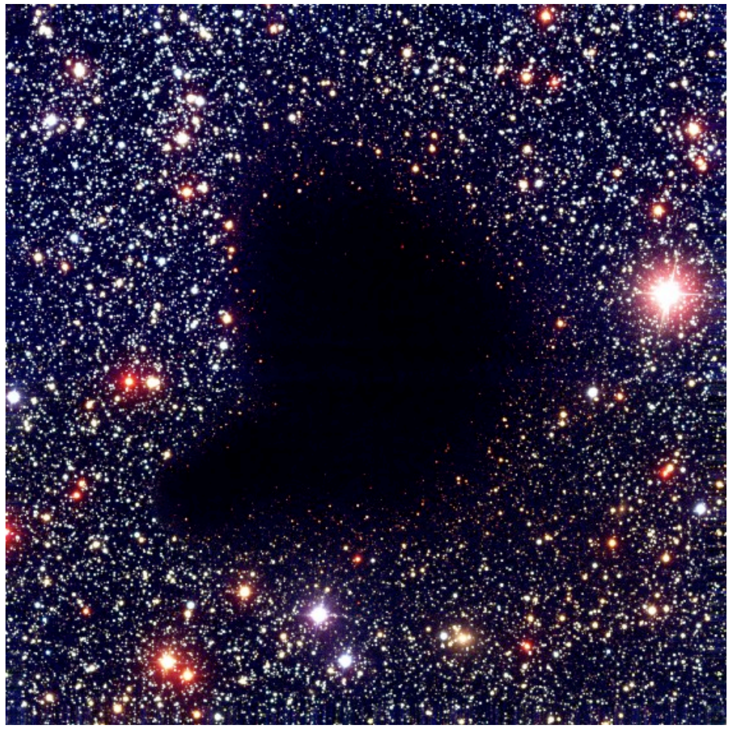
- Also sometimes talk about **translucent molecular clouds**

- These are intermediate between diffuse, dark clouds

- Typically $A_V \sim 1$, $n_{H2} >> n_H$ but still little CO

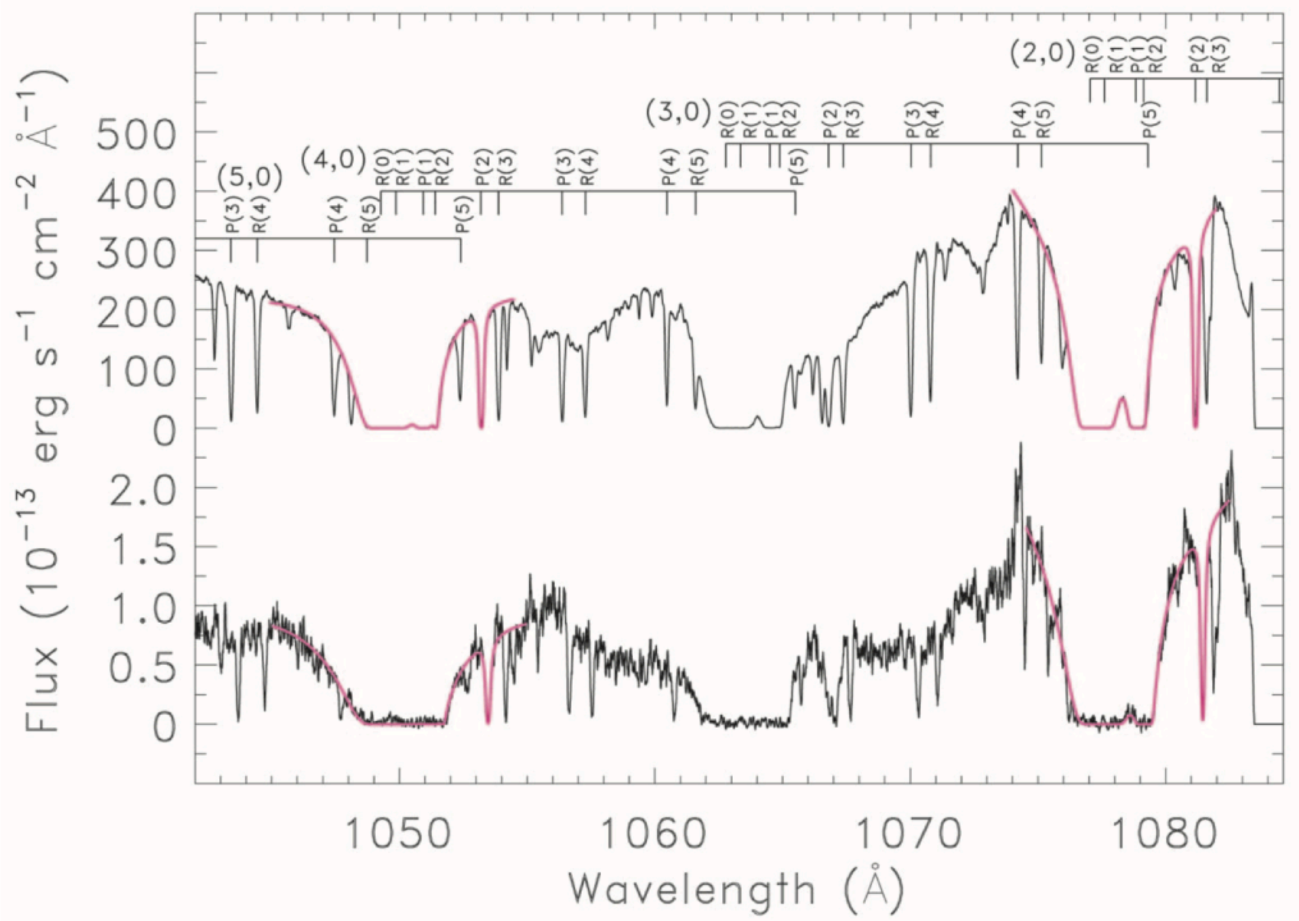
- Dark molecular clouds have wide range of sizes

- Small examples often referred to as **Bok globules**

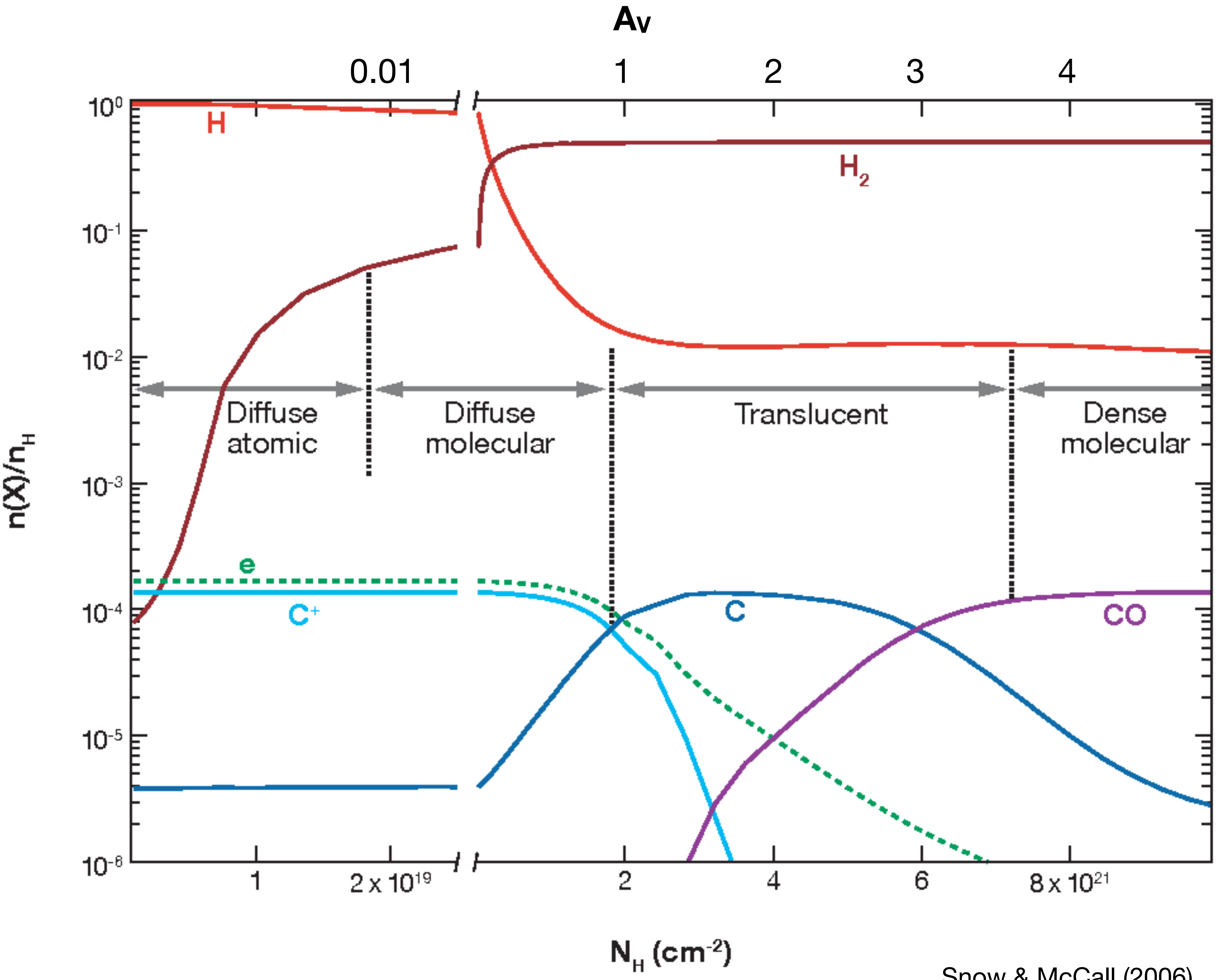


- Large examples are **giant molecular clouds (GMCs)**

- Dark clouds are opaque at optical wavelengths, bright in CO emission, so it’s obvious how we detect them
- What about diffuse/translucent clouds?
- Primarily studied in absorption, particularly in UV



Rachford et al (2002)



Snow & McCall (2006)

- Transition from H to H_2 does not coincide with transition of C from C^+ to CO

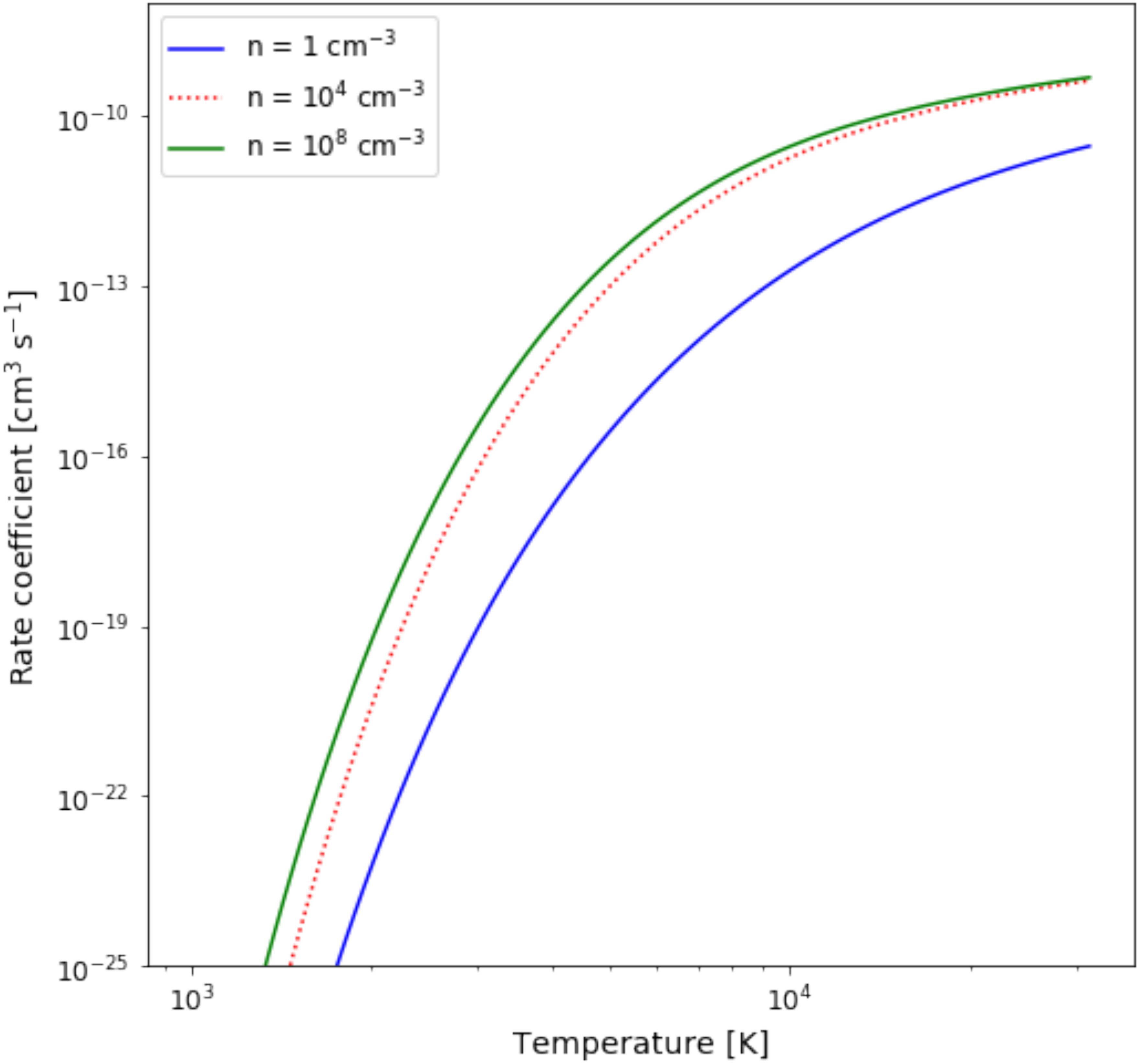
- In this lecture, we'll examine why this is so

- Our starting point is the chemistry of H_2

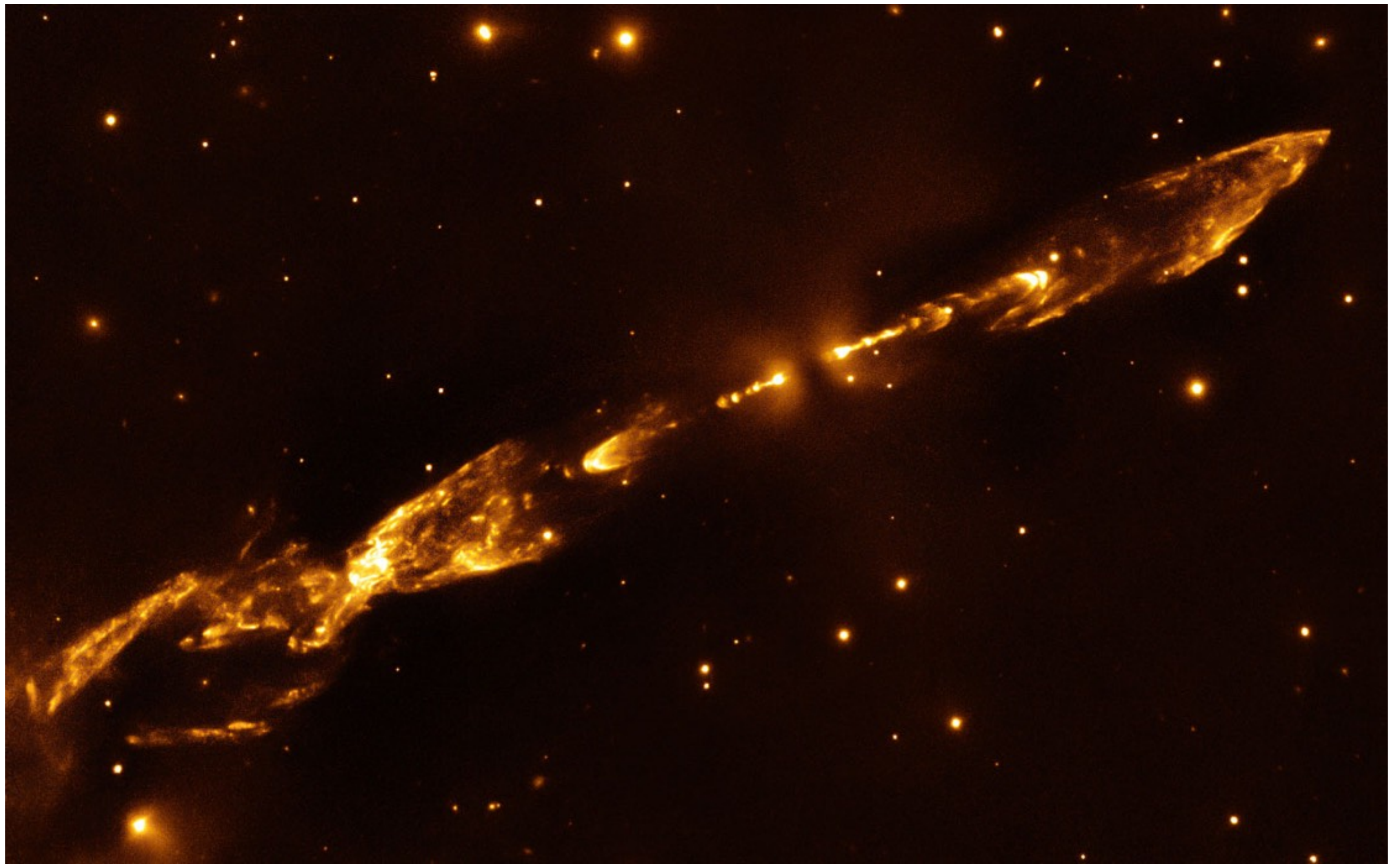
- As we discussed earlier, in the local ISM molecular hydrogen forms primarily on the surface of dust grains

- What we didn't yet discuss is how H_2 is destroyed

- H_2 has a binding energy of ~4.5 eV
- Collisional dissociation therefore requires high T
- Dissociation rate also density-dependent:
  - $v > 0$ levels become populated at high n
  - Dissociation from these levels requires less energy
- This behaviour allows H_2 in dense gas to be dissociated by series of collisions, each requiring < 4.5 eV
- Don’t get same behaviour at low n as excited H_2 radiatively decays before next collision


n = 1 cm^{-3}
n = 10^{4} cm^{-3}
n = 10^{8} cm^{-3}
Rate coefficient [cm^{3} s^{-1}]
10^{-10}
10^{-13}
10^{-16}
10^{-19}
10^{-22}
10^{-25}
10^{3}
10^{4}
Temperature [K]

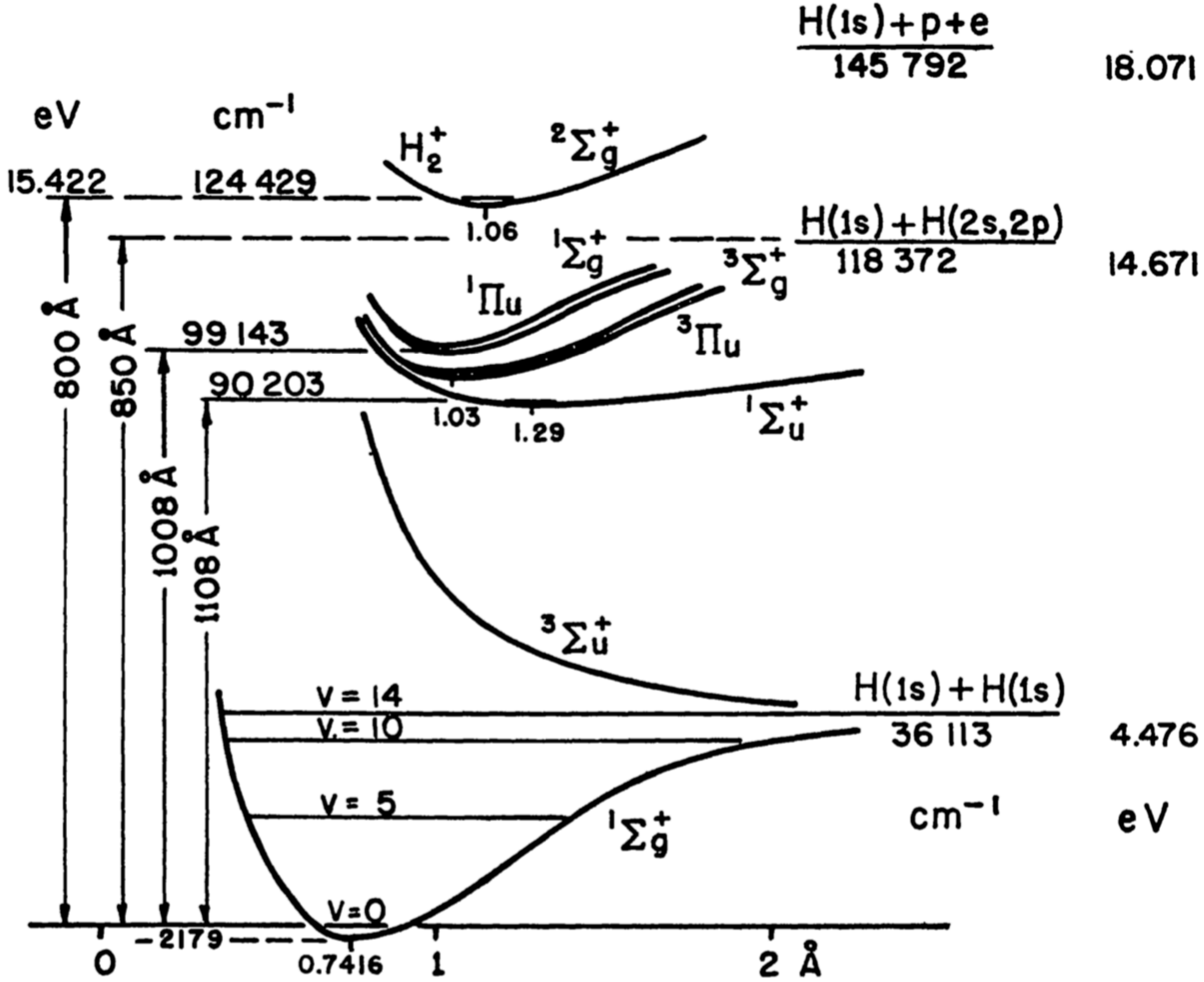
- Even in dense gas, need T >> 1000 K to get effective collisional dissociation of H_2
- In CNM, molecular clouds, T << 1000 K, so collisional dissociation is ineffective here
- Does play a role in strong shocks



- In cold gas, main destruction process is photodissociation:

$$H_2 + \text{photon} \rightarrow H + H$$

- To understand how this takes place, we need to consider the different electronic states of H_2


H(1s) + p + e
145 792
18.071
eV
cm^{-1}
H_2^+
$^2\Sigma_g^+$
15.422
124 429
1.06
H(1s) + H(2s,2p)
118 372
14.671
$^1\Sigma_g^+$
$^3\Sigma_g^+$
$^1\Pi_u$
$^3\Pi_u$
99 143
90 203
1.03
1.29
$^1\Sigma_u^+$
800 Å
850 Å
1008 Å
1108 Å
$^3\Sigma_u^+$
H(1s) + H(1s)
v = 14
v = 10
36 113
4.476
v = 5
$^1\Sigma_g^+$
cm^{-1}
eV
v = 0
-2179
0
0.7416
1
2 Å

Field (1966)

- Transition to $^3\Sigma_u^+$ anti-bonding orbital needs only ~4.5eV, but is highly forbidden — negligible destruction rate

- H_2 photodissociation instead dominated by two-step **Solomon process**

- **Step 1**: absorption of UV photon excites H_2 molecule to Lyman (B) or Werner (C) electronic state

- This transition is allowed, hence cross-section is large

- B, C states also bound, with quantized v, J

- v, J can change during excitation: $(v, J) \rightarrow (v', J')$

- Absorption occurs in discrete spectral lines: the Lyman and Werner bands

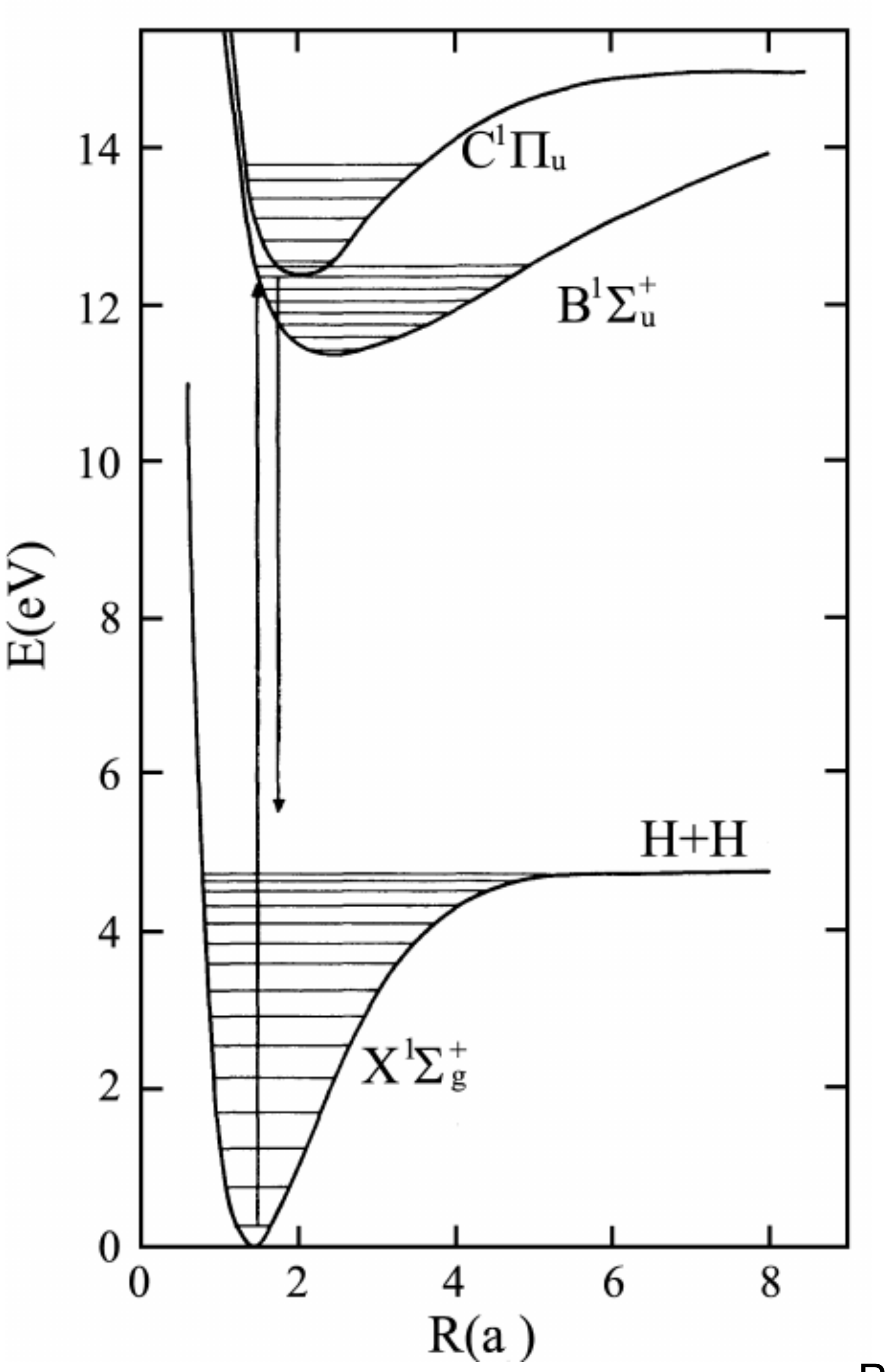
- **Step 2:** radiative de-excitation from B or C state returns molecule to electronic ground state

- Most of the time (~85%), molecule ends up back in bound state (although often with high v and/or J)

- Small fraction of time (~15%), molecule ends up in vibrational continuum, leading to photodissociation

- For H_2 in vibrational ground state, minimum energy required to reach Lyman state is ~11.2 eV

- UV photons capable of exciting H_2 to Lyman or Werner states commonly referred to as **Lyman-Werner photons**



Pak et al (2003)

- Total H_2 photodissociation rate:

$$\zeta_{\rm diss} = \sum_u \frac{\pi e^2}{m_{\rm e} c^2 h} f_{lu} \lambda_{lu}^3 u_{\lambda_{lu}} p_{{\rm diss},u}$$

f_{lu} = oscillator strength of transition

λ_{lu} = wavelength of transition

u_λ = radiation field energy density at that wavelength

$p_{\rm diss,u}$ = dissociation probability

- We sum here over all levels u accessible in the B, C states given our initial (v, J) in the ground state

- What makes a level accessible?
  - Energy difference < 13.6 eV — higher energy photons are absorbed by atomic H, hence not available
  - Rotational selection rule: $\Delta J = 0, +1$ or -1 (plus transitions from $J = 0$ to $J = 0$ not allowed)
  - No constraint on change in v

- B, C states in H_2 are analogous to 2s, 2p in atomic H
- Higher energy bound states also exist, analogous to states with $n > 2$, but energy separation from ground state exceeds 13.6 eV

- H_2 can also be photoionized to H_2^+ or photodissociated via single-step bound-free absorption

- However, both processes again require > 13.6 eV, hence don't occur in regions where H is present to absorb UV

- For rotationally cold H_2 (i.e. all molecules in ortho or para ground state), can easily compute photodissociation rate. For local value of ISRF, we find:

$$\zeta_{\rm diss} \simeq 5.6 \times 10^{-11}\,{\rm s}^{-1}$$

- Total radiative excitation rate is factor of ~7 larger

- In chemical equilibrium:

$$\zeta_{\rm diss} n_{\rm H_2} = R_{\rm H_2,dust}.$$

- Evaluating this for the local ISRF we find:

$$\frac{n_{\rm H_2}}{n_{\rm H}} = \frac{3 \times 10^{-17} (T/100)^{1/2} n}{5.6 \times 10^{-11}} \simeq 5.4 \times 10^{-7} \left(\frac{T}{100}\right)^{1/2} n.$$

- For typical CNM density, temperature, this yields an equilibrium H_2 fraction ~ 4×10^{-5}

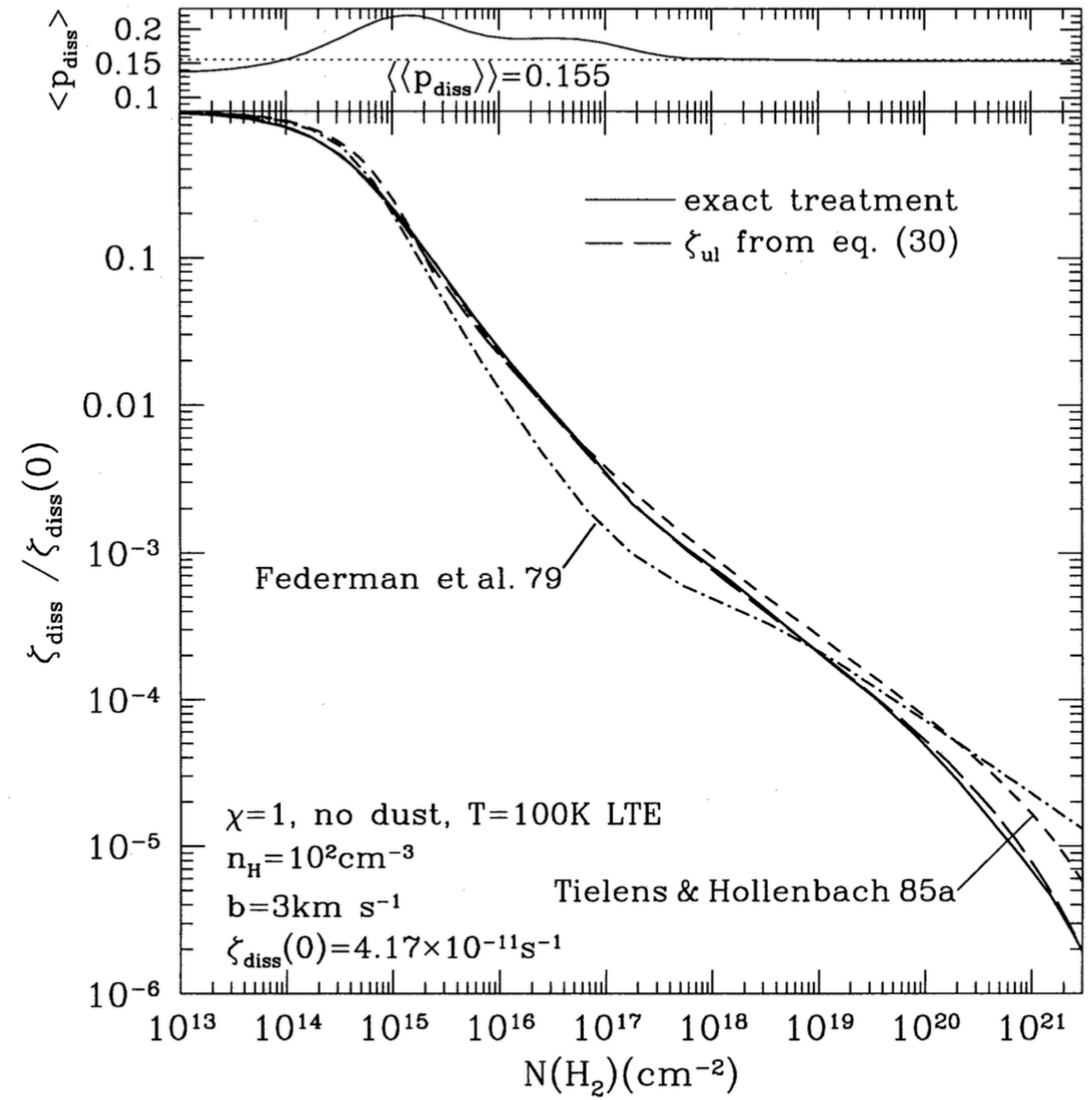
- In the diffuse ISM, destruction dominates. So how do we wind up with clouds with $n_{H2} >> n_H$?

- Answer: **shielding**!
- Photodissociation requires presence of UV photons at wavelengths corresponding to Lyman-Werner lines
- Photodissociation selectively removes these photons from the radiation field
- As beam of radiation propagates through a cloud containing H_2, it gradually loses the photons needed to destroy H_2
- Hence: destruction of H_2 steadily becomes less effective.
- H_2 molecules near surface of cloud shield H_2 molecules further in — process known as **self-shielding**

- Strong lines become optically thick before weaker lines

- Different transitions dominate H_2 photodissociation rate for different H_2 column densities
  - Strong lines dominate for low N_{H2}
  - Weak lines dominate for large N_{H2}

- Dependence of photodissociation rate on N_{H2} weaker than for process dominated by single spectral line



Draine & Bertoldi (1996)

- Define a self-shielding function f_{shield} such that:

$$\zeta_{\text{diss}} = f_{\text{shield}} \zeta_{\text{diss},0},$$

- Simple but fairly inaccurate approximation:

$$f_{\text{shield}} = \begin{cases} 1 & \text{for } N_{\text{H}_2} < 10^{14}\ \text{cm}^{-2}, \\ (N_{\text{H}_2}/10^{14}\ \text{cm}^{-2})^{-0.75} & \text{for } N_{\text{H}_2} \geq 10^{14}\ \text{cm}^{-2}. \end{cases}$$

- More accurate approximation:

$$f_{\text{shield}} = \frac{0.965}{(1 + x/b_5)^2} + \frac{0.035}{(1+x)^{0.5}} \exp\left[-8.5 \times 10^{-4} (1+x)^{0.5}\right],$$

where $x = N_{H2} / 5 \times 10^{14}$ cm^{-2}, $b_5 = b / 10^5$ cm s^{-1}

- One additional complication: absorption by dust

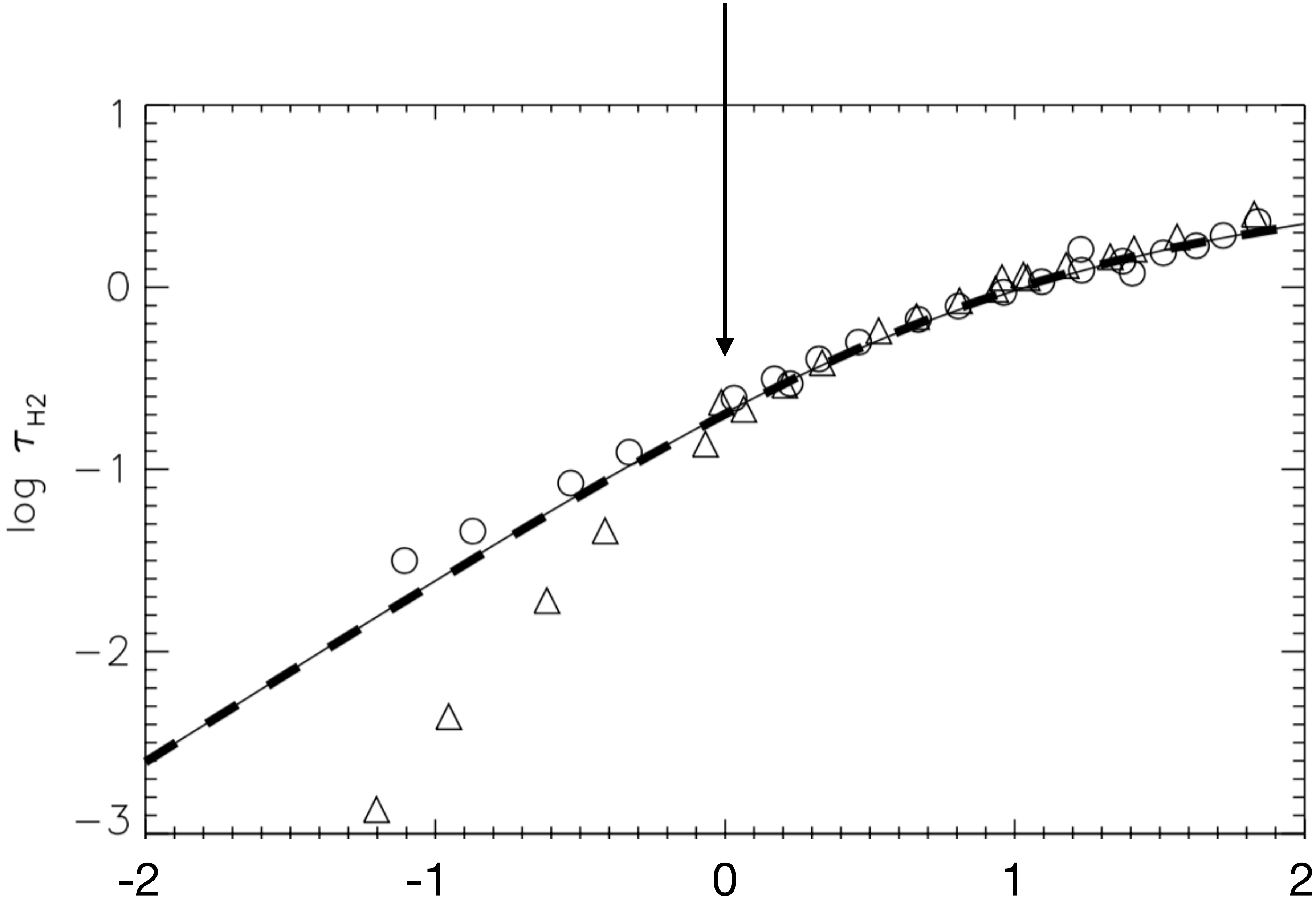
- Dust absorption cross-section in LW bands:

$$\sigma_d \approx 2 \times 10^{-21} \text{ cm}^2$$

- Importance of dust absorption depends on total column density required for $H \rightarrow H_2$ transition

- Column density required depends on strength of radiation field — dust plays greater role when radiation field strong

Milky Way



Dust optical
depth in atomic
gas layer

Log (Radiation field strength)

$A_V \sim 0.25\ \tau_{H2}$

McKee & Krumholz (2010)

- In self-shielding dominated regime, equilibrium H_2 fraction given approximately by:

$$\begin{aligned}\frac{n_{\mathrm{H}_2}}{n_{\mathrm{H}}} &= \frac{3 \times 10^{-17} (T/100)^{1/2} n}{5.6 \times 10^{-11} f_{\mathrm{shield}}}, \\ &\simeq 1.7 \times 10^{-17} \left(\frac{T}{100}\right)^{1/2} n \, N_{\mathrm{H}_2}^{0.75}.\end{aligned}$$

- If cloud has radius L, with $N_{H2} = n_{H2}$ L at centre, then:

$$n_{\mathrm{H}_2} = 2.4 \times 10^{-12} \left(\frac{T}{100}\right)^2 n^4 \, n_{\mathrm{H}}^4 L_{\mathrm{pc}}^3,$$

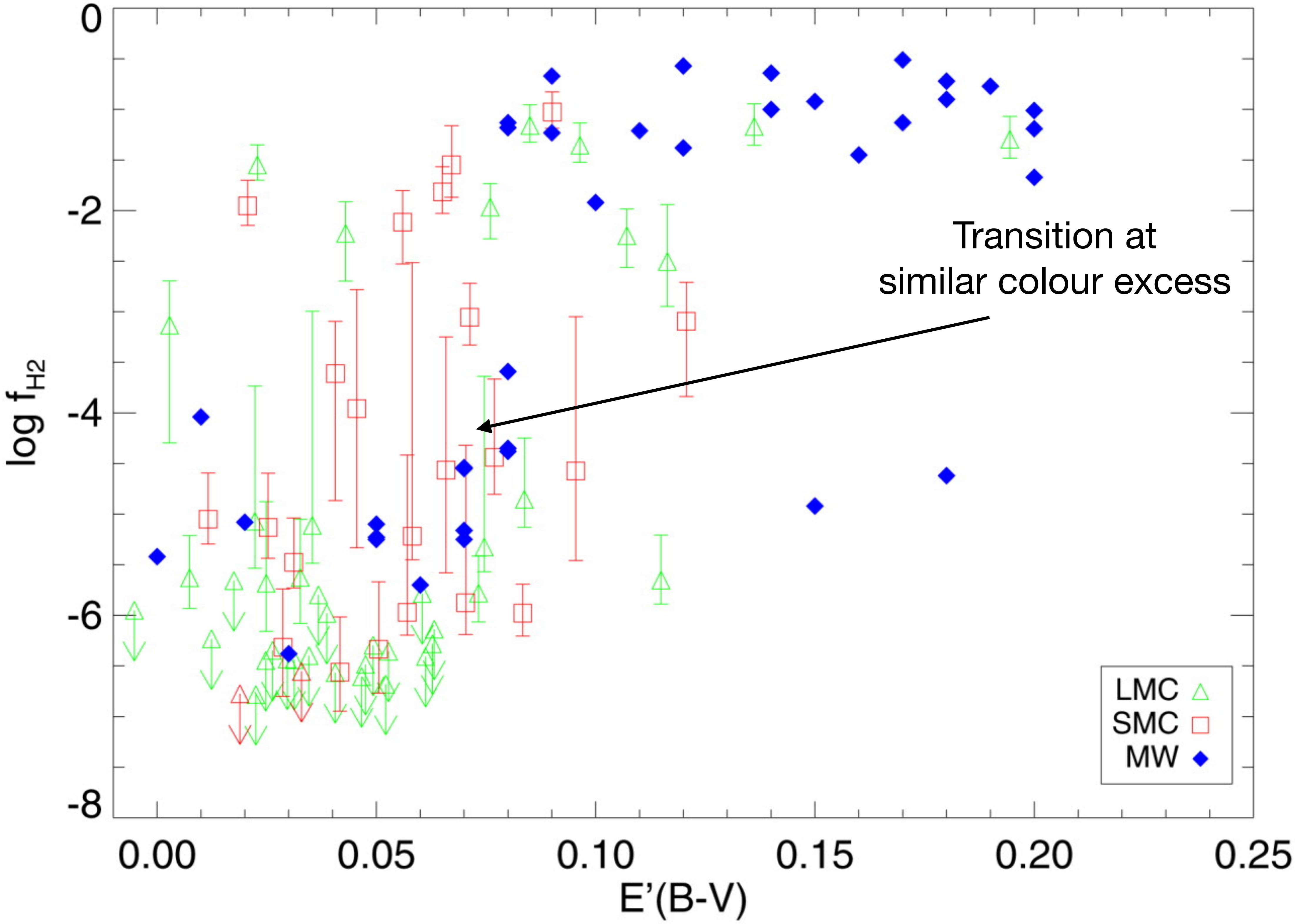
- H_2 fraction is a very steep function of number density, cloud size

- Expect rapid transition from optically thin regime with very low H_2 fraction to self-shielded regime with $x_{H2} \sim 1$

- Can test this observationally using UV absorption spectroscopy to measure H_2, H column densities

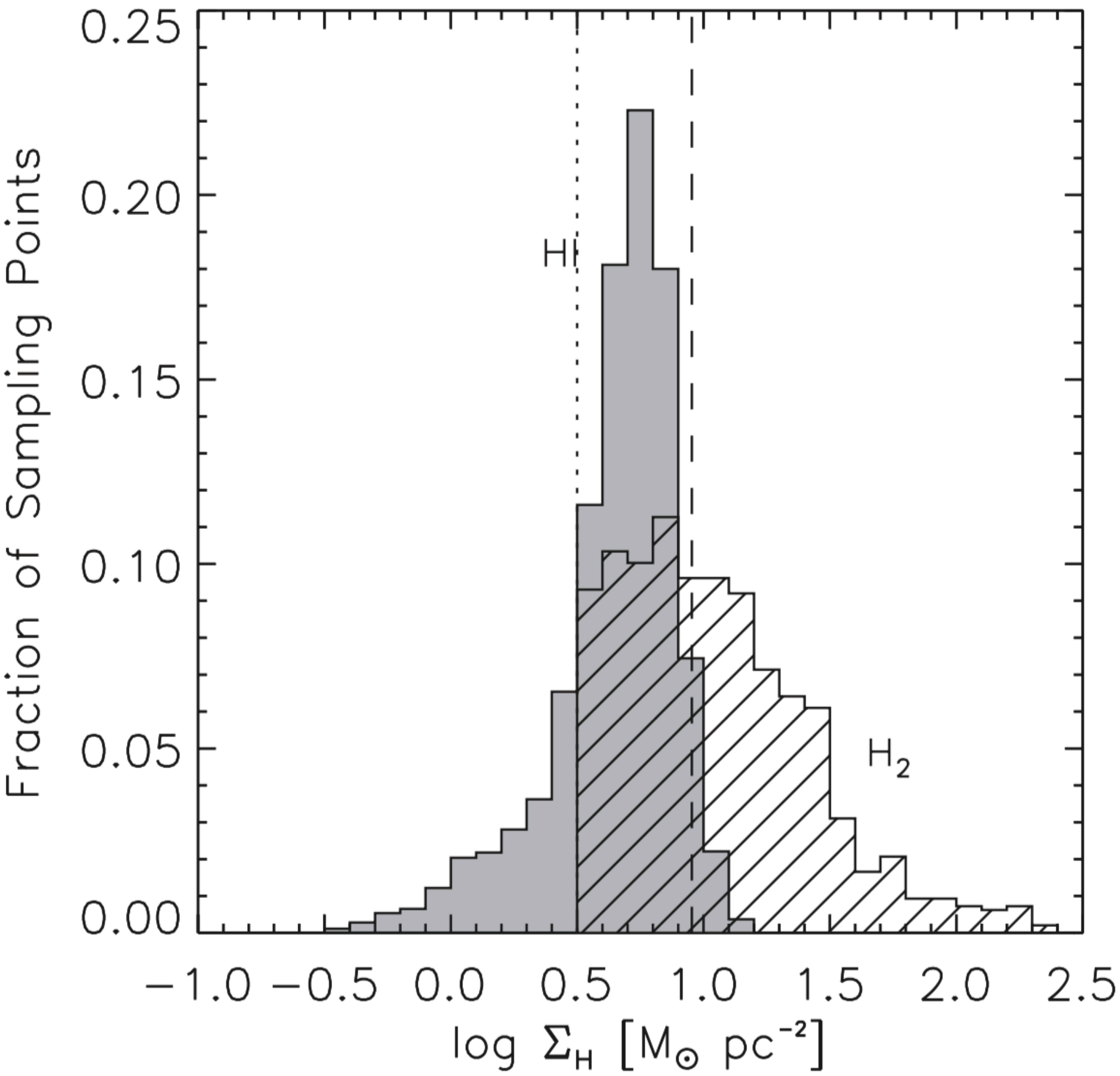
- First done in Milky Way in 1970s by Copernicus satellite, more recently for MW, LMC, SMC by FUSE

$E'(B-V)_{crit} \sim 0.07$



Transition at
similar colour excess

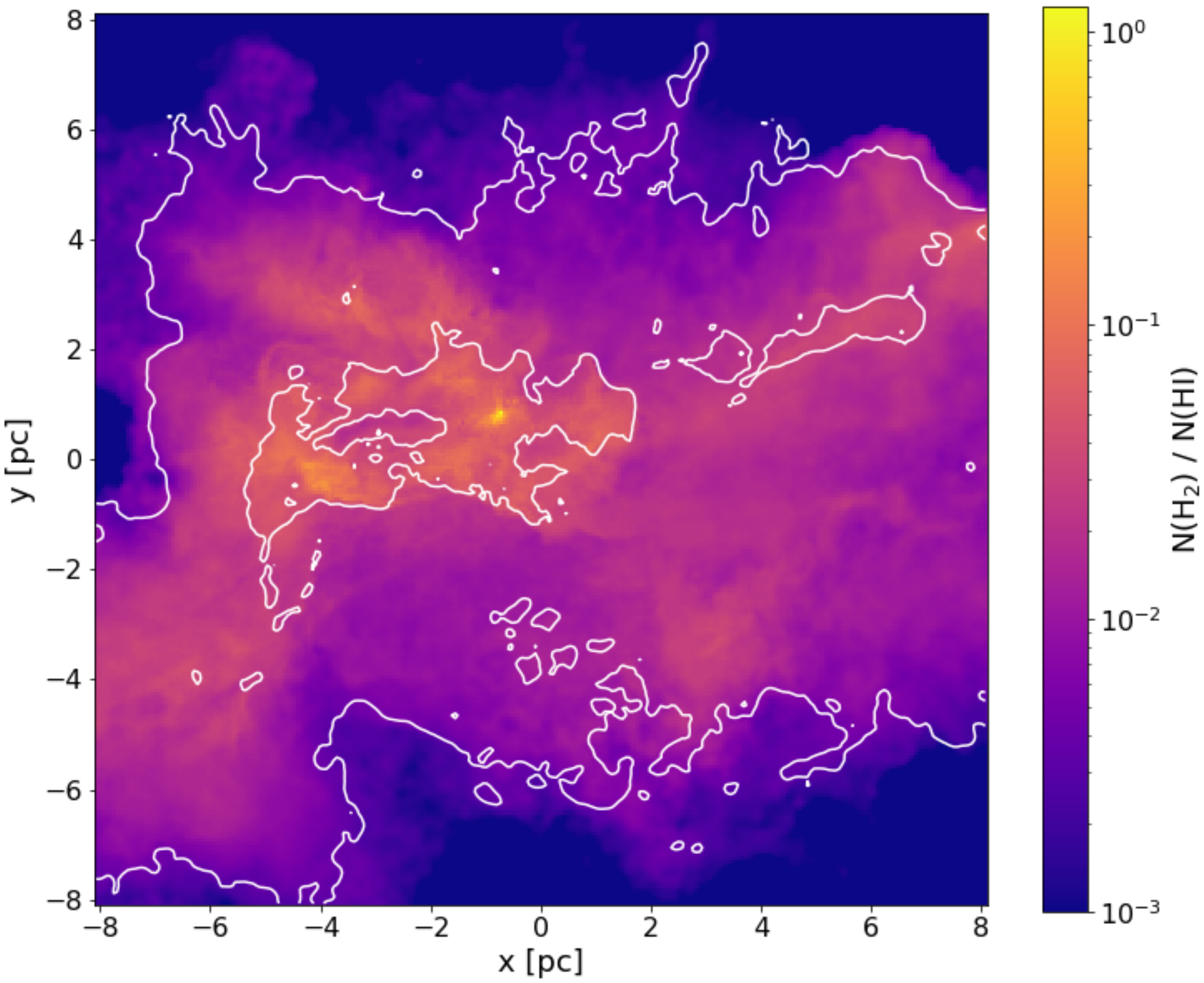
Tumlinson et al (2002)



Bigiel et al (2008)

- Does H_2 fraction actually reach equilibrium in the ISM?
- At typical CNM density, H_2 formation time ~ 10 Myr
- Turbulence accelerates this by creating transient density enhancements, can reduce timescale by factor of few
- For comparison: free-fall collapse time ~ 5 Myr
- H_2 fraction may be out of equilibrium in CNM, but not wildly so — equilibrium results good guide to behaviour

- But this is at solar metallicity. What happens at low metallicity?
- Formation time inversely proportional to dust abundance
- If dust abundance ~ metallicity, formation time increases as 1/Z
- At low Z, evidence for steeper dependence of dust abundance on metallicity, so this probably underestimates t_{form} in low Z systems
- At sufficiently low Z, equilibrium not guaranteed — collapse and star formation may occur in H-dominated regime



Simulated star-forming cloud in galaxy with $Z = 0.03\ Z_{sun}$

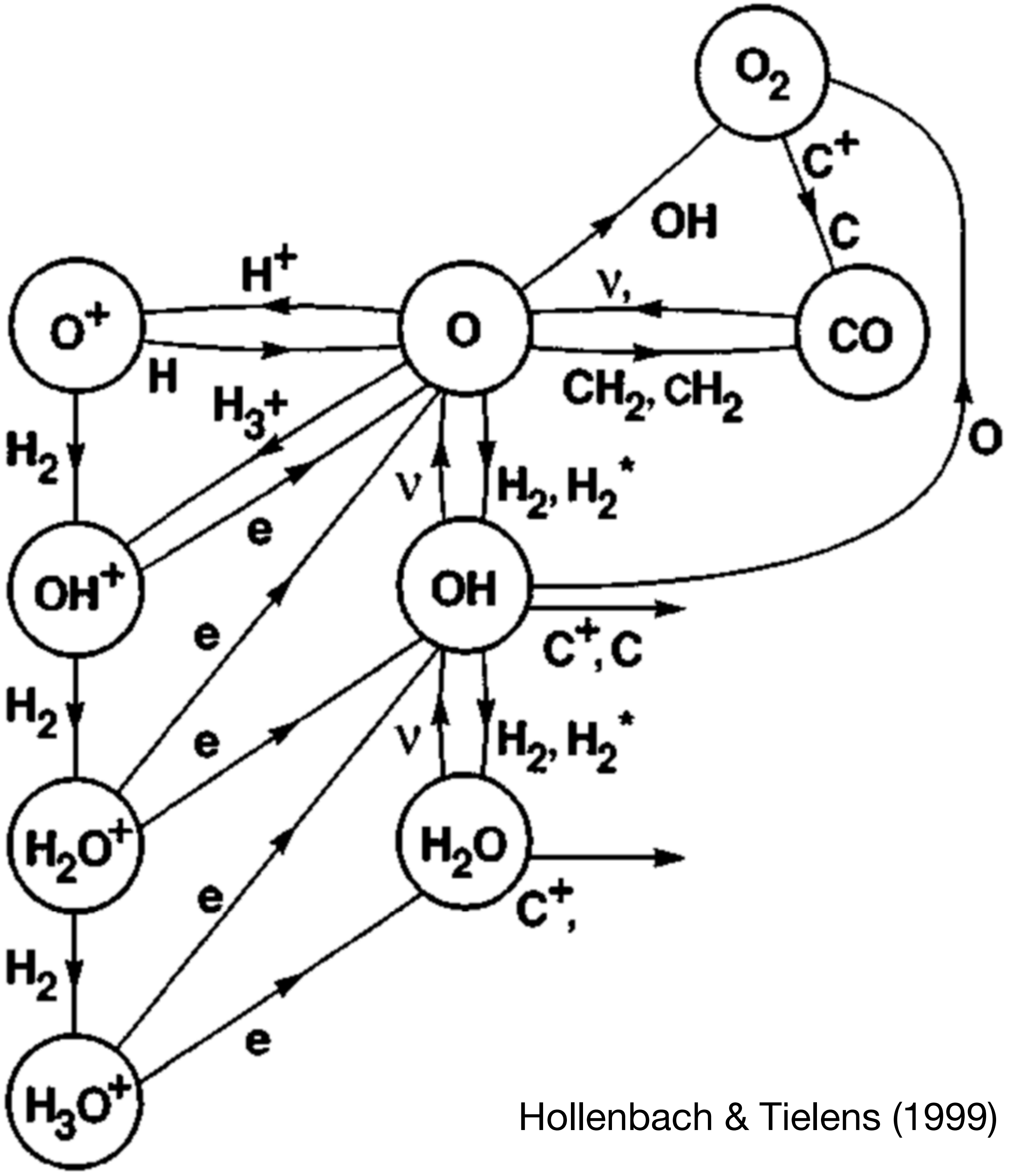
CO formation

- As with H_2, the simplest way to form CO in the ISM is via radiative association:

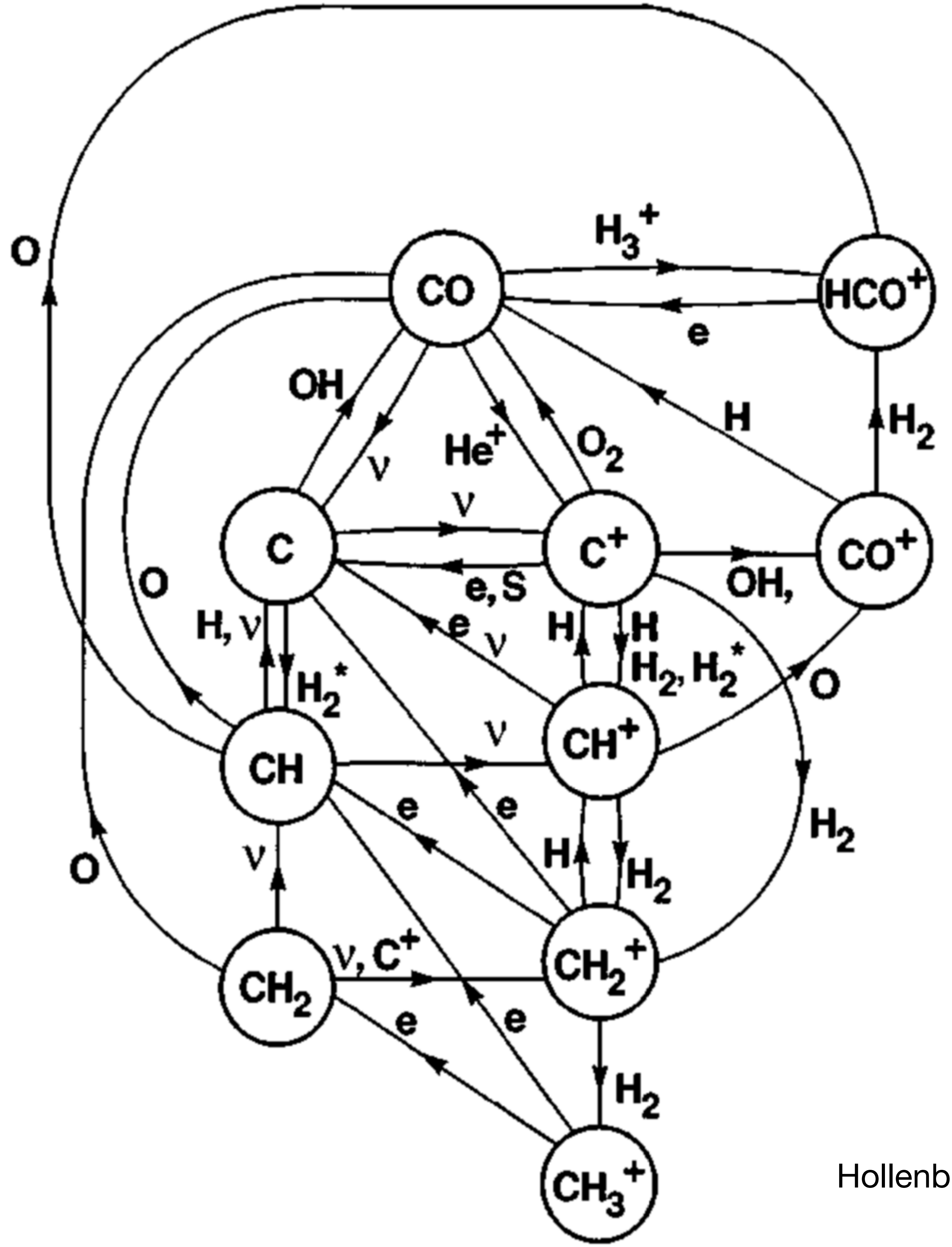
$$C + O \rightarrow CO + \text{photon}$$

- However, this reaction is slow (albeit not as slow as the corresponding reaction for H_2), hence usually unimportant

- CO formation is instead dominated by a variety of gas-phase ion-neutral reactions



Hollenbach & Tielens (1999)



Hollenbach & Tielens (1999)

- At first glance, this complexity is rather daunting
- In practice, not all of these reactions are equally important, so safe to focus on a few of the key chains
- First of these involves hydroxyl (OH). One way to form this is the chain:

$$\begin{aligned} \mathrm{O^+ + H_2} &\rightarrow \mathrm{OH^+ + H}, \\ \mathrm{OH^+ + H_2} &\rightarrow \mathrm{H_2O^+ + H}, \\ \mathrm{H_2O^+ + H_2} &\rightarrow \mathrm{H_3O^+ + H}, \end{aligned}$$

- H_3O^+ doesn't react further with H_2, but destroyed by dissociative recombination:

$$\mathrm{H_3O^+ + e^- \rightarrow OH + (H_2 \ or \ H + H)}$$

- Alternatively, we can form OH starting with:

$$\begin{aligned} \mathrm{O} + \mathrm{H_3^+} &\rightarrow \mathrm{OH^+} + \mathrm{H_2}, \\ \mathrm{O} + \mathrm{H_2^+} &\rightarrow \mathrm{OH^+} + \mathrm{H} \end{aligned}$$

- OH^+ ions formed via one of these reactions then follow same pathway as above

- OH is an interesting ISM tracer in its own right, but is also a stepping stone to CO:

$$\begin{aligned} \mathrm{C^+} + \mathrm{OH} &\rightarrow \mathrm{CO^+} + \mathrm{H}, \\ \mathrm{CO^+} + \mathrm{H_2} &\rightarrow \mathrm{HCO^+} + \mathrm{H}, \\ \mathrm{HCO^+} + \mathrm{e^-} &\rightarrow \mathrm{CO} + \mathrm{H}. \end{aligned}$$

- If carbon is present as C rather than C^+, can also form CO directly from OH via:

$$\mathrm{C} + \mathrm{OH} \rightarrow \mathrm{CO} + \mathrm{H}.$$

- All of these reactions are non-radiative and exothermic (i.e. they produce energy).

- In every case, $p_{\mathrm{react}} \sim 1$ and the reactions proceed at rates close to the collision rate

- Typical reaction rate coefficients at 100 K range from $\sim 10^{-6}$ cm^3 s^{-1} for dissociative recombination to $\sim 10^{-11}$ cm^3 s^{-1} for neutral-neutral reactions such as C + OH

- In each version of the OH pathway, rate-limiting step for forming OH is formation of the initial ion (O^+, H_2^+ or H_3^+)

- Main source: **cosmic ray ionisation**

- Cosmic ray ionisation produces O^+ and H_2^+ ions at a total rate ~ 2×10^{-15} s^{-1}

- Most H_2^+ immediately destroyed by the reaction:

$$H_2 + H_2^+ \rightarrow H_3^+ + H$$

- Some fraction of O^+, H_3^+ ions resulting from cosmic ray ionisation then react to form OH^+, initiating pathway to OH

- How large is this fraction?

- For O^+, reaction with H_2 is main destruction mechanism in gas with $n_{H2} > n_H$, so fraction ~ 1

- For H_3^+, dissociative recombination is far more effective than reaction with O — fraction ~ 0.01 (x_O / x_e)

- If we assume all OH converted to CO, then net CO formation rate per unit volume is:

$$R_{\rm CO} = 4 \times 10^{-18} \zeta_{\rm H,16} \, n_{\rm H_2} \ {\rm cm^{-3} \, s^{-1}},$$

- Corresponding CO formation timescale:

$$t_{\rm form,CO} \simeq 1.0 \, x_{\rm H_2}^{-1} \zeta_{\rm H,16}^{-1} \ {\rm Myr},$$

- CO can also form via several reaction chains starting from CH^+ or CH_2^+ ions

- Unlike OH^+, these ions are primarily formed via radiative association of C^+ with H or H_2:

$$\begin{aligned} \mathrm{C^+ + H} &\rightarrow \mathrm{CH^+} + \gamma \\ \mathrm{C^+ + H_2} &\rightarrow \mathrm{CH_2^+} + \gamma. \end{aligned}$$

- In CNM conditions, resulting CO formation rate is same order of magnitude as that due to OH^+ and OH

- Both routes also depend crucially on presence of H_2

- Important points to take away from this analysis:

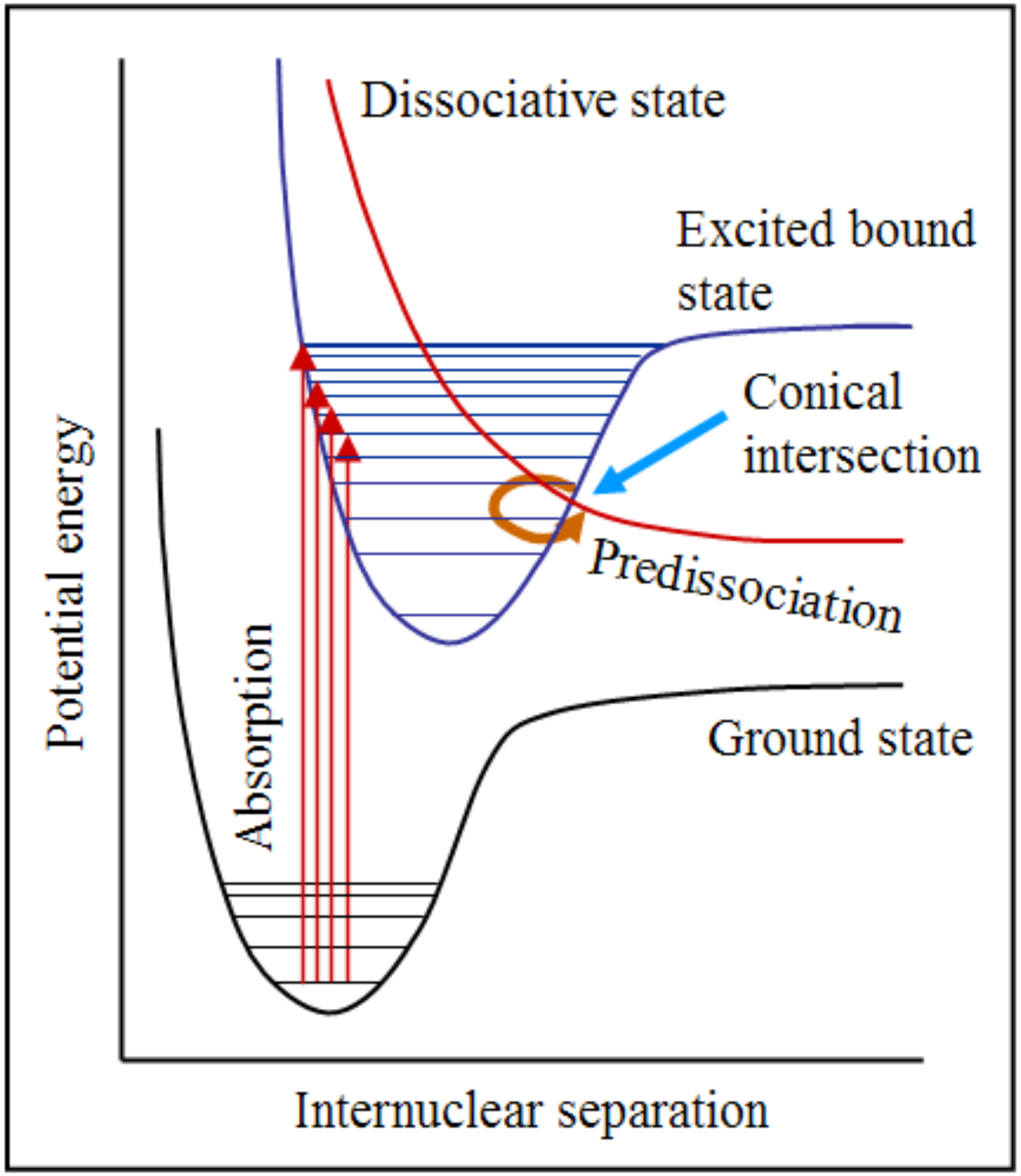
  1) CO formation occurs in less than one dynamical time in moderate density gas (n ~ 1000 cm^{-3} or less)

  2) CO formation requires the presence of H_2

  3) Point (2) implies that the <u>most important chemical timescale for GMCs is the H_2 formation timescale</u>

CO destruction

- As with H_2, collisional dissociation of CO is highly endothermic and hence important only at high T
- At low T and low column densities, destruction of CO is dominated by photodissociation
- CO photodissociation differs from H_2, occurs via a process known as **predissociation**


Dissociative state
Excited bound state
Conical intersection
Predissociation
Absorption
Ground state
Potential energy
Internuclear separation

Iqbal (2010)

- Key differences to H_2 photodissociation:
  - Transition to unbound state highly likely, so $p_{diss} \sim 1$
  - Excited state very short-lived, so lines are broad

- Similarities to H_2 photodissociation:
  - Line-driven process, hence self-shielding is possible
  - Requires UV photons, minimum energy 11.5eV

- In practice, CO self-shielding not very efficient

- Two main reasons for this:
  - Absorption lines often broader than for H_2, hence need more column density to produce τ ~ 1
  - CO column densities << H_2 column densities in fully molecular gas, since C, O much less abundant than H

- CO shielding dominated by dust, although also a significant contribution from H_2

- In typical CNM conditions, require A_V ~ 1-2 in order to make photodissociation rate smaller than formation rate

- Therefore expect transition from C^+ to CO to occur at approximately this visual extinction

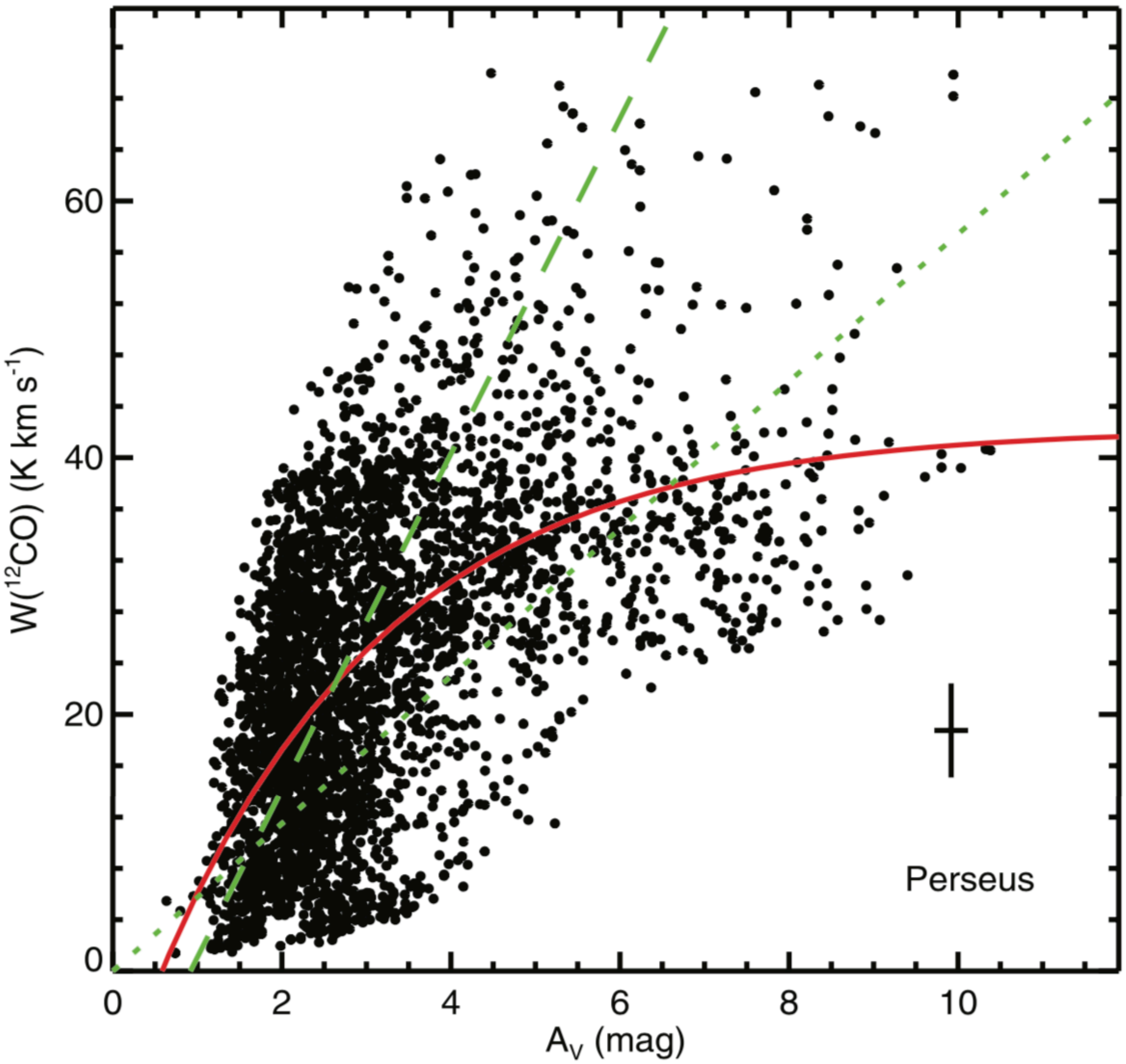
- Cf. the transition from H to H_2, which requires $A_V \sim 0.1$

- This mismatch between the column densities required for efficient shielding of H_2, CO explains existence of two classes of molecular clouds

- Diffuse, translucent clouds have high enough column density to shield H_2 but not CO

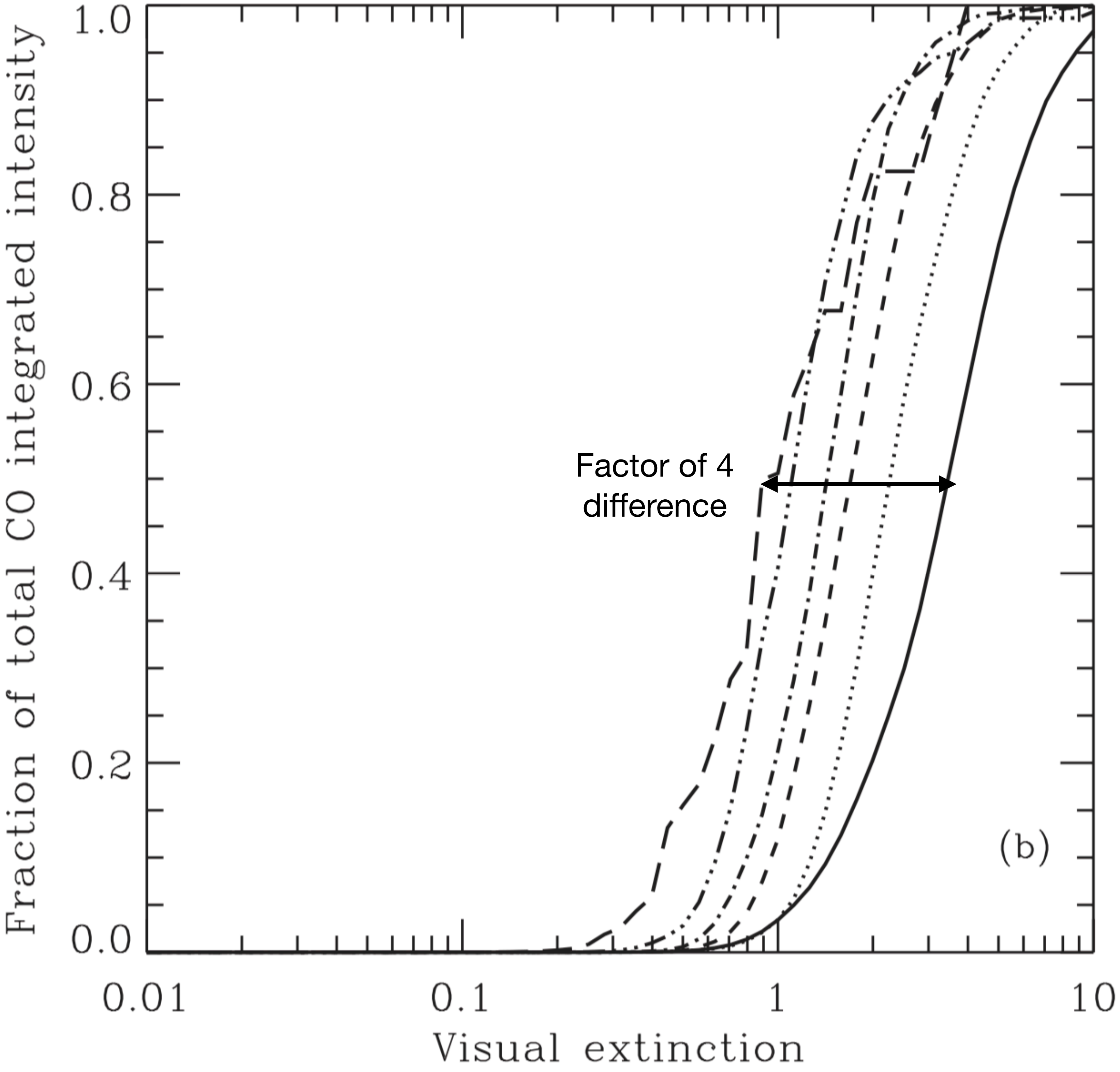
- GMCs shield both molecules effectively in their interiors

Observations of an A_V threshold for bright CO emission



Pineda et al (2008)

Simulation results for clouds of varying metallicity



Factor of 4 difference

Glover & Clark (2016)

Simulated Z ranges from 0.03 — 1 Z_{sun}

- Outer regions of GMCs have $A_V < 1$

- Expect these regions to be dominated by H_2 but to have very little associated CO — **CO-dark molecular gas**

- For the Milky Way, CO-dark H_2 associated with GMCs is around 10-20% of total

- Total fraction of CO-dark gas (including diffuse, translucent clouds) much higher, but uncertain

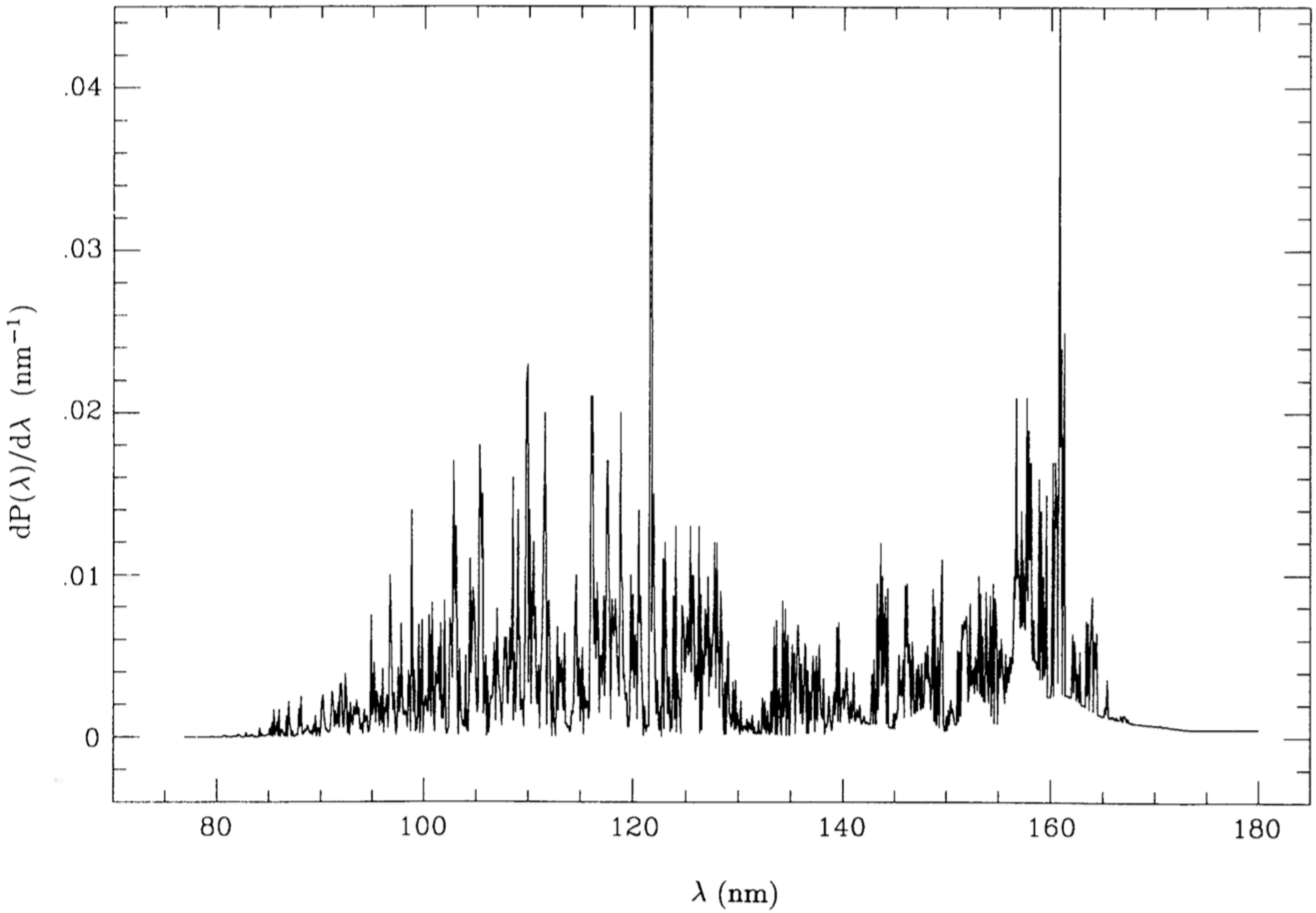
- At low Z, these numbers are much, much larger

- At high A_V, CO well-shielded from external radiation field
- CO in these regions can still be destroyed by cosmic rays
- Direct ionization of CO by cosmic rays ineffective, since resulting CO^+ ions quickly reform CO
- More effective: dissociative charge transfer with He^+

$$\begin{aligned} \mathrm{He} + \mathrm{c.r.} &\rightarrow \mathrm{He}^+ + \mathrm{e}^-, \\ \mathrm{He}^+ + \mathrm{CO} &\rightarrow \mathrm{He} + \mathrm{C}^+ + \mathrm{O}. \end{aligned}$$

- When cosmic ray fluxes are very large, this may strongly suppress CO fraction

- CRs also destroy CO via the **Prasad-Tarafdar mechanism**
- As previously mentioned, cosmic ray ionization produces energetic electrons
- These electrons can lose energy by exciting higher electronic states in H, H_2
- Decay of these states to the ground state produces local flux of UV photons
- These photons can then photodissociate CO



Gredel et al (1989)

Atomic carbon

- In our discussion of CO formation and discussion, we’ve largely ignored atomic carbon (C)

- In CNM, C abundance set by balance between radiative recombination of C^+

$$C^+ + e^- \rightarrow C + \text{photon}$$

and photoionization of C:

$$C + \text{photon} \rightarrow C^+ + e^-$$

- At a typical CNM temperature of 60 K, the recombination rate is approximately:

$$R_{\mathrm{rec,C^+}} \simeq 1.2 \times 10^{-11} n_{\mathrm{C^+}} n_{\mathrm{e^-}} \ \mathrm{cm^{-3}\,s^{-1}}$$

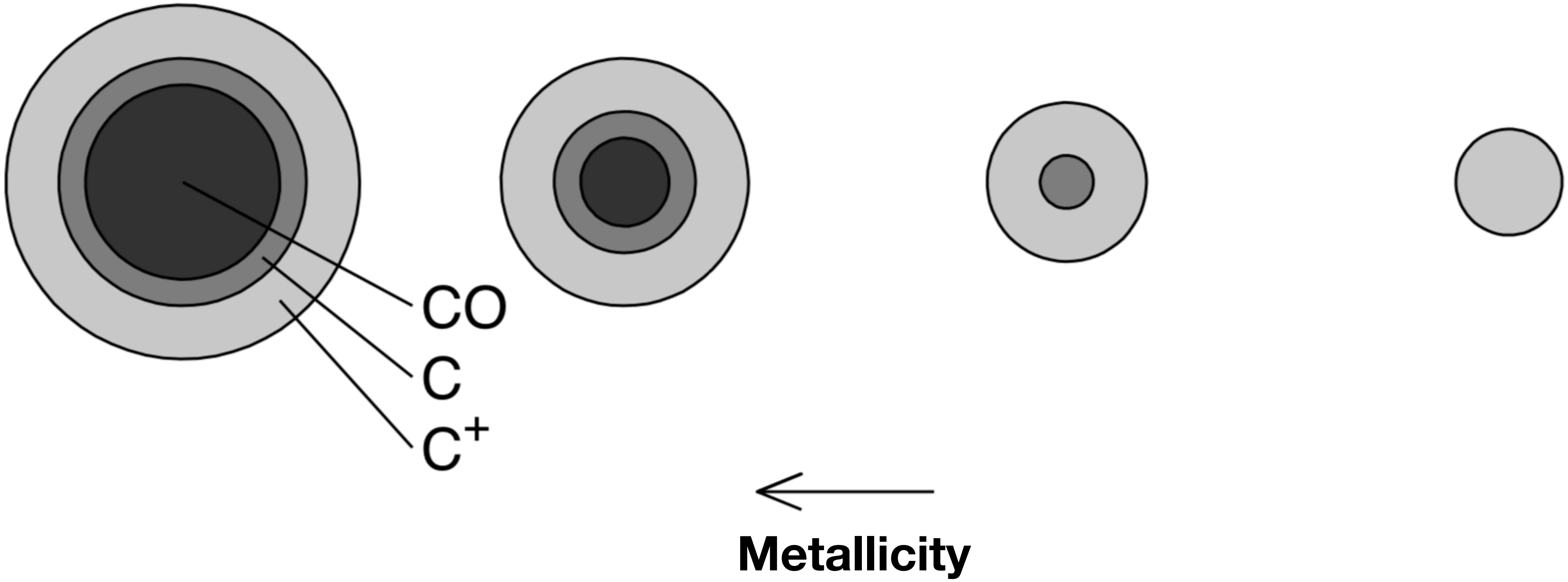
- For the local ISRF, the photoionization rate is

$$R_{\mathrm{pi,C}} = 3.5 \times 10^{-10} \exp\left(-3.76 A_{\mathrm{V}}\right) \, n_{\mathrm{C}} \, \mathrm{cm^{-3}\,s^{-1}}$$

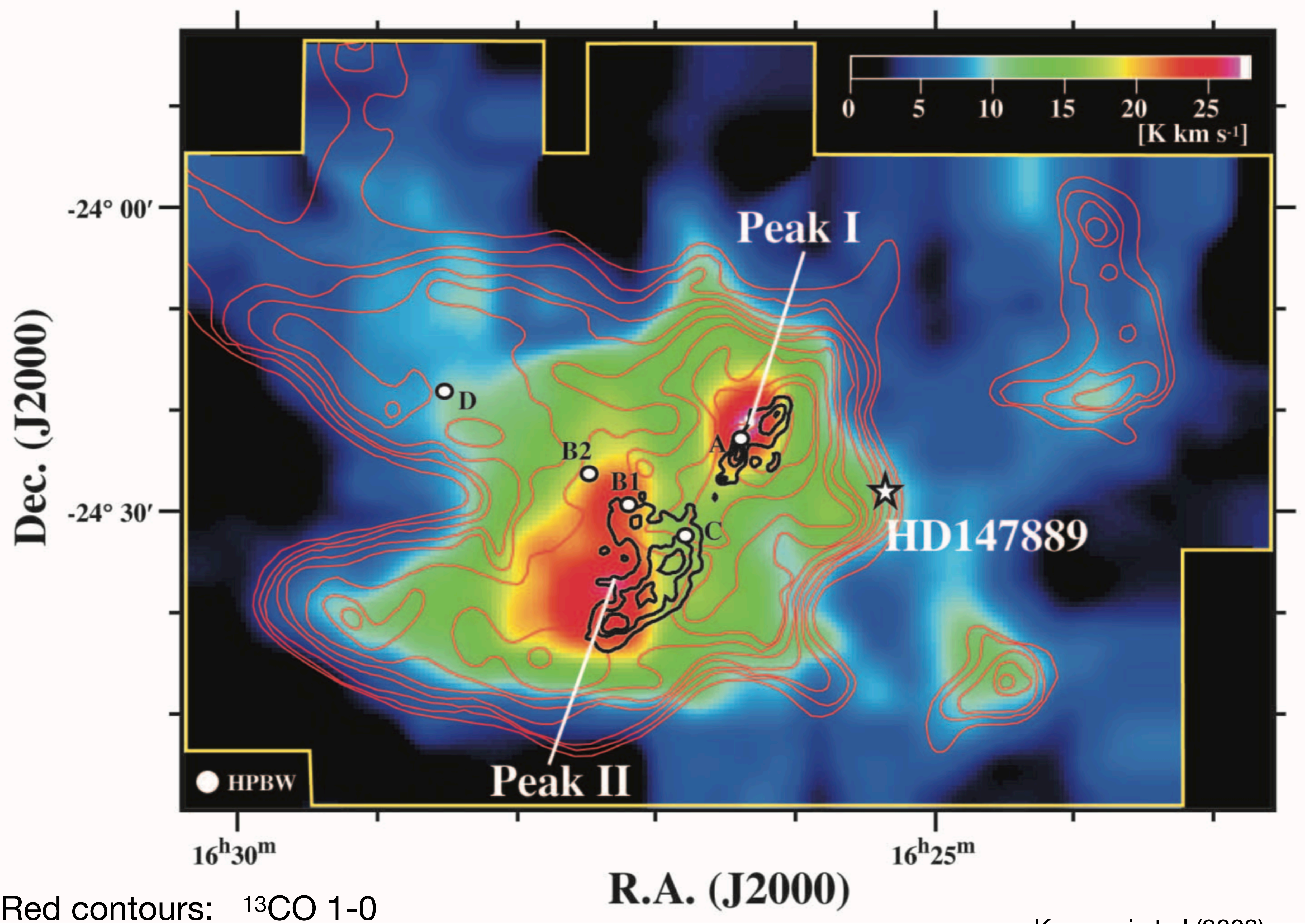
- Equating these, we find that the equilibrium C+ / C ratio is given by:

$$\frac{n_{\mathrm{C}}}{n_{\mathrm{C^+}}} = 3.4 \times 10^{-2} n_{\mathrm{e^-}} \exp\left(+3.76 A_{\mathrm{V}}\right)$$

- For densities, fractional ionizations typical of the CNM, we get $C/C^+ \sim 1$ for $A_V \sim 2$
- Transition from C^+ to C occurs in similar conditions to transition from C to CO
- C should form a “skin” around regions traced by CO
- Is this what we see?



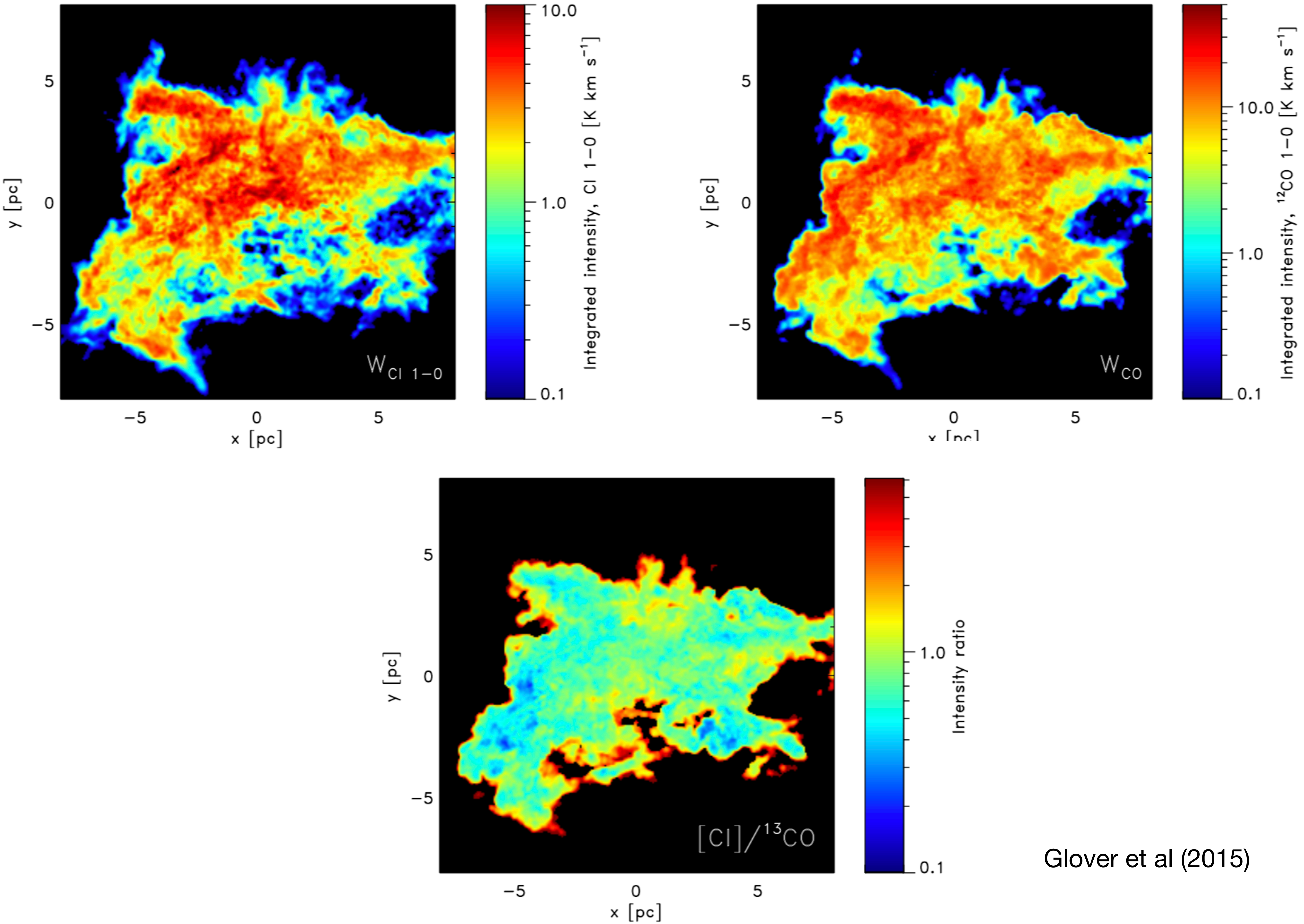
Bolatto et al (1999)



Red contours: ^{13}CO 1-0
Black contours: C^{18}O 1-0

Kamegai et al (2003)

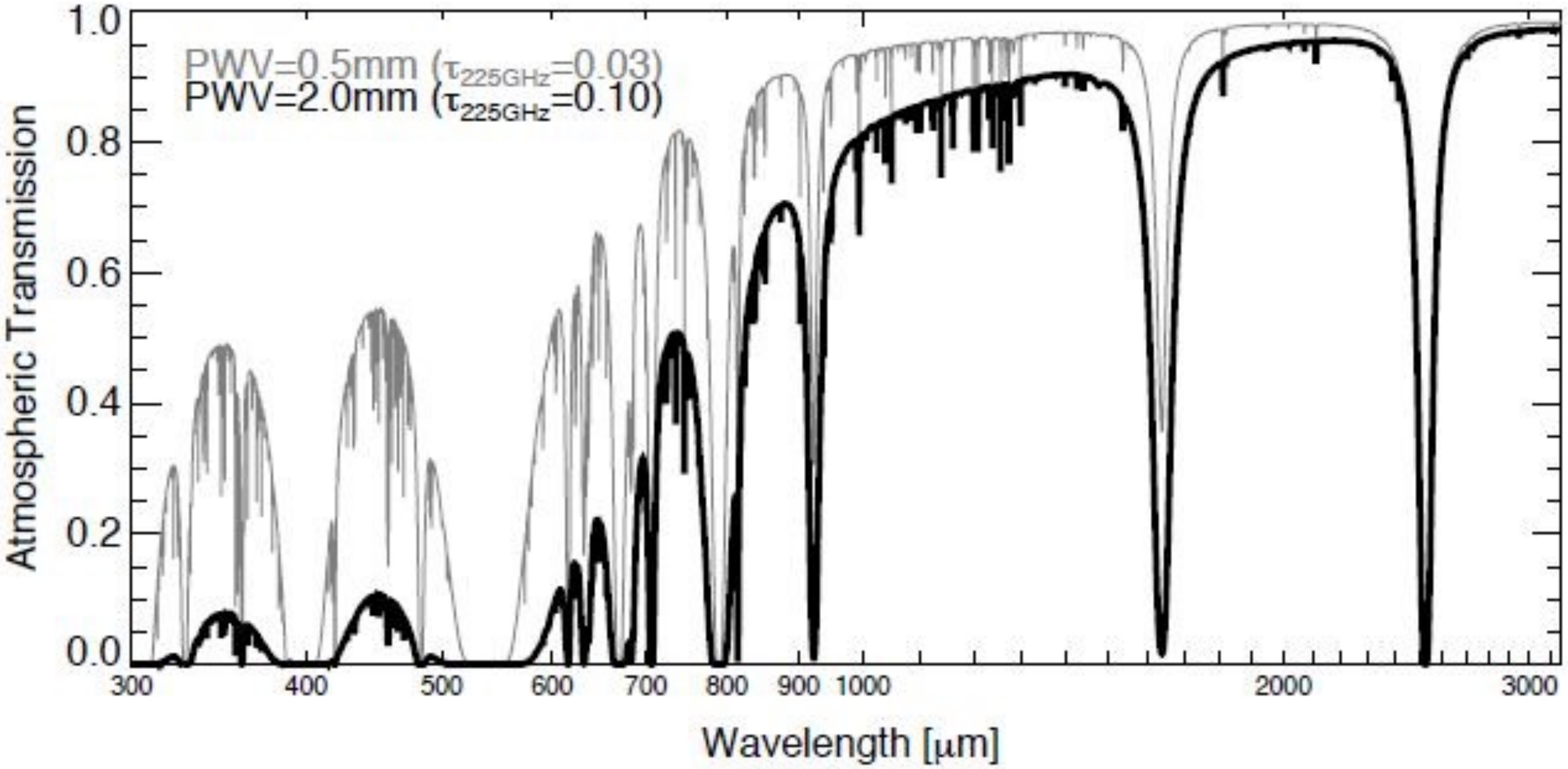
- Observations don’t look much like onion-skin toy model
- Why? Because clouds have substructure
- [CI] emission traces envelopes of many small-scale clumps, filaments within GMC
- When smoothed, result is that [CI] emission traces optically thin CO emission well
- We can reproduce this behaviour well in models that account for cloud substructure



Glover et al (2015)

- If [CI] traces cloud structure as well as CO, why don't we use [CI] as our main tracer of molecular gas?

- Answer: the atmosphere — much harder to observe the [CI] 1-0 line at 609μm than the CO 1-0 line at 2.6 mm



Casey et al (2014)

Summary

- H_2 forms primarily on dust grain surfaces
- CO forms in gas phase, via ion-neutral chemistry, largely driven by cosmic ray ionization
- H_2 destroyed by two-step Solomon process (line-driven, but only ~15% of absorptions lead to dissociation)
- CO destroyed by predissociation (still line driven, but more effective than the Solomon process)
- Shielding of H_2 dominated by self-shielding, dust
- Shielding of CO dominated by dust

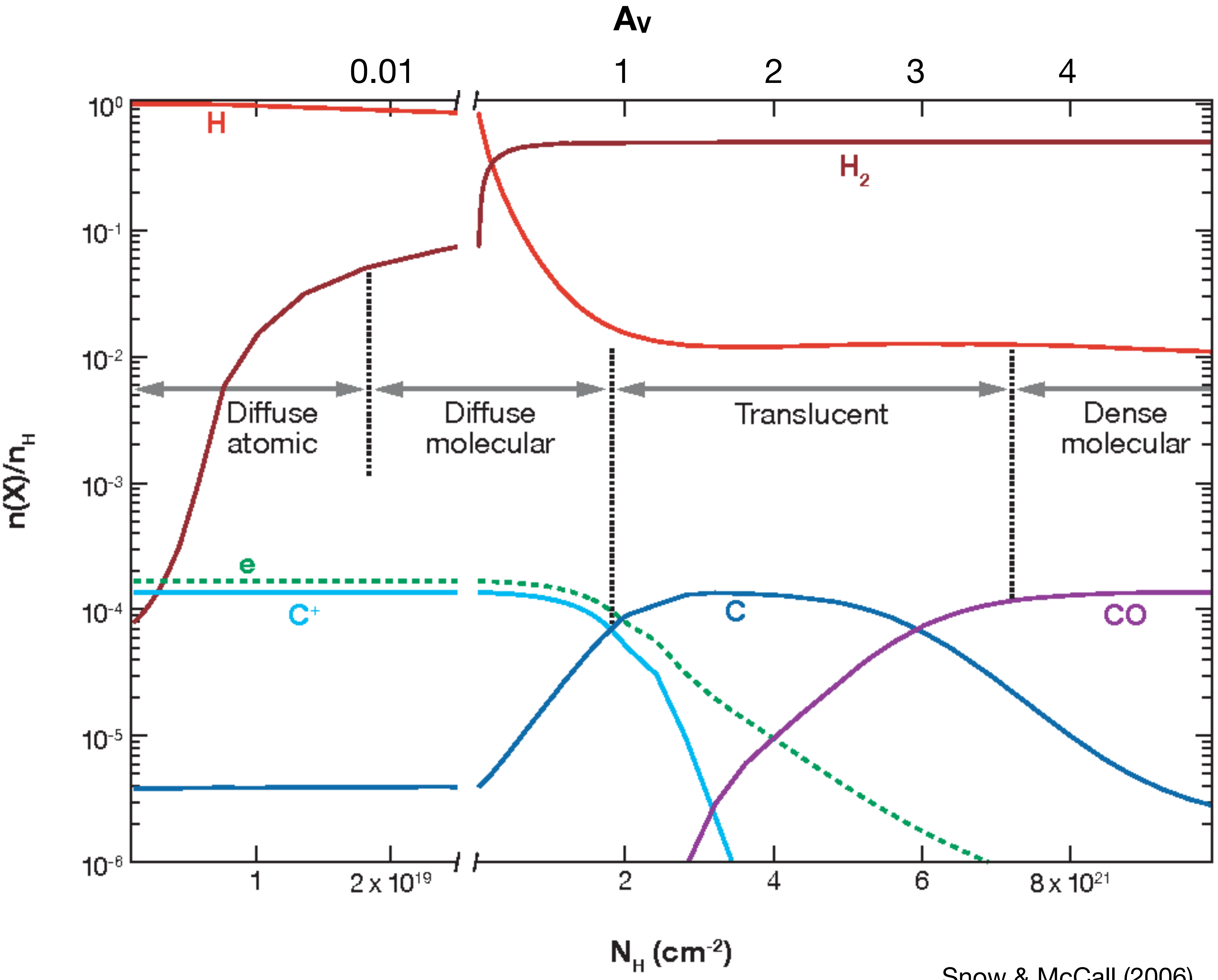
- Transition from H to H_2 occurs once gas sufficiently shielded that destruction rate ~ formation rate

- In the local ISM, this requires $A_V \sim 0.1$

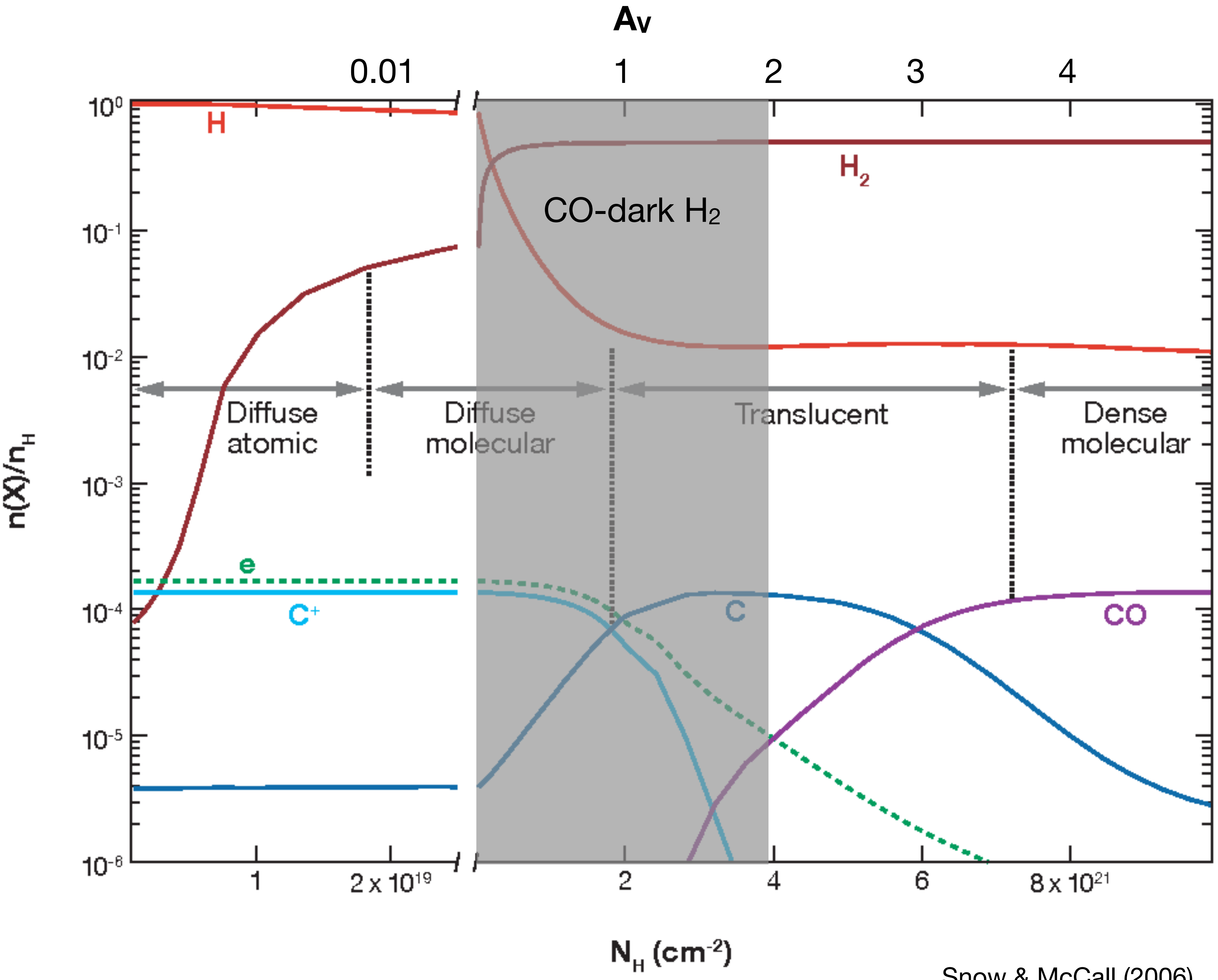
- Transition from C^+/C to CO requires more dust shielding, occurs at $A_V \sim 1 - 2$

- Difference in critical A_V → existence of CO-dark H_2 (diffuse & translucent clouds, envelopes of GMCs)

- Transition from C^+ to C requires A_V only slightly smaller than for transition to CO — C traces CO in GMCs



Snow & McCall (2006)



Snow & McCall (2006)

- Classic layered photodissociation region (PDR) structure good description of behaviour of slabs, spheres

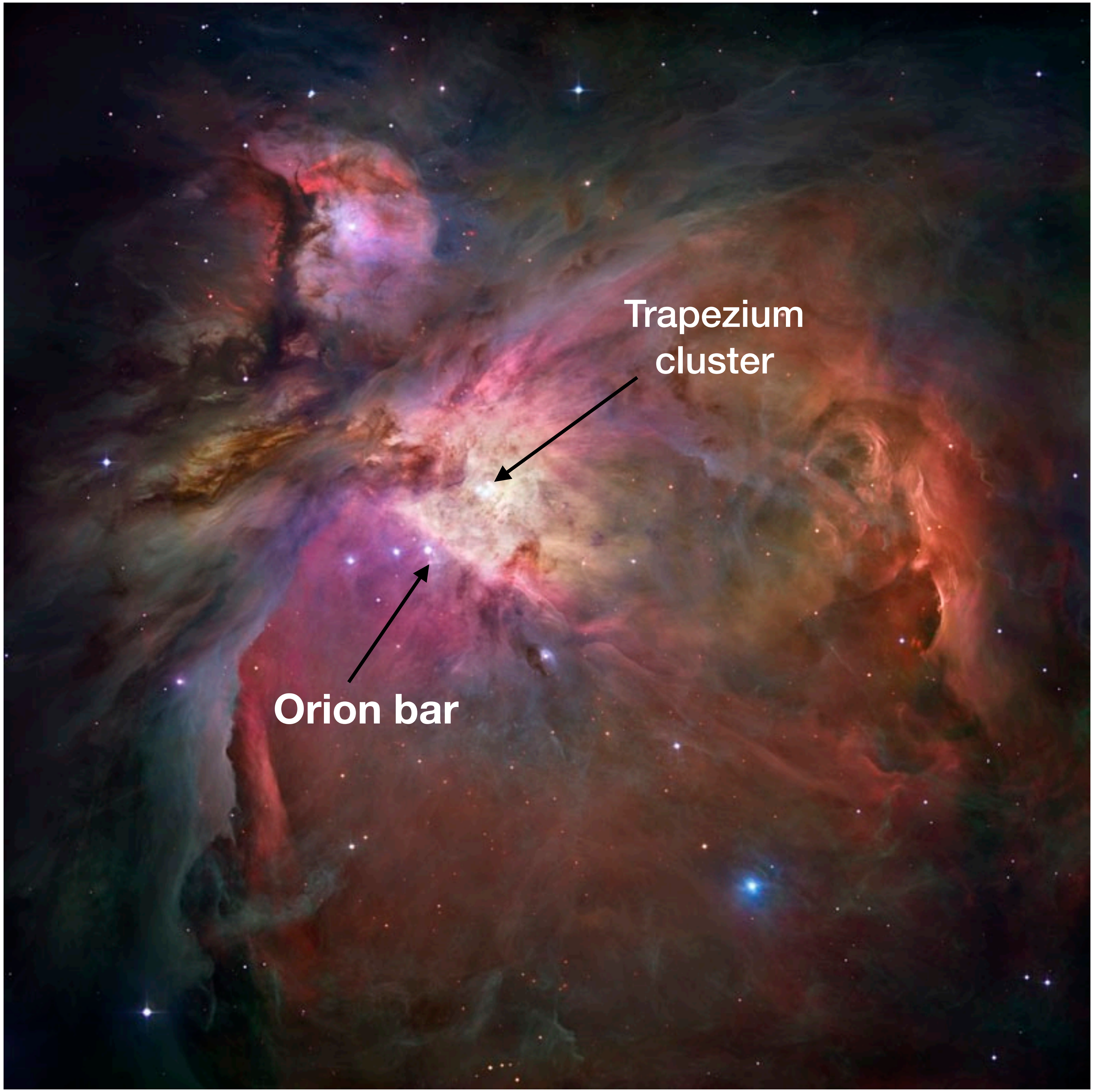
- Real GMCs are clumpy, so don’t look much like this idealized structure

- However, we do see something like this if we zoom in on individual substructures

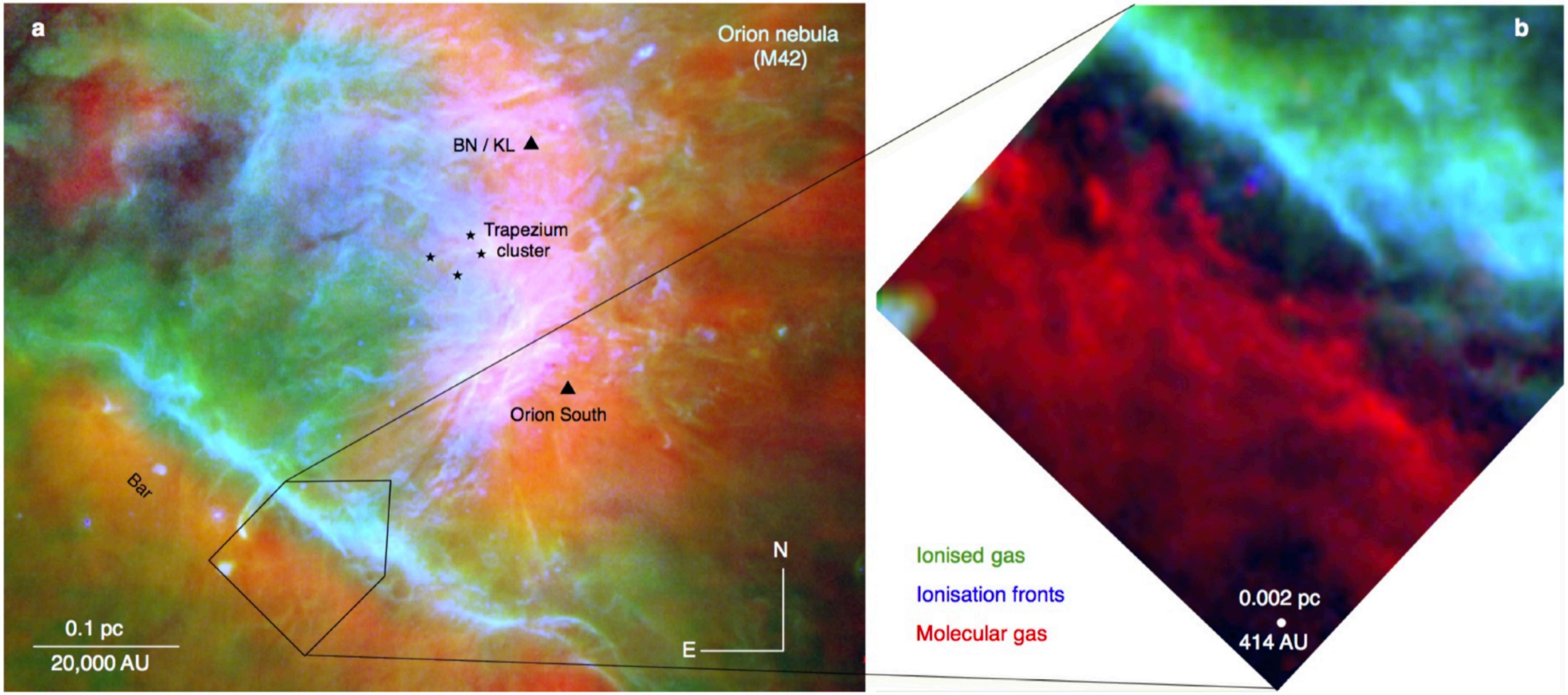
Example: the Orion Bar

Credit: NASA/ESA/M. Robberto

Example: the Orion Bar



Credit: NASA / O’Dell & Wong



Green: [SII] 6731Å
Blue: [OI] 6300 Å
Red: HCO^+ J=3-2