H_2 in Space©

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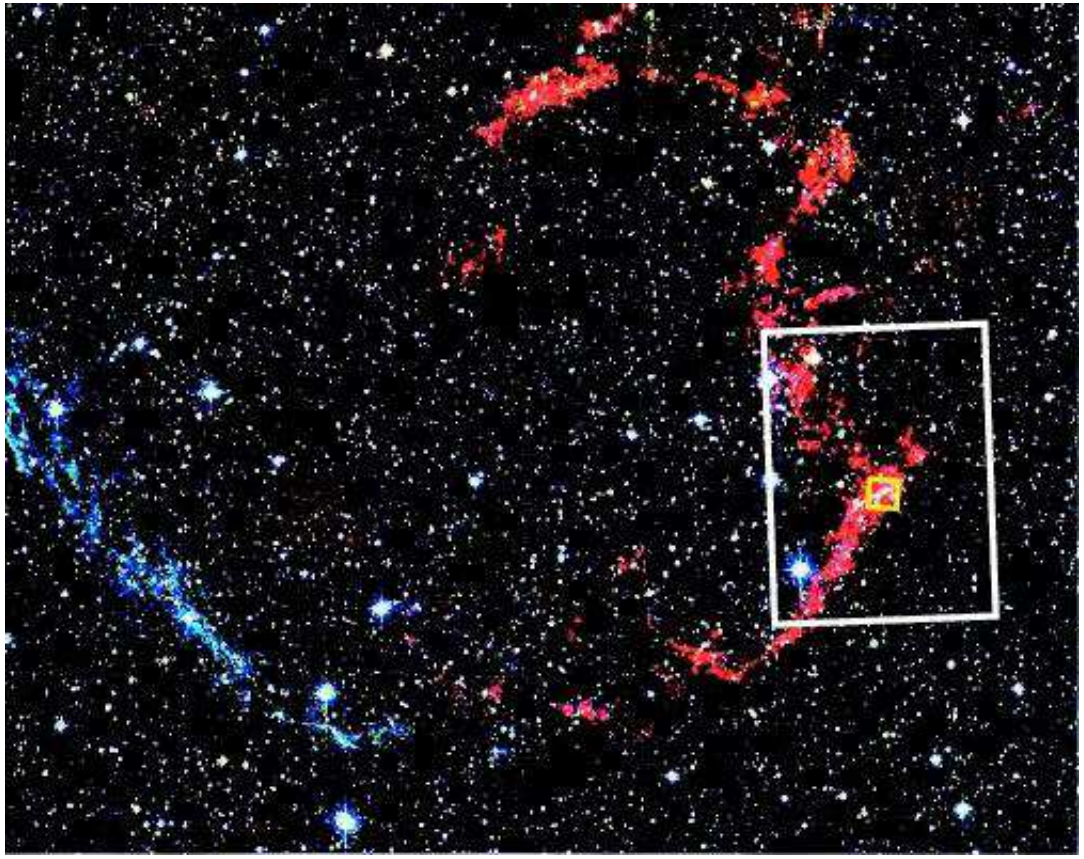
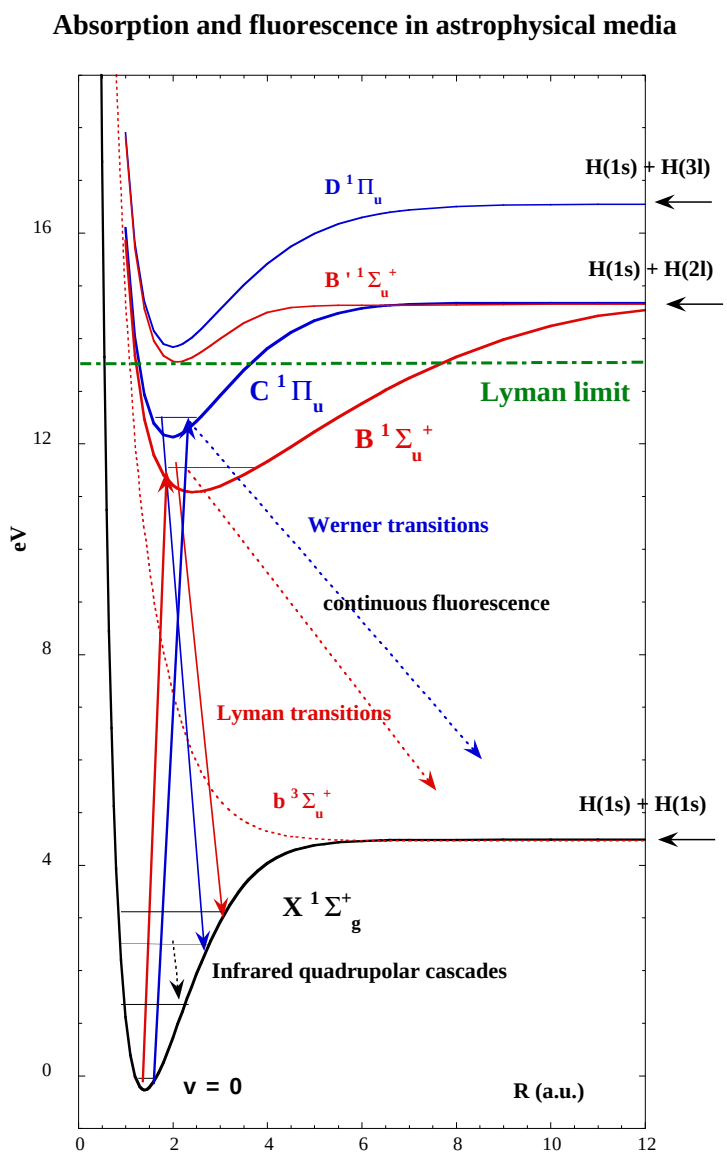
October 2014

H_2 in Space



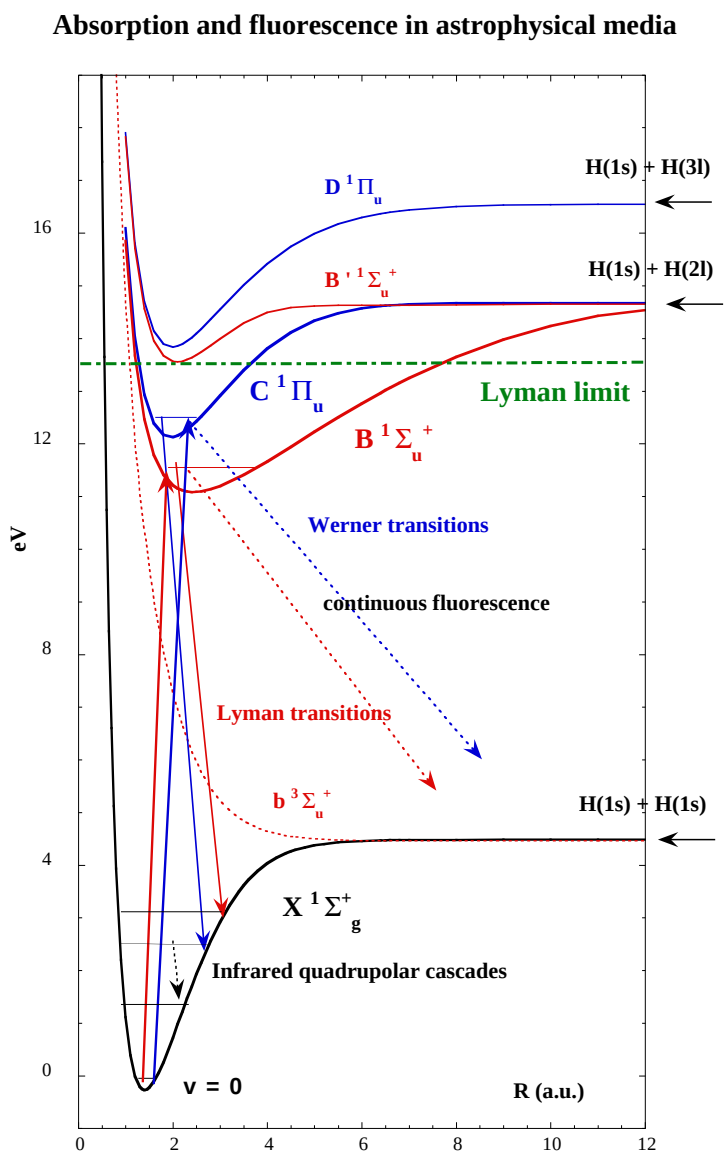
Neufeld & Yuan, ApJ, 2008 - S443 SNR
Red: K band $H_2\, 1-0\, S(1)$

H_2 Structure



Homonuclear and light ⇒

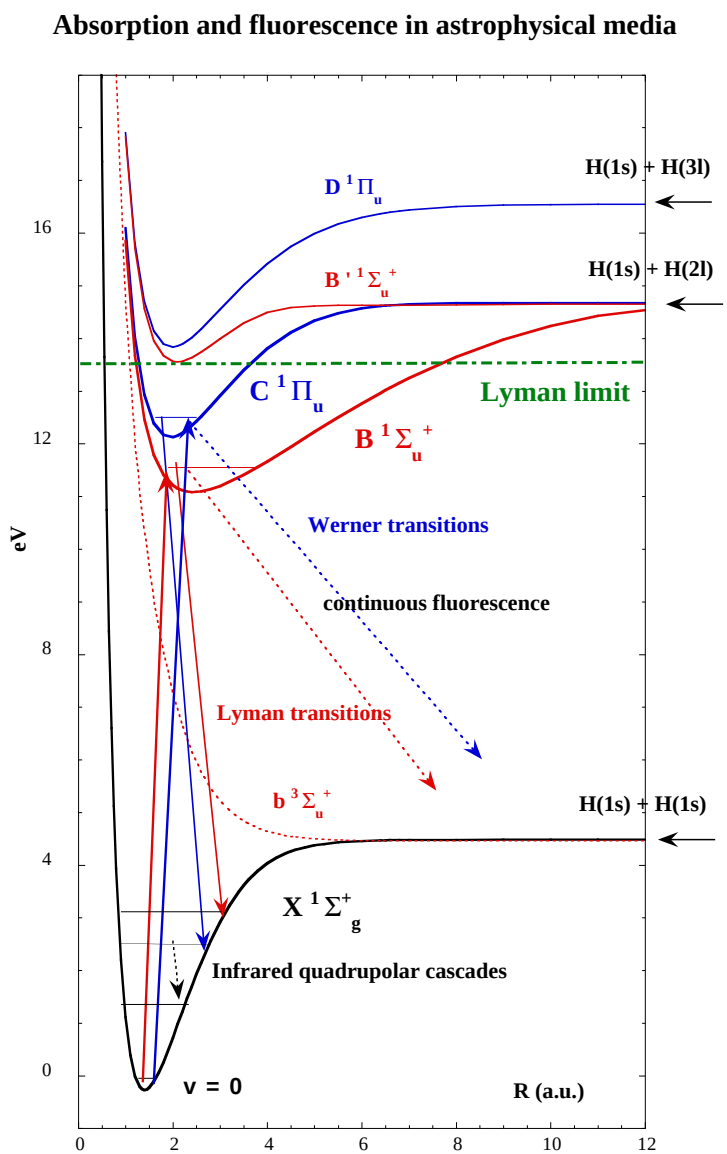
H_2 Structure



Homonuclear and light ⇒

- No dipolar transitions

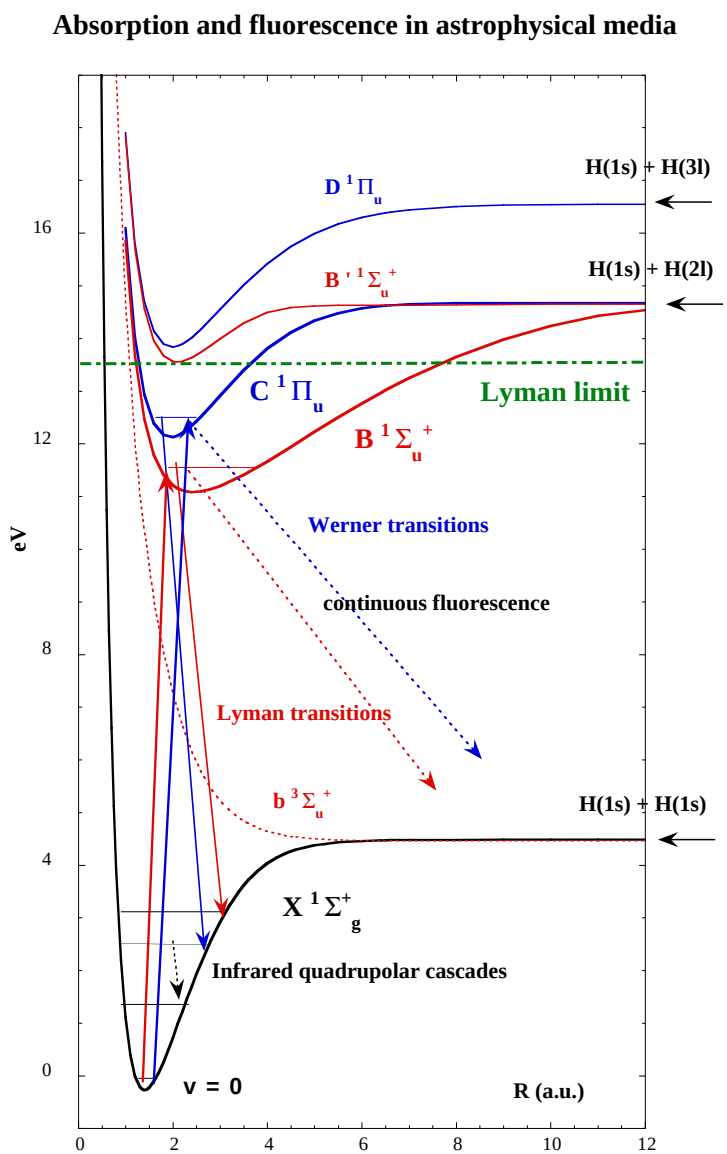
H_2 Structure



Homonuclear and light ⇒

- No dipolar transitions
- No formation in gas phase

H_2 Structure



Homonuclear and light $\Rightarrow$

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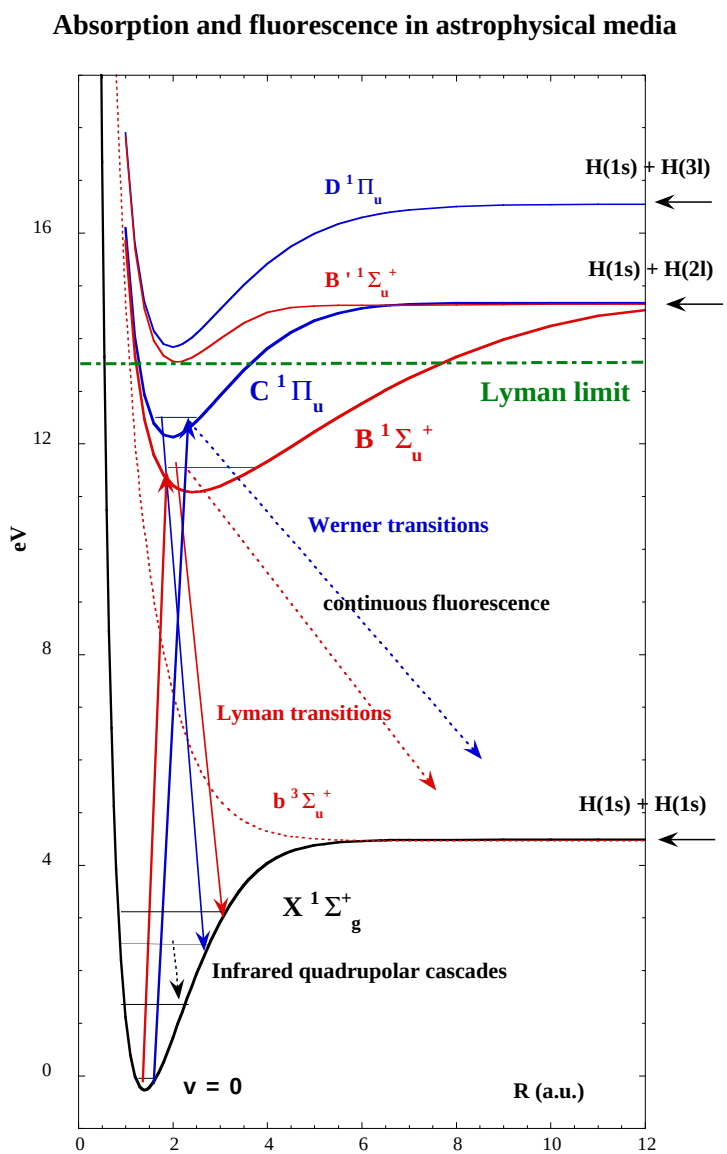
- No formation in gas phase
- No direct UV dissociation

H_2 Structure



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- Formation releases $4.5\,\mathrm{eV}$

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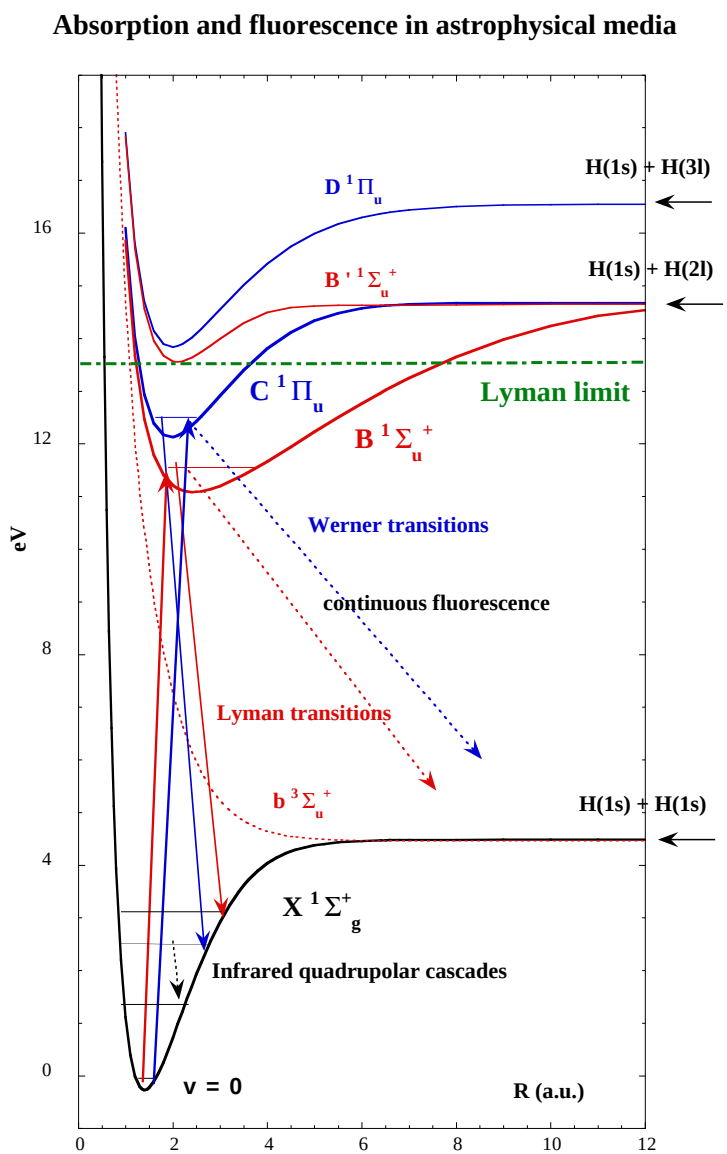

Homonuclear and light $\Rightarrow$

- No dipolar transitions
- No formation in gas phase
- No direct UV dissociation
- Formation releases $4.5\,\mathrm{eV}$
- Lowest transitions are high:
  $J = 2 \rightarrow 0 : \; 509.8\,\mathrm{K}$
  $J = 3 \rightarrow 1 : \; 844.6\,\mathrm{K}$
- Source of secondary photons.

H_2 Destruction

- UV transitions:
  - Pumping in Lyman ($B\,^1\Sigma_u^+$) and Werner systems ($C\,^1\Pi_u$)
  - Discrete transition, either to $X\,^1\Sigma_g^+$ (88 %) or to the continuum.
  - In free space, for Draine's field $k_D^0 = 5.8\,10^{-11}\,\mathrm{s}^{-1}$.

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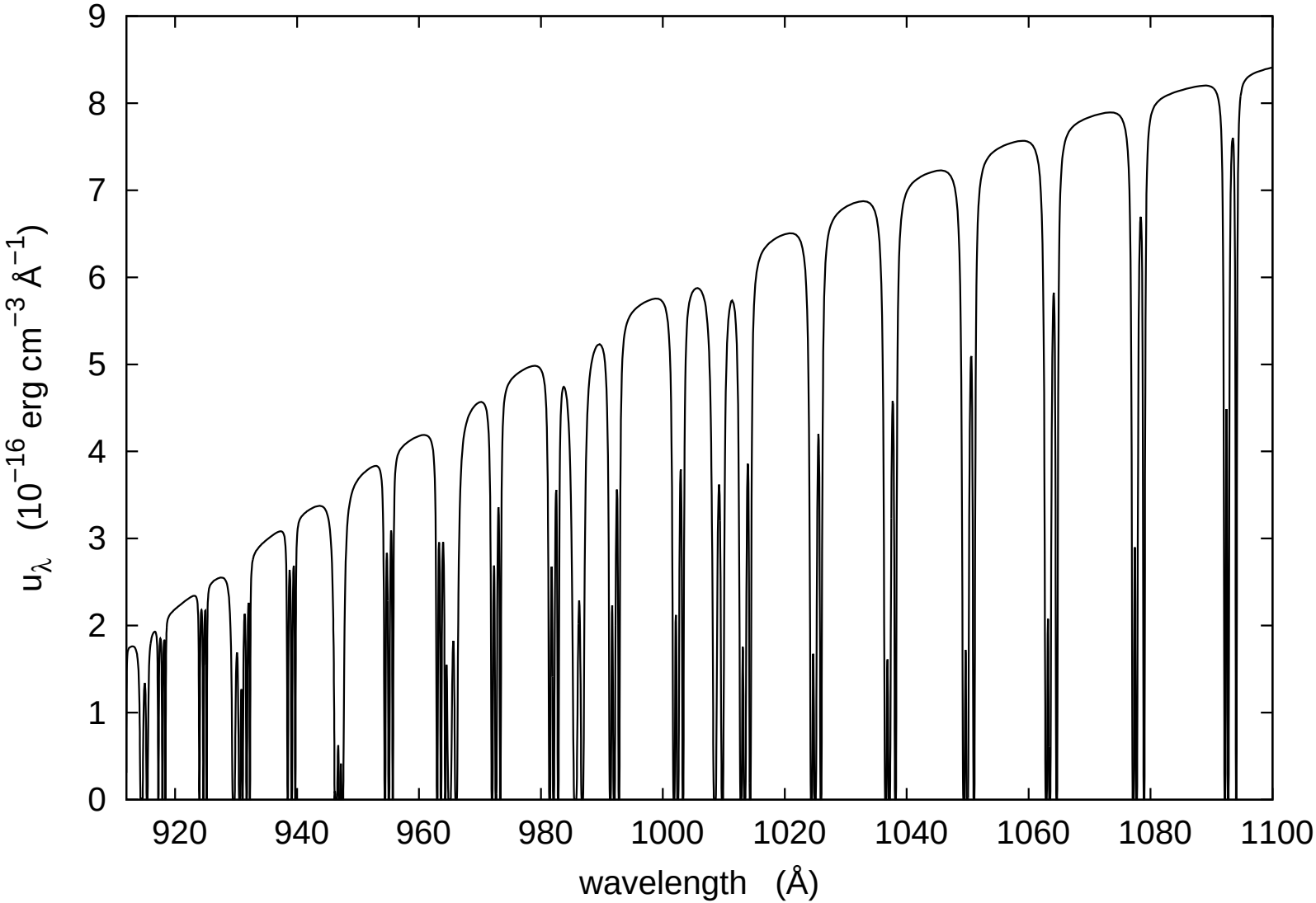
  - Discrete transition, either to $X\,^1\Sigma_g^+$ (88 %) or to the continuum.
  - In free space, for Draine's field $k_D^0 = 5.8\,10^{-11}\,\mathrm{s}^{-1}$.
- Within a cloud:

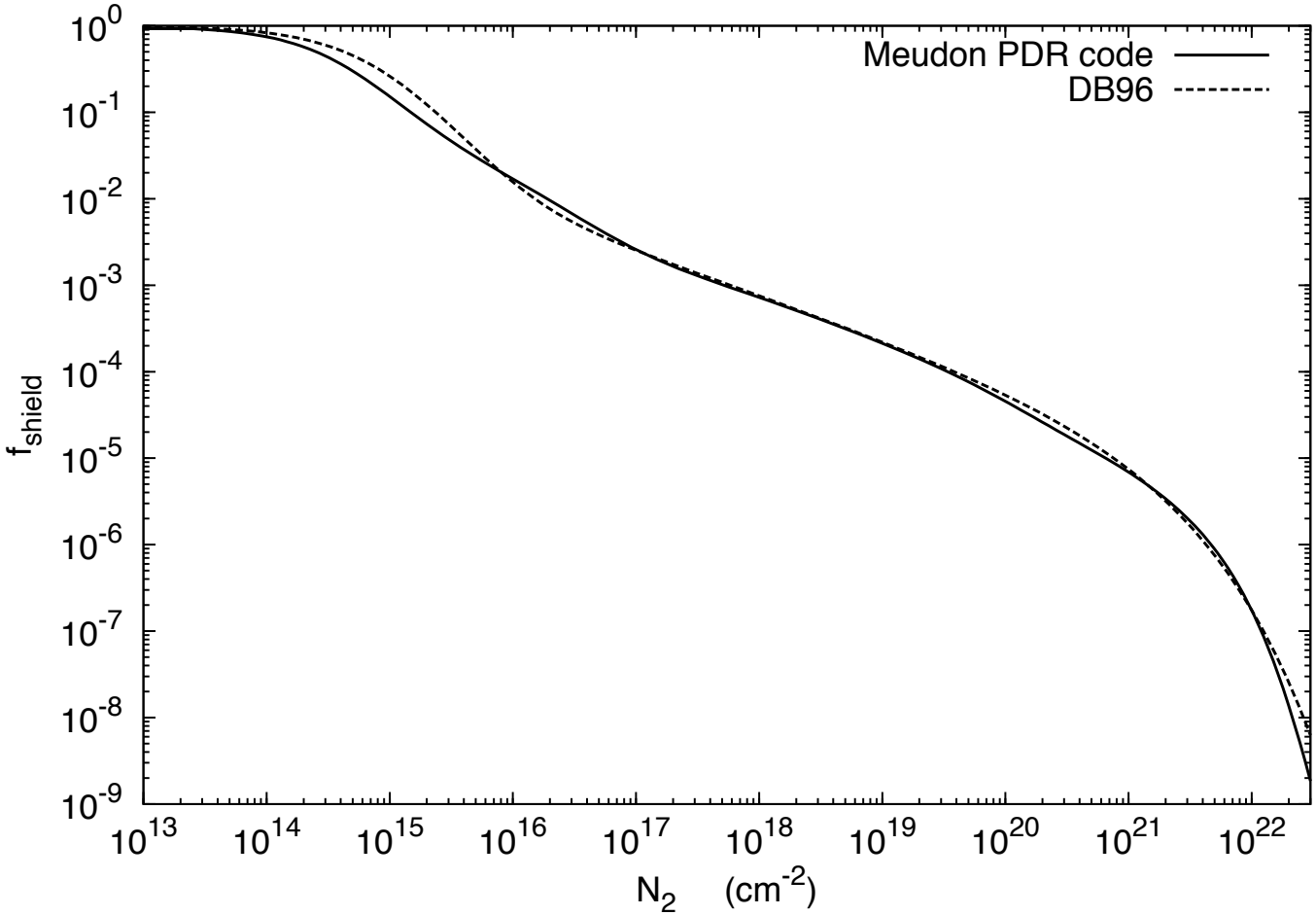
$$k_D = k_D^0\, I_{UV}\, \exp\left(-\sigma_g\left(N_1 + 2\,N_2\right)\right)\, f_{shield}(N_2)$$

N_1 & N_2: Column densities of H and H_2,
σ_g: grain absorption, I_{UV}: radiation field strength.

H_2 Self-Shielding



H_2 Self-Shielding



Self-shielding function: $f_{shield} = \frac{1}{\sigma_d}\frac{dW_d}{dN_2}$. $\sigma_d \simeq 2.36\,10^{-3}\,\mathrm{cm}^2\,\mathrm{Hz}$

H_2 Formation

- Formation on grains ⇒ by default

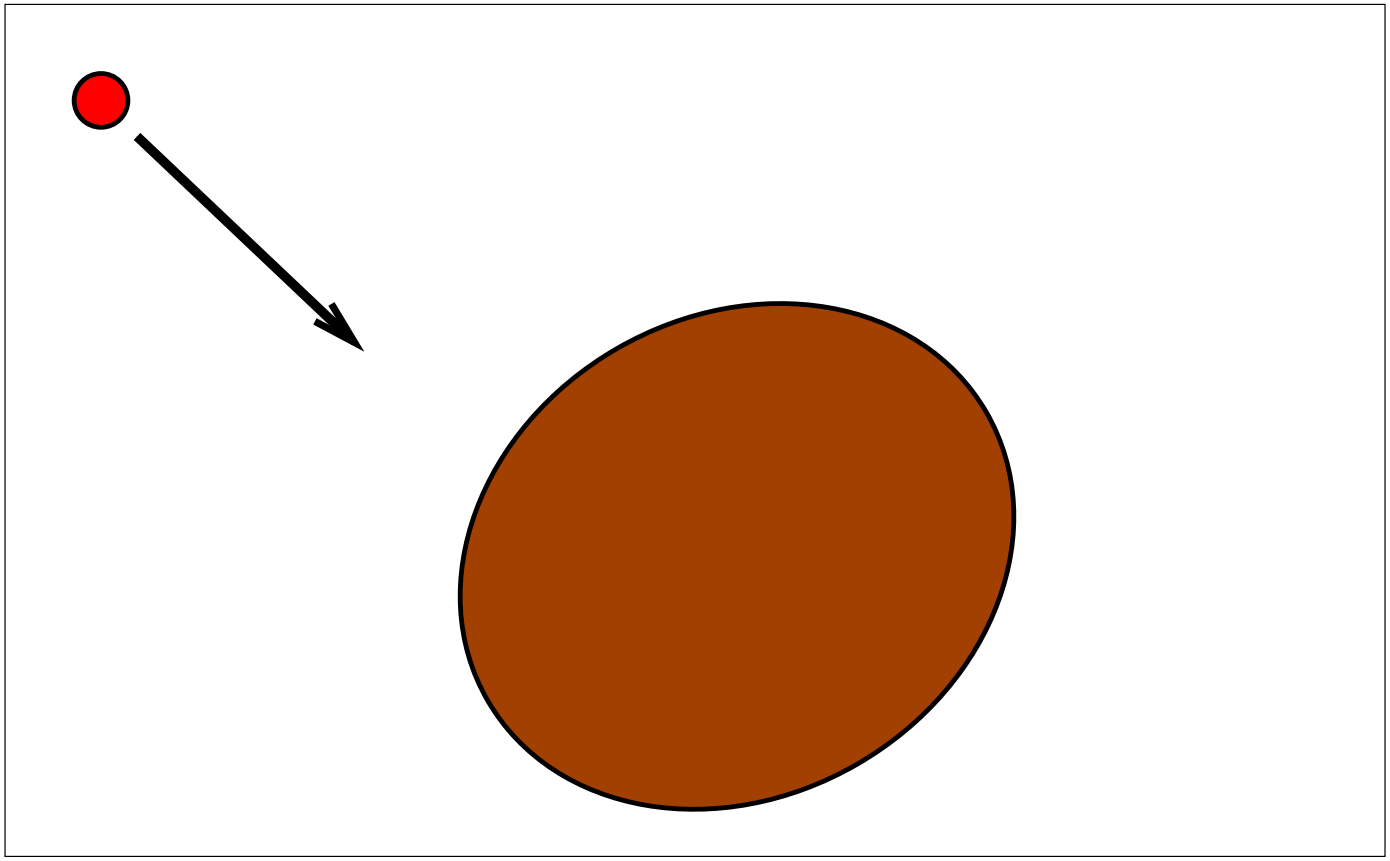
$$\frac{d[\mathrm{H_2}]}{dt} = R_f \, n_{\mathrm{H}} \, n(\mathrm{H})$$

- Copernicus (Jura, (1975) ApJ 197, 575):

$$R_f \sim 3\,10^{-17}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

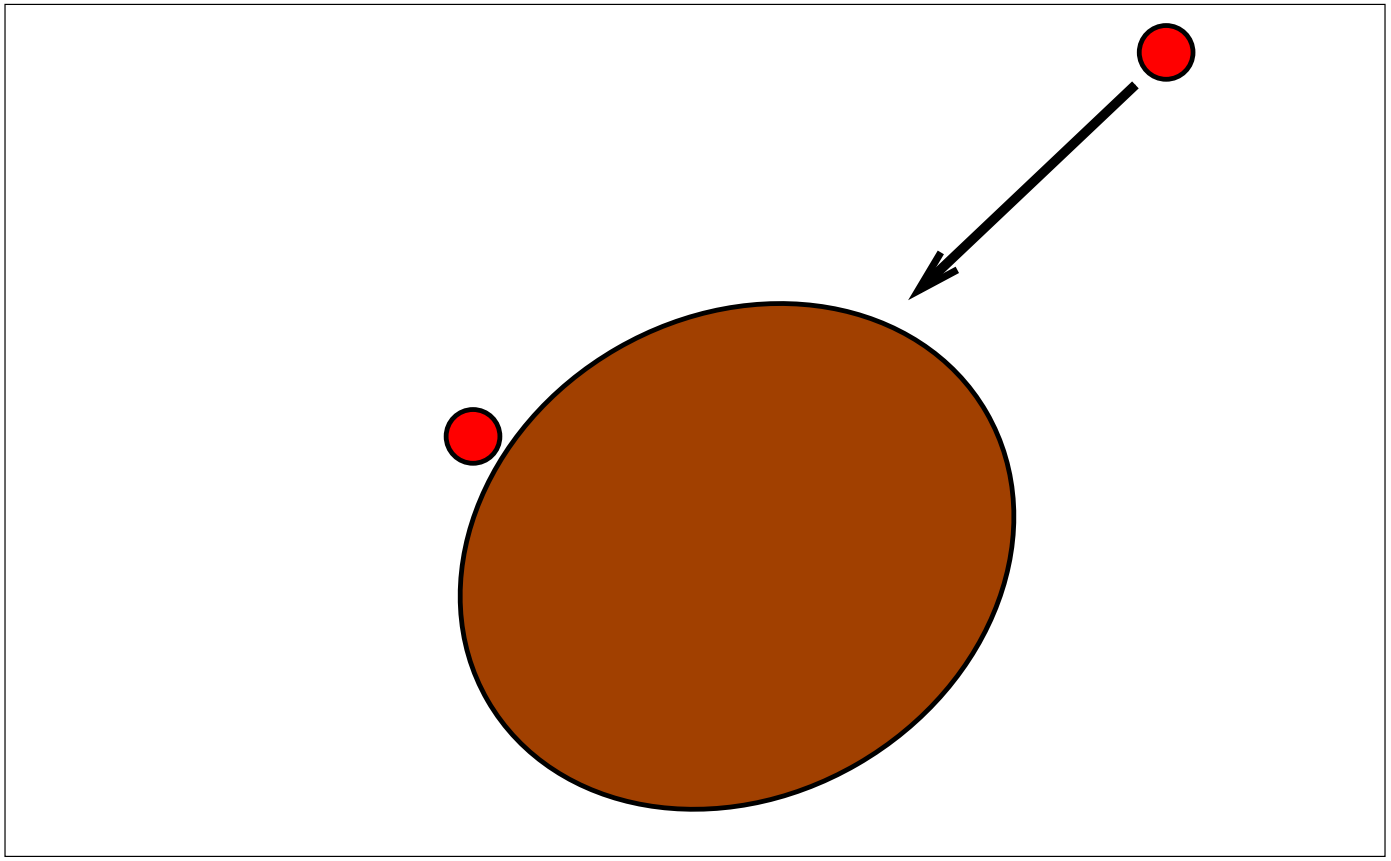
- Details still under investigation
  (see talk by Emeric Bron, following mine)

H_2 formation(traditional view)



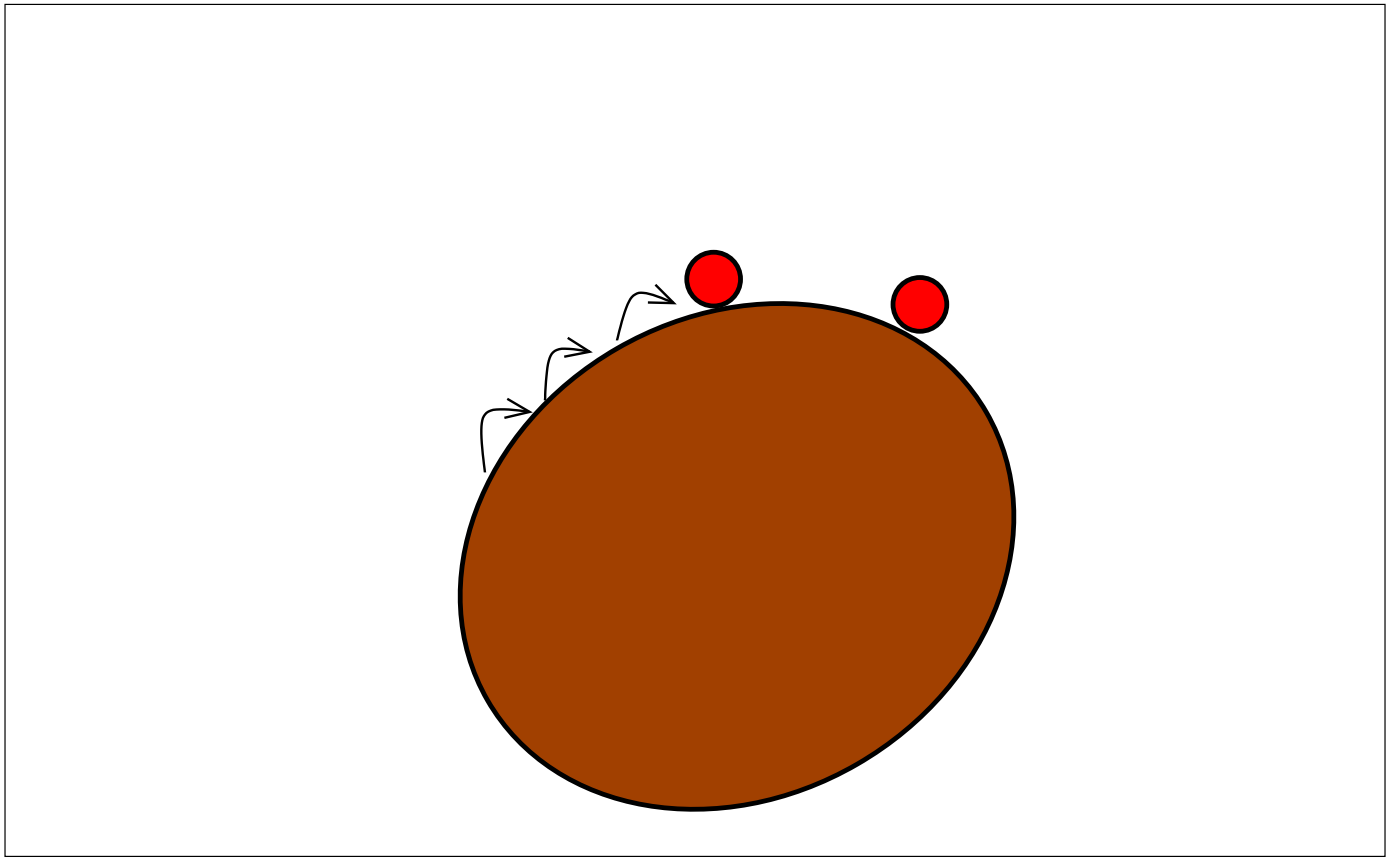
- Rate: ?

H_2 formation (traditional view)



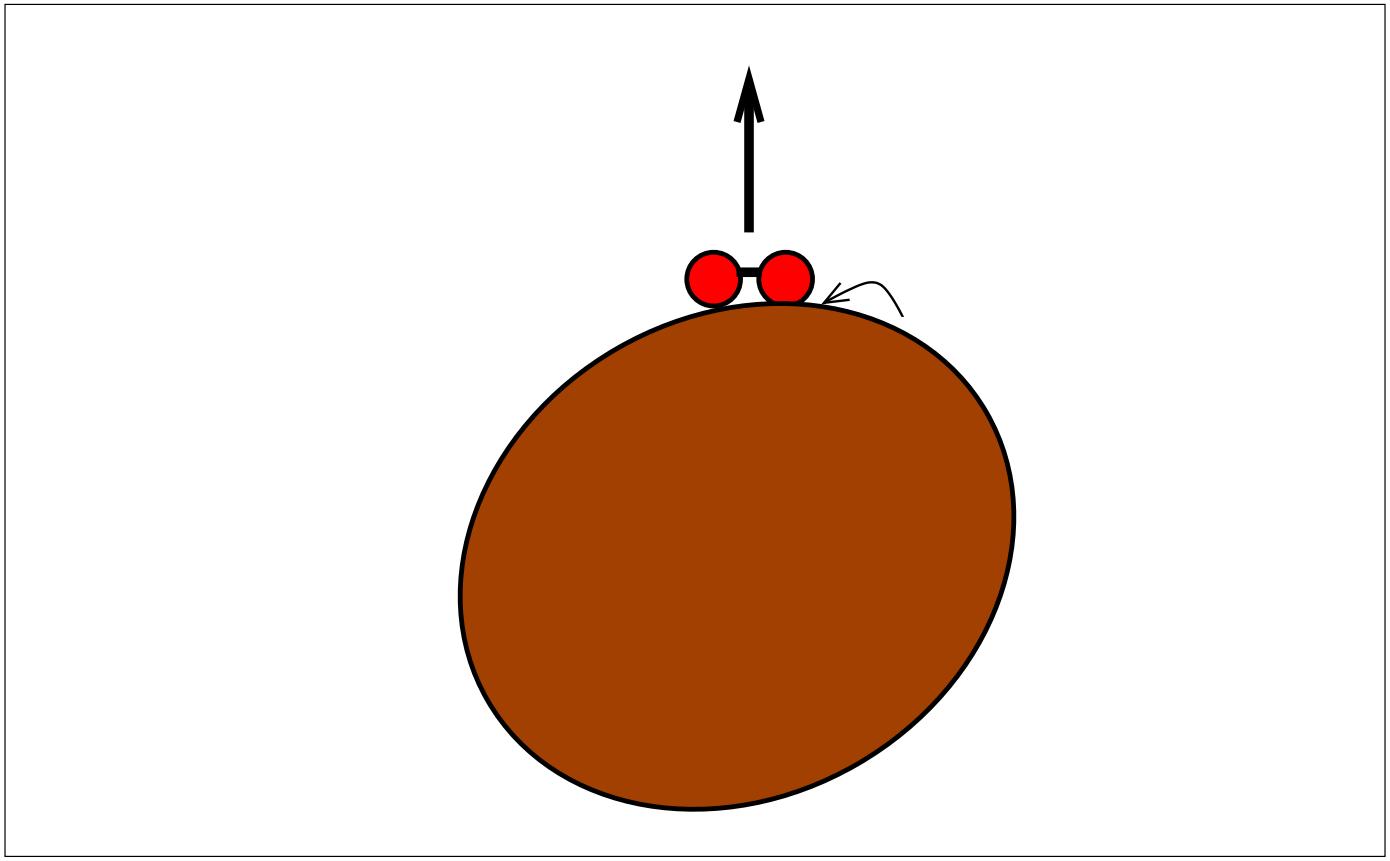
- Rate: known from observations

H_2 formation (traditional view)



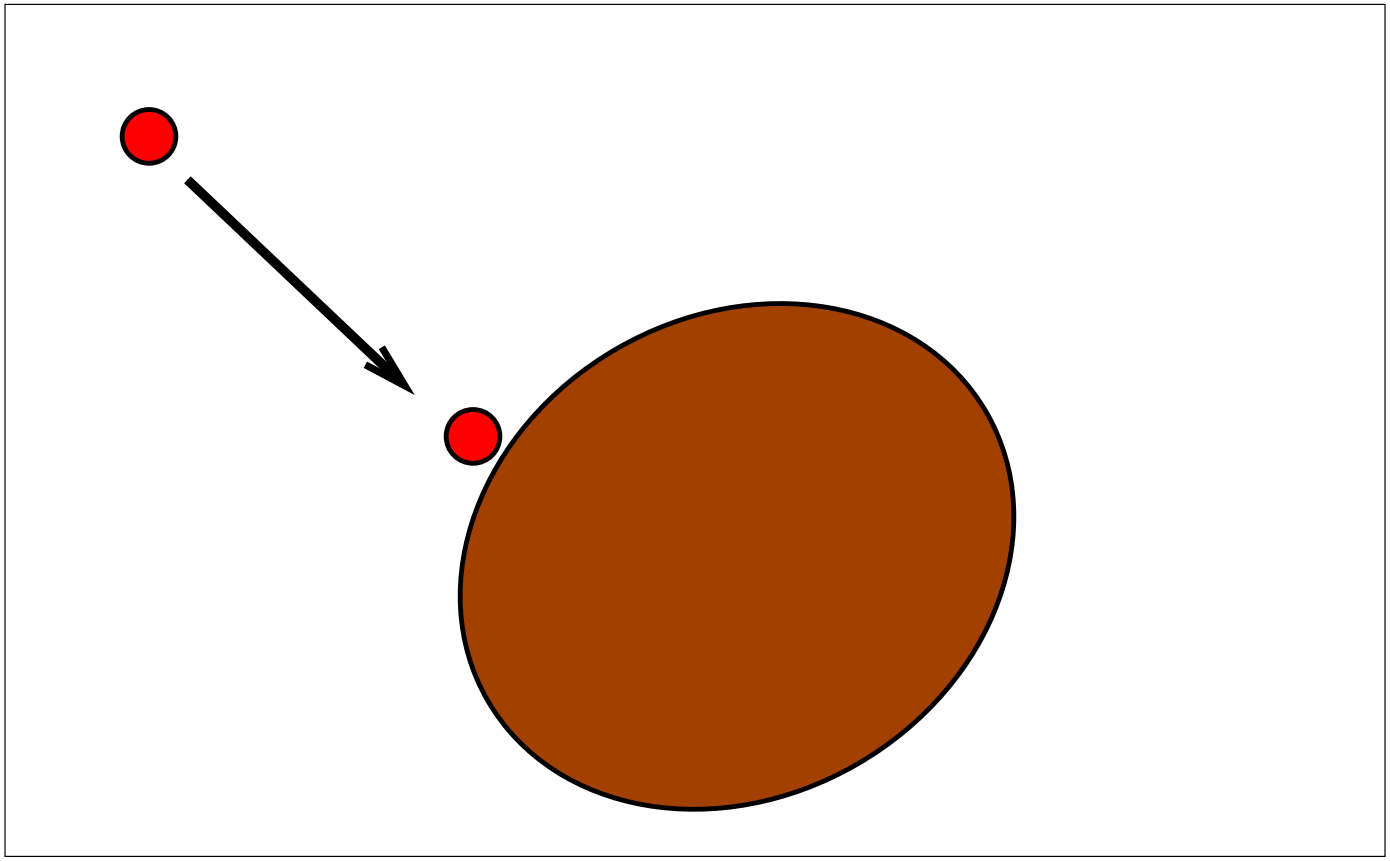
- Rate: Proportional to v_T, $n(\mathrm{H})$ and n_{gr}

H_2 formation (traditional view)



- Rate: $\sim 3\,10^{-17}\sqrt{\frac{T}{100}}\,Z'\,n_H\,n(\mathrm{H})\,\mathrm{cm}^{-3}\,\mathrm{s}^{-1}$
  - Langmuir-Hinshelwood (LH)

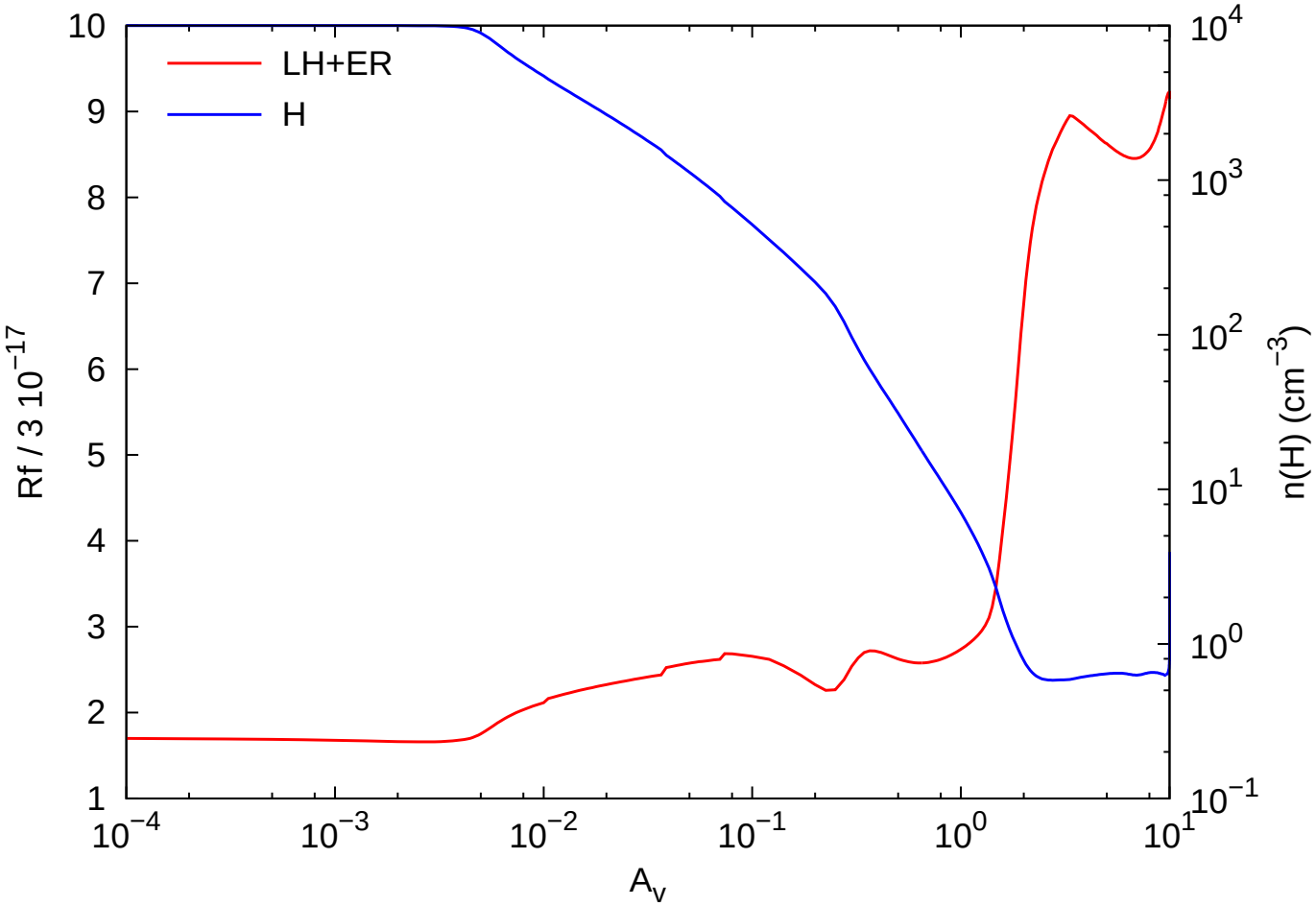
H_2 formation (traditional view)



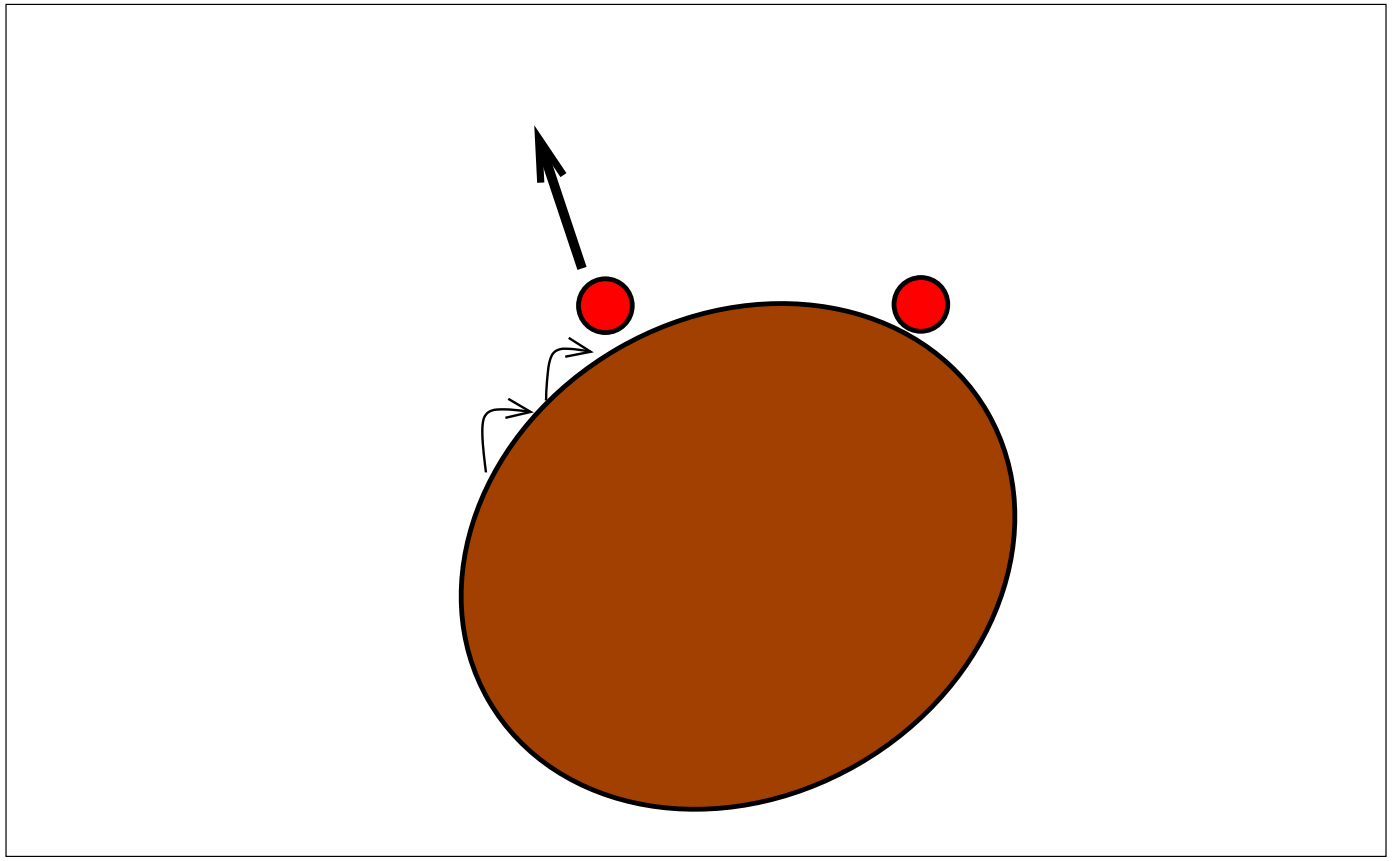
- Rate: $\sim 3\,10^{-17}\sqrt{\frac{T}{100}}\,Z'\,n_H\,n(\mathrm{H})\,\mathrm{cm}^{-3}\,\mathrm{s}^{-1}$
  - Eley-Rideal (ER)

H_2 formation - Full computation

- $n_{\mathrm{H}} = 10^4\,\mathrm{cm}^{-3}$, Mathis $\times 100$

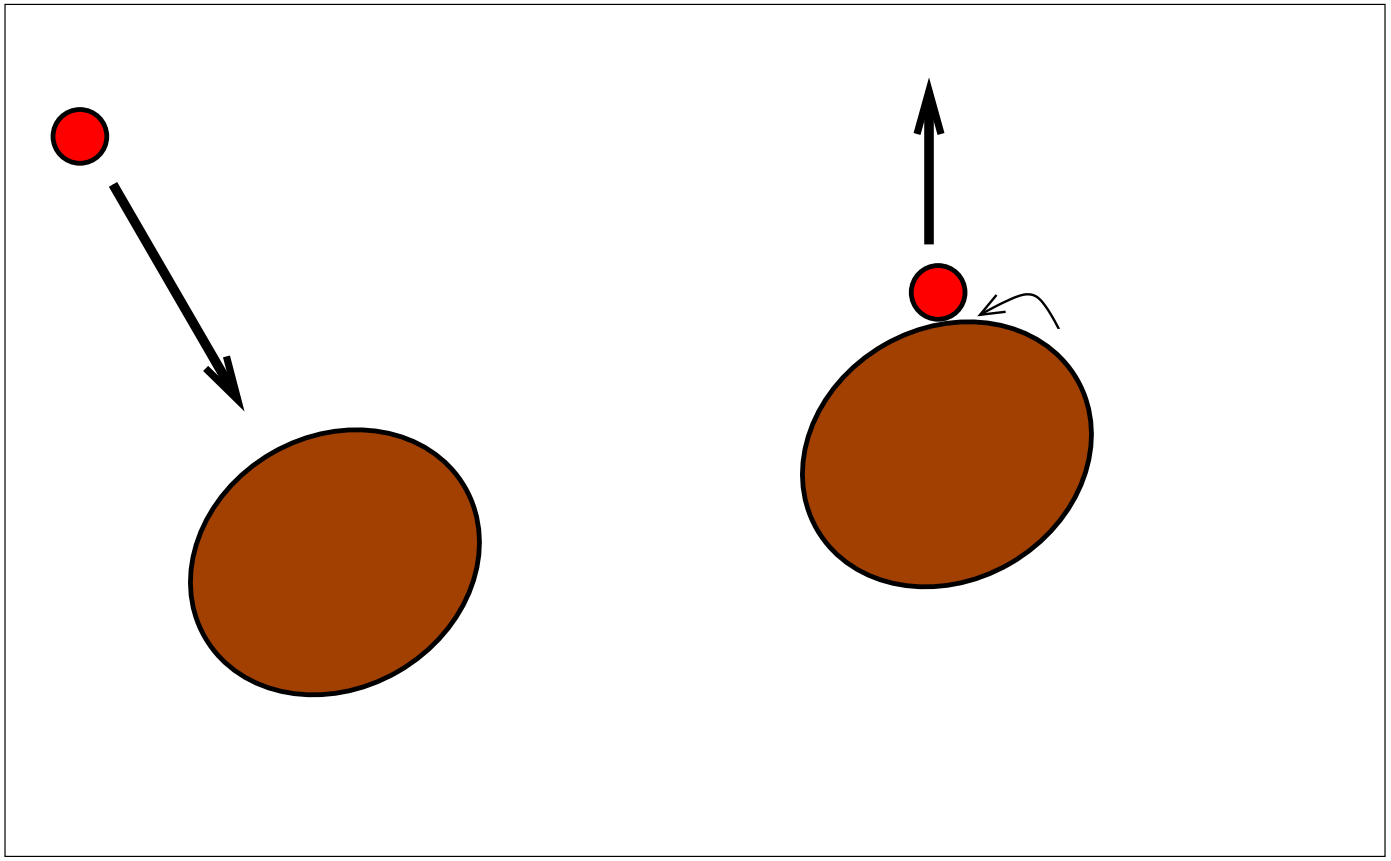


H_2 formation - Problem I



- Evaporation is fast from hot grains.

H_2 formation - Problem II



- Grains are **very** small.

H_2 formation - Fluctuations rescue!

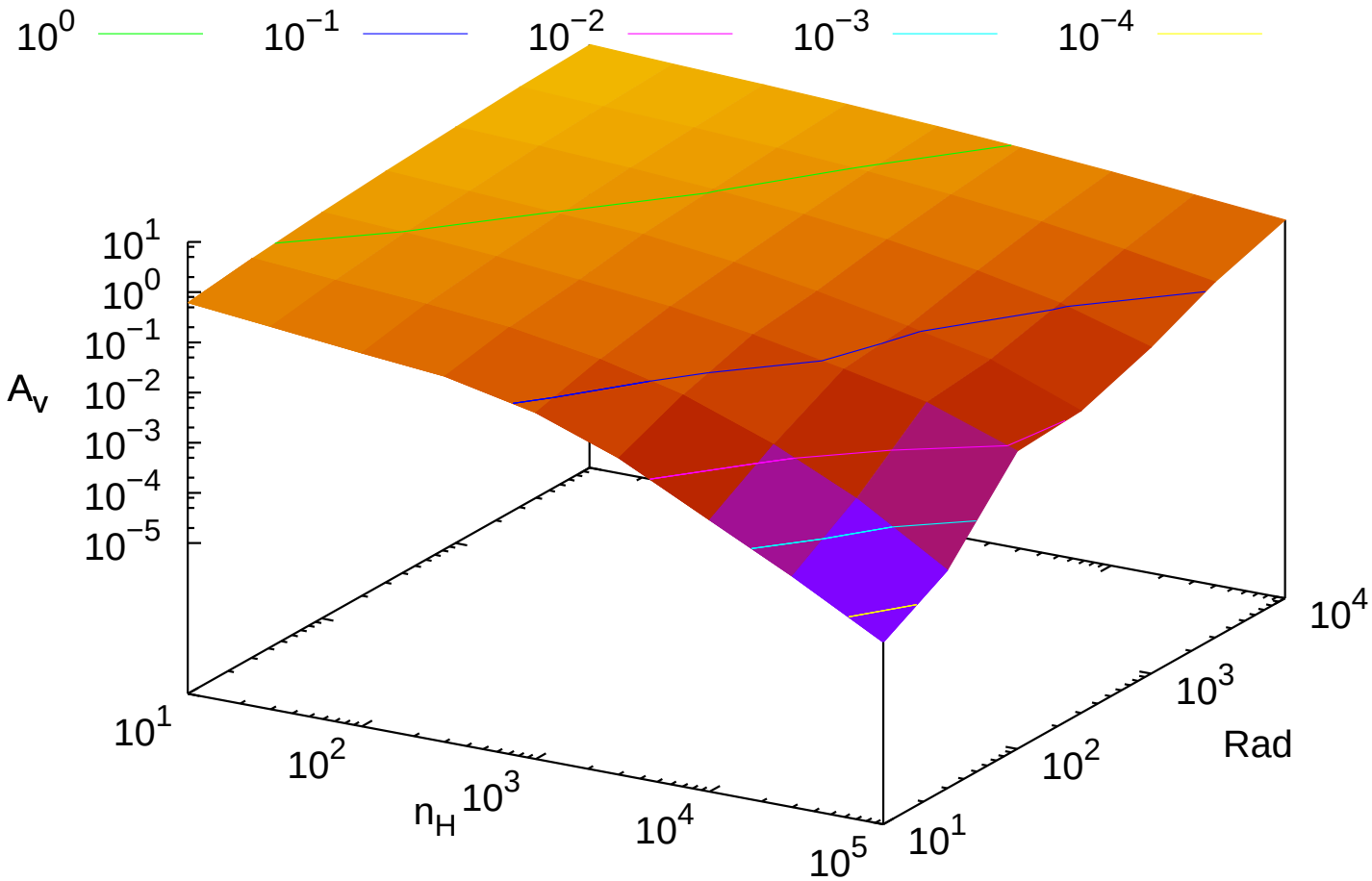
- Requires statistical computation of fluctuations
- See following presentation by Emeric Bron
  Bron et al. (2014), A&A 569, 100

H_2 formation - Fluctuations rescue!

- Requires statistical computation of fluctuations
- See following presentation by Emeric Bron
  Bron et al. (2014), A&A 569, 100
- Take home message:
  - Crude evaluation: rate equations OK (e.g. in MHD codes).
  - Grain physics: full statistical formalism required.

H/H_2 transition

- To first order, depends on I_{UV}/n_H:



H/H_2 transition

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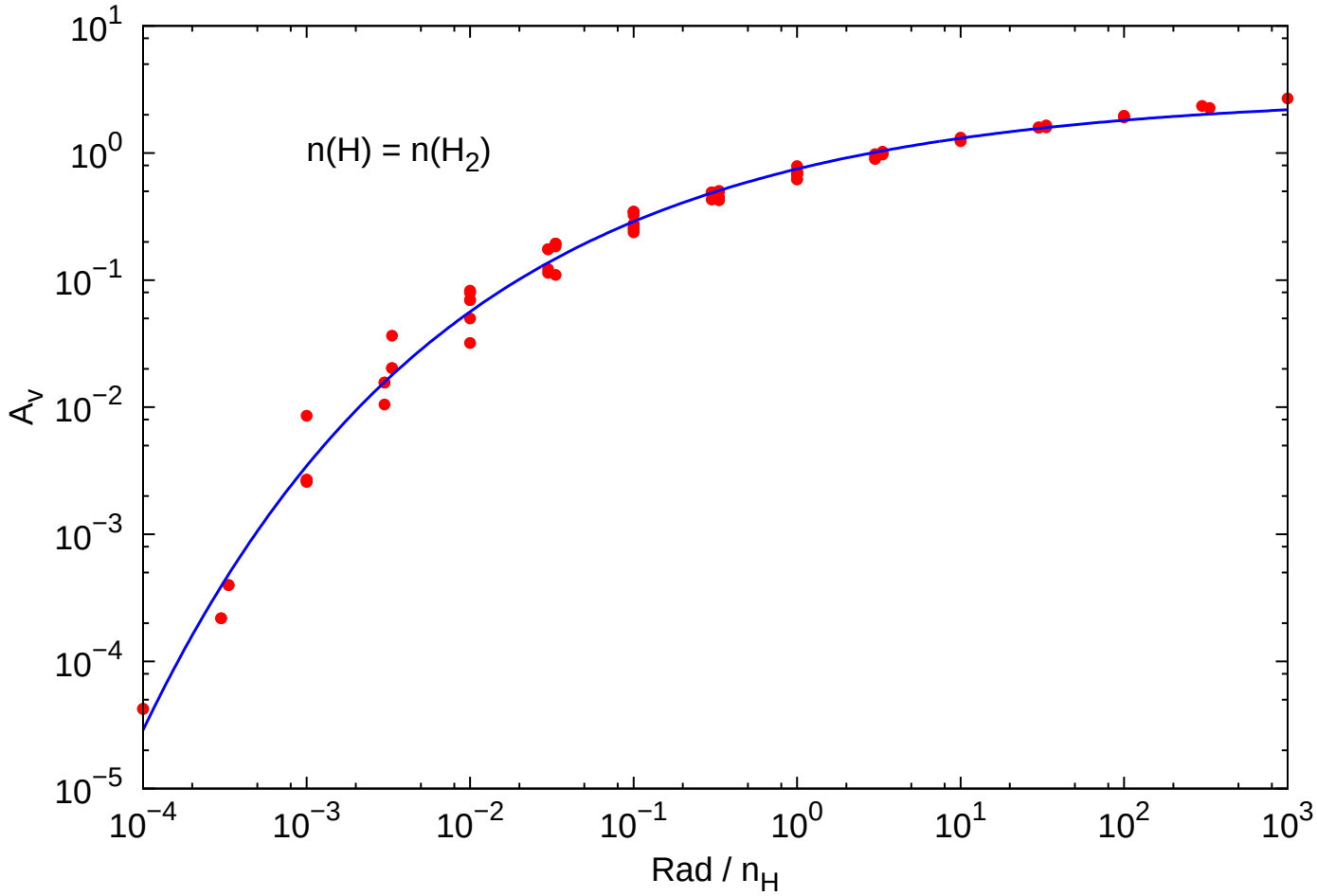
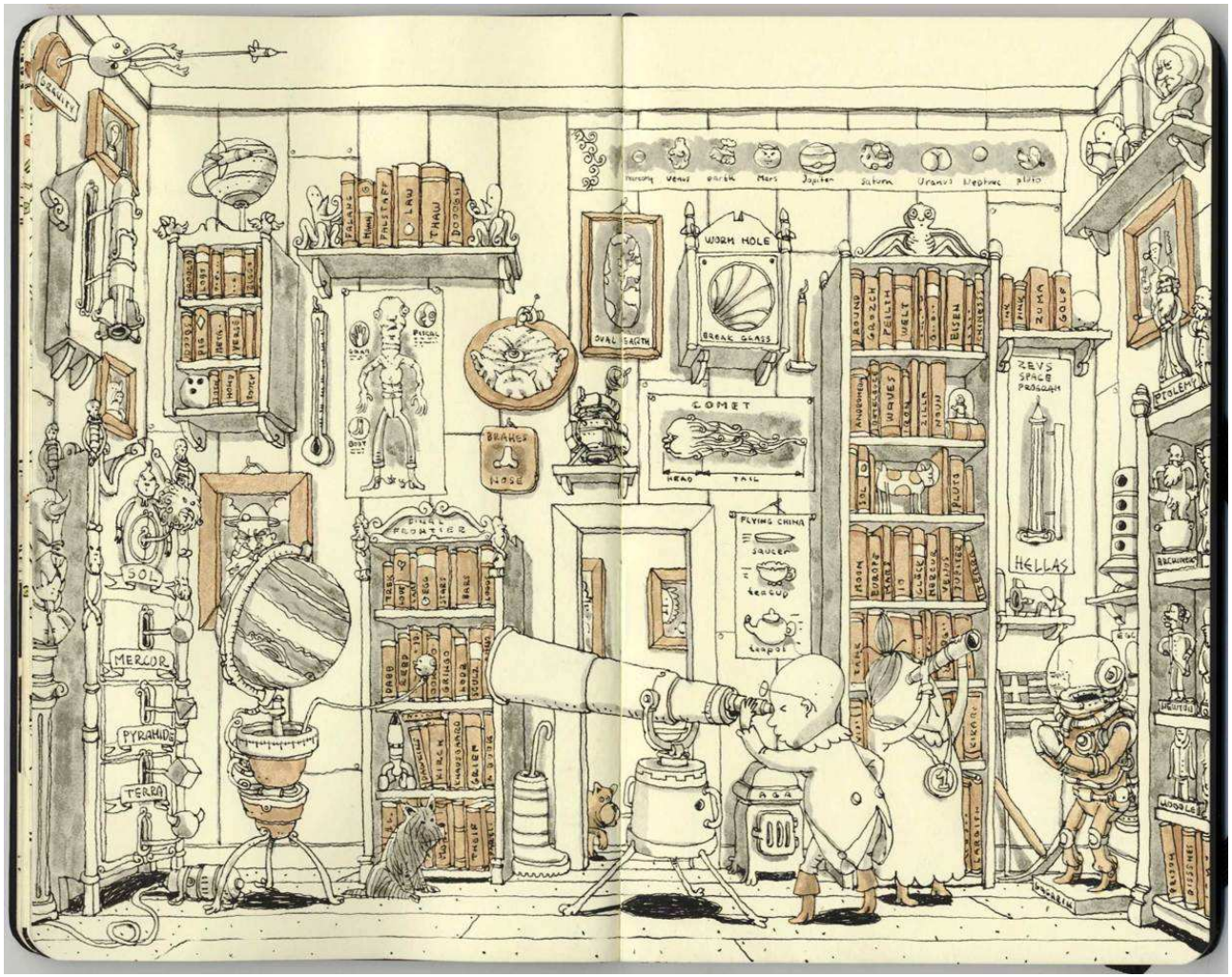


Adapted from Sternberg et al. (2014), ApJ 790, 10.



www.behance.net/MattiasA

H_2 Constant Formation/Destruction Approximation

- With a constant formation rate R_f and density n_{H}:

$$R_f \, n_{\mathrm{H}} \, n(\mathrm{H}) = k_D \, n(\mathrm{H}_2)$$

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$$R_f = 3\,10^{-17} \sqrt{\frac{T}{100}} \, Z' \, \mathrm{cm}^3 \, \mathrm{s}^{-1}$$

$$k_D = k_D^0 \, f(N_2) \, \exp\left(-\sigma_g \, (N_1 + 2N_2)\right) \, \mathrm{s}^{-1}$$

$$\sigma_g \simeq 1.9\,10^{-21} \, Z' \, \mathrm{cm}^2 \, \mathrm{H}^{-1}$$

H_2 Constant Formation/Destruction Approximation

- With a constant formation rate R_f and density $n_{\rm H}$:

$$R_f \, n_{\rm H} \, n({\rm H}) = k_D \, n({\rm H}_2)$$

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$$\sigma_g \simeq 1.9\,10^{-21} \, Z' \, {\rm cm}^2 \, {\rm H}^{-1}$$

- Equation is separable:

$$n({\rm H}) = \frac{dN({\rm H})}{ds} = \frac{dN_1}{ds} \, ; \quad n({\rm H}_2) = \frac{dN({\rm H}_2)}{ds} = \frac{dN_2}{ds}$$

$$R_f \, n_{\rm H} \, \exp\left(\sigma_g \, N_1\right) \, dN_1 = k_D^0 \, f(N_2) \, \exp\left(-\sigma_g \, 2N_2\right) \, dN_2$$

H_2 Constant Formation Approximation

$$N_1 = \frac{1}{\sigma_g} \log \left(1 + \frac{k_D^0 \, \sigma_g}{R_f \, n_{\mathrm{H}}} \int_0^{N_2} f(N) \, \exp\left(-2\sigma_g \, N\right) \, dN \right)$$

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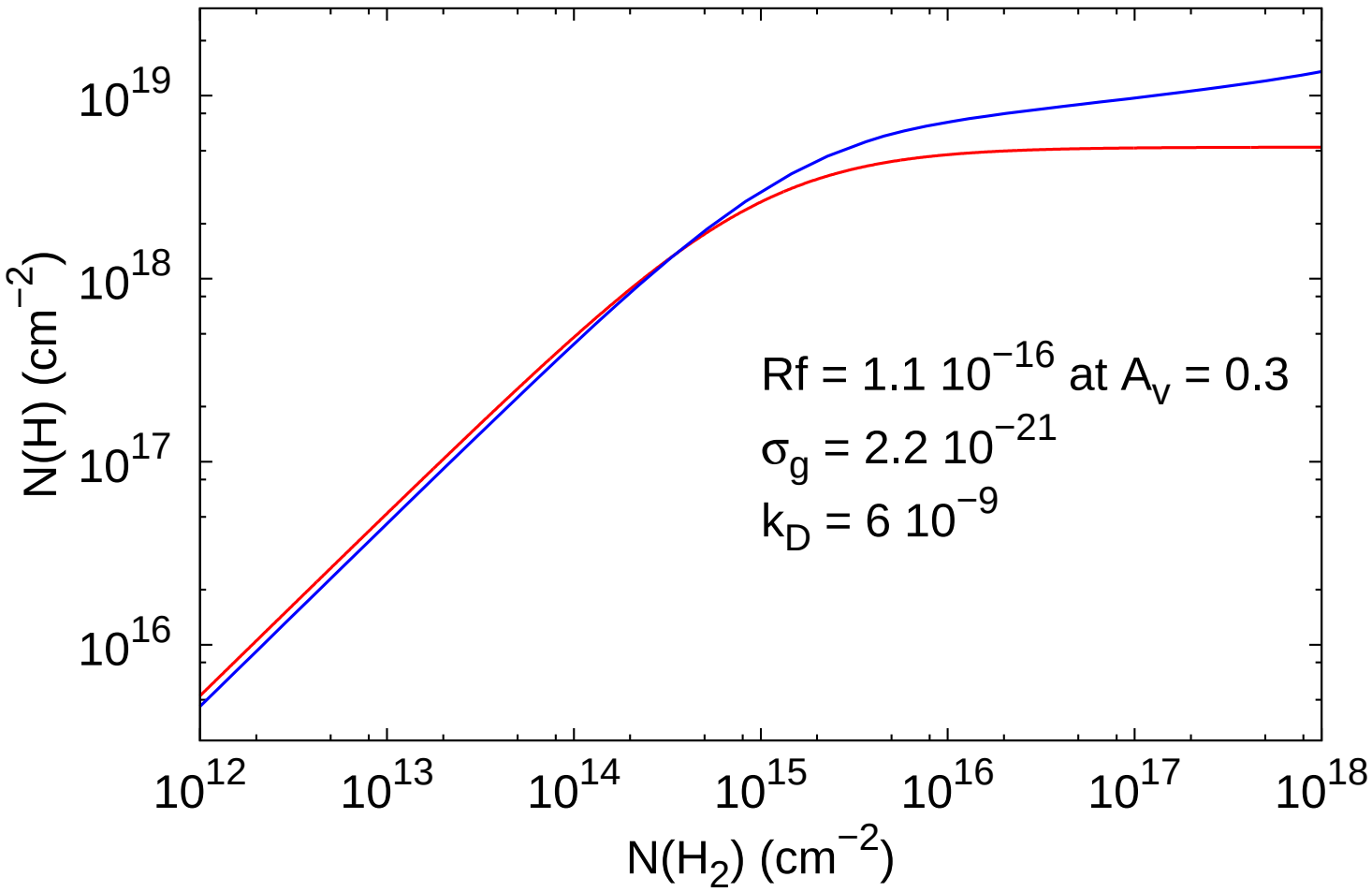
Draine and Bertoldi (1996) give:

$$f(x) = \frac{0.965}{\left(1 + \frac{x}{b_5}\right)^2} + \frac{0.035}{(1+x)^{0.5}} \exp\left(-8.5\,10^{-4} \, (1+x)^{0.5}\right)$$

with $x = \dfrac{N}{N_0}$, $N_0 = 5\,10^{14}\,\mathrm{cm}^{-2}$ and $b_5 = \dfrac{b}{10^5\,\mathrm{cm\,s}^{-1}}$
$\Rightarrow$ Analytical integration is possible.

Comparison to model



Notice effect of chemistry at high $N(\mathrm{H}_2)$.

Analytical analysis

Back to:

$$N_1(N_2) = \frac{1}{\sigma_g} \log \left(1 + \frac{k_D^0 \, \sigma_g}{R_f \, n_{\mathrm{H}}} \int_0^{N_2} f(N) \, \exp\left(-2\sigma_g \, N\right) \, dN \right)$$

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We set:

$$\alpha = \frac{2\,k_D^0}{R_f\,n_{\rm H}}\,; \quad G(N_2) = \sigma_g \int_0^{N_2} f(N)\,\exp\left(-2\sigma_g\,N\right)\,dN$$

$$N_1(N_2) = \frac{1}{\sigma_g} \log\left(1 + \frac{\alpha\,G(N_2)}{2}\right)$$

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$$N_1(N_2) = \frac{1}{\sigma_g} \log\left(1 + \frac{\alpha\,G(N_2)}{2}\right)$$

- $\alpha = \dfrac{n_1}{n_2}$ in free space (typically: $\alpha \sim 2\,10^4$)
- G: Average H_2 self-shielding factor. (typically $G \sim 5\,10^{-5}$)

Analytical analysis

- Asymptotically:

$$N_{1,tot} = \frac{1}{\sigma_g} \log\left(1 + \frac{\alpha\, G}{2}\right) \; ; \quad G = \lim_{N_2 \to \infty} G(N_2)$$

- Most Z' dependancies cancel, but one:

$$\alpha\, G \simeq 1.5\, \frac{I_{UV}}{(n_{\rm H}/100\,{\rm cm}^{-3})}\, \frac{1}{1 + \sqrt{2.64\, Z'}}$$

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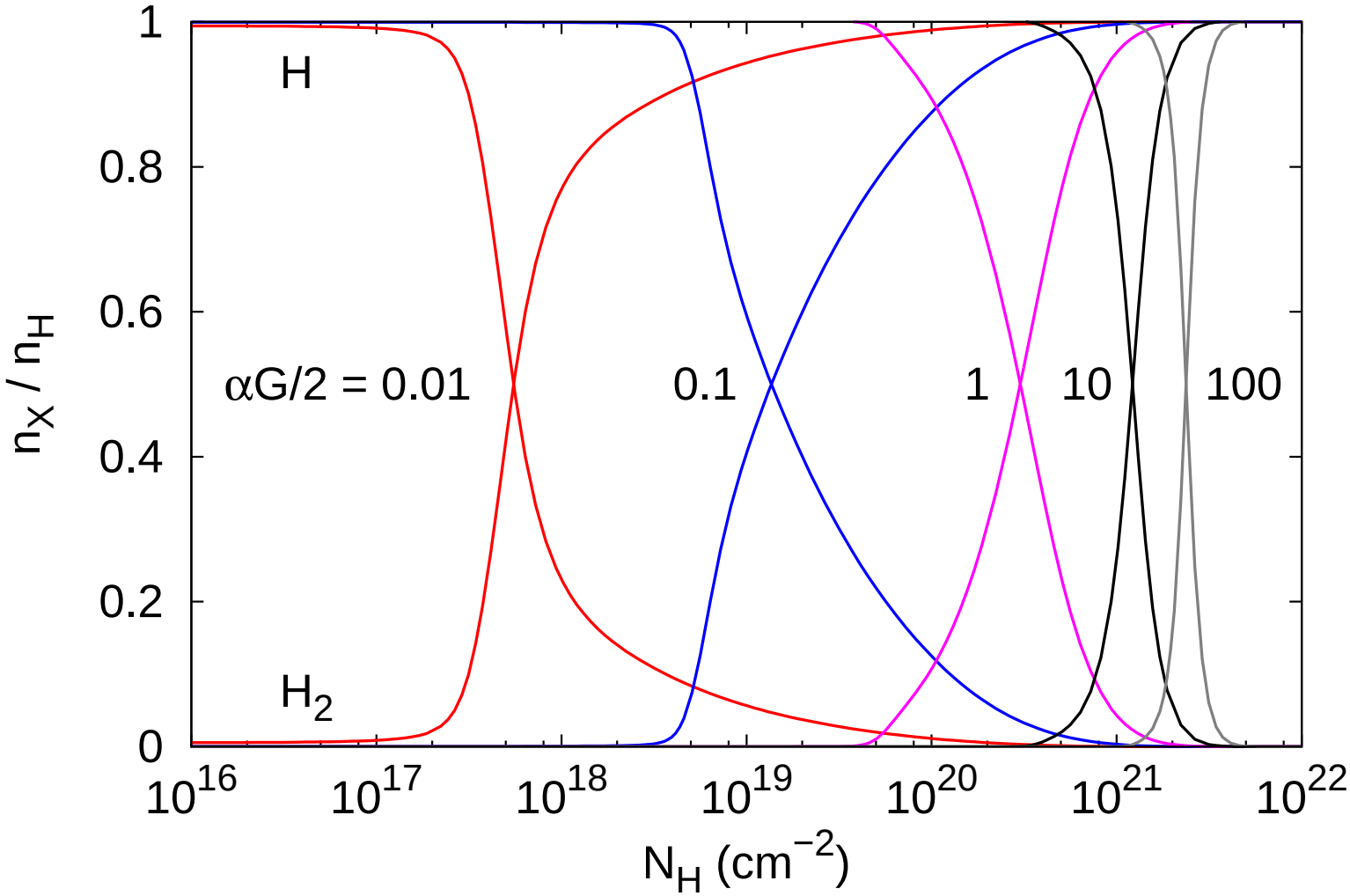
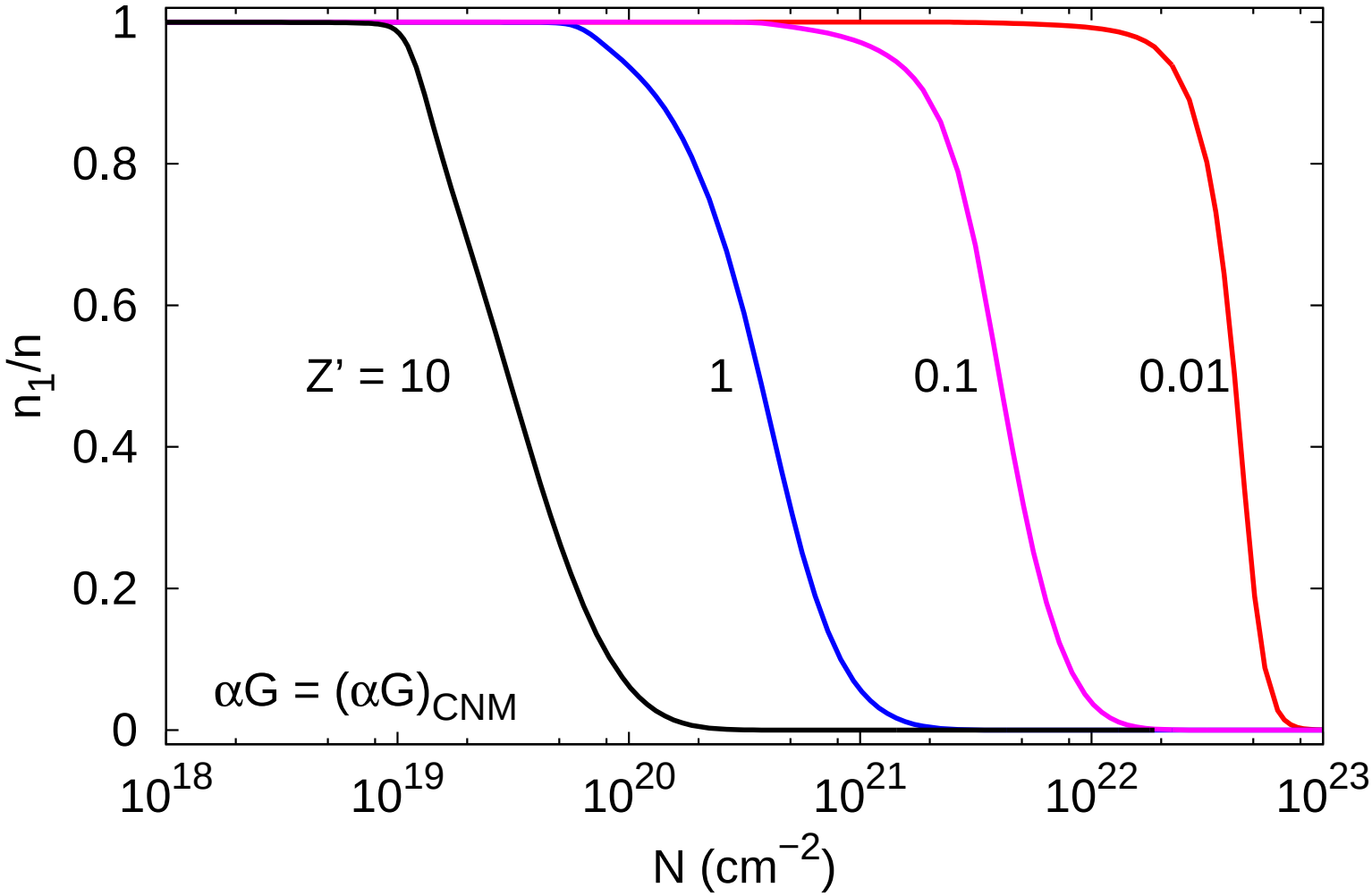
- $\alpha\, G << 1$: weak field limit:
  Absorption by H_2 lines and H_2-dust dominates.
- $\alpha\, G >> 1$: strong field limit:
  Absorption by HI-dust dominates.

See complete discussion in Sternberg et al. (2014)

Weak to strong field



Effects of metallicity



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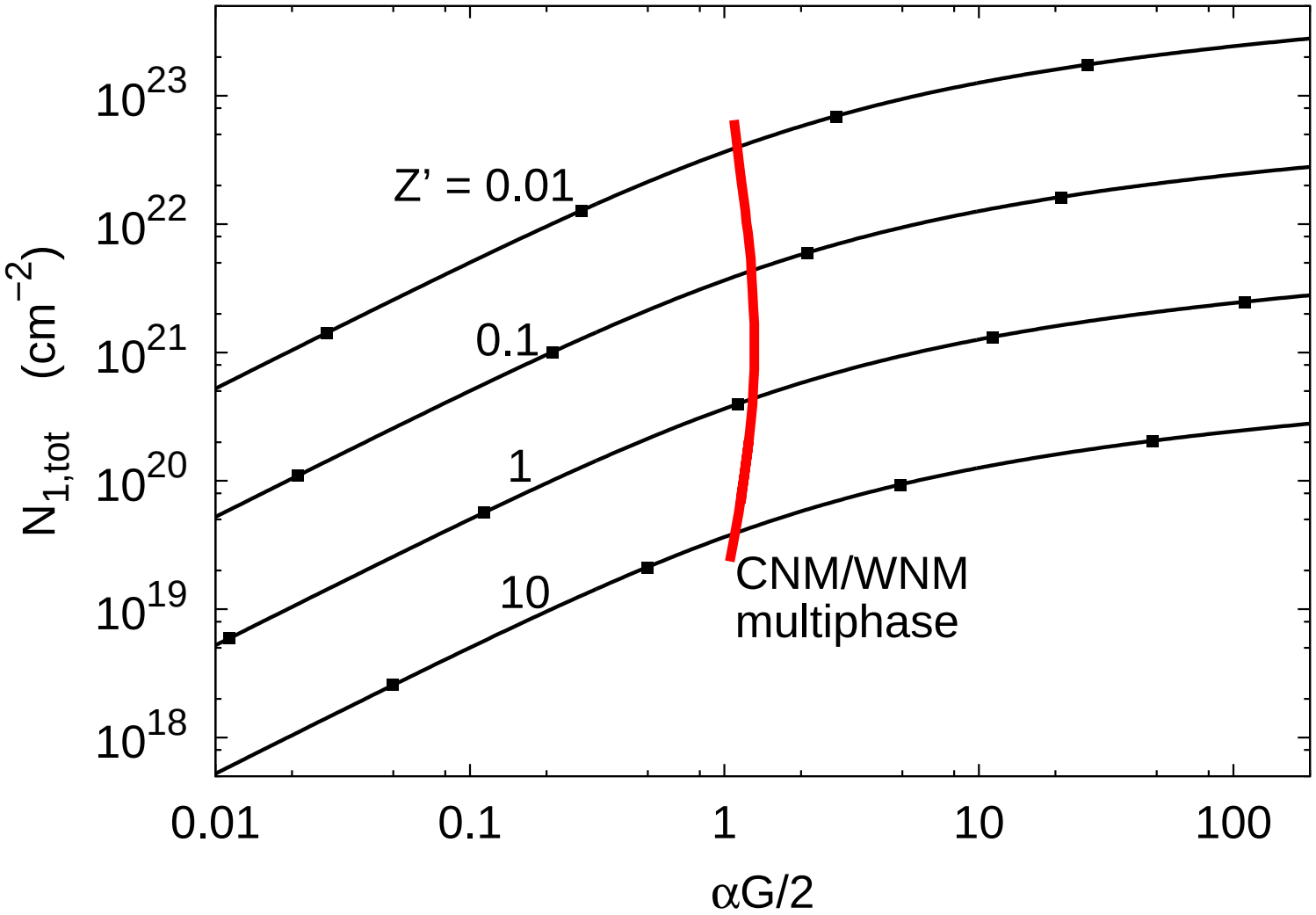


Effects of metallicity

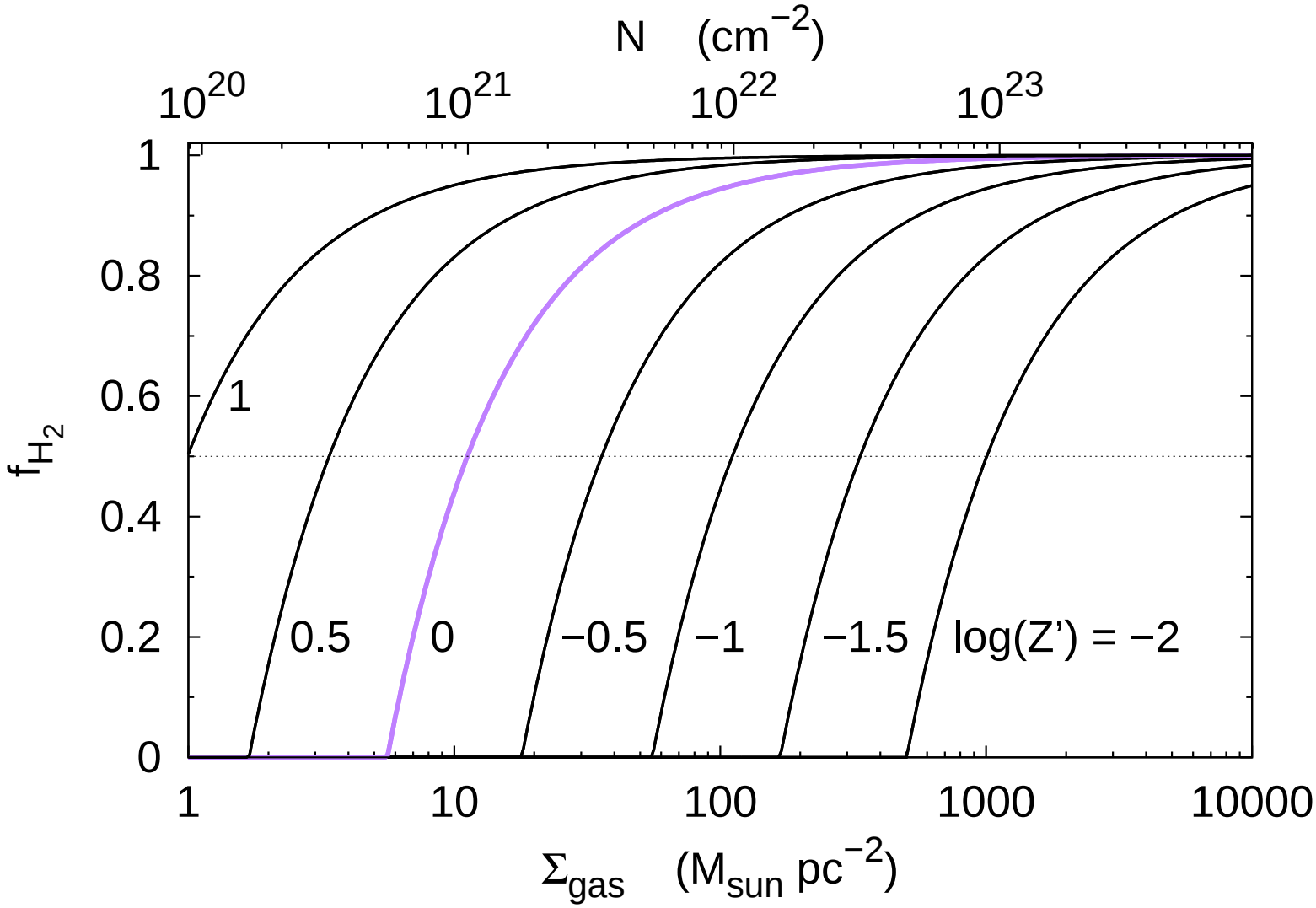
For isotropic radiation field:

$$N_{1,tot} = \frac{<\mu>}{\sigma_g} \log\left(1 + \frac{1}{<\mu>}\frac{\alpha\, G}{4}\right)$$

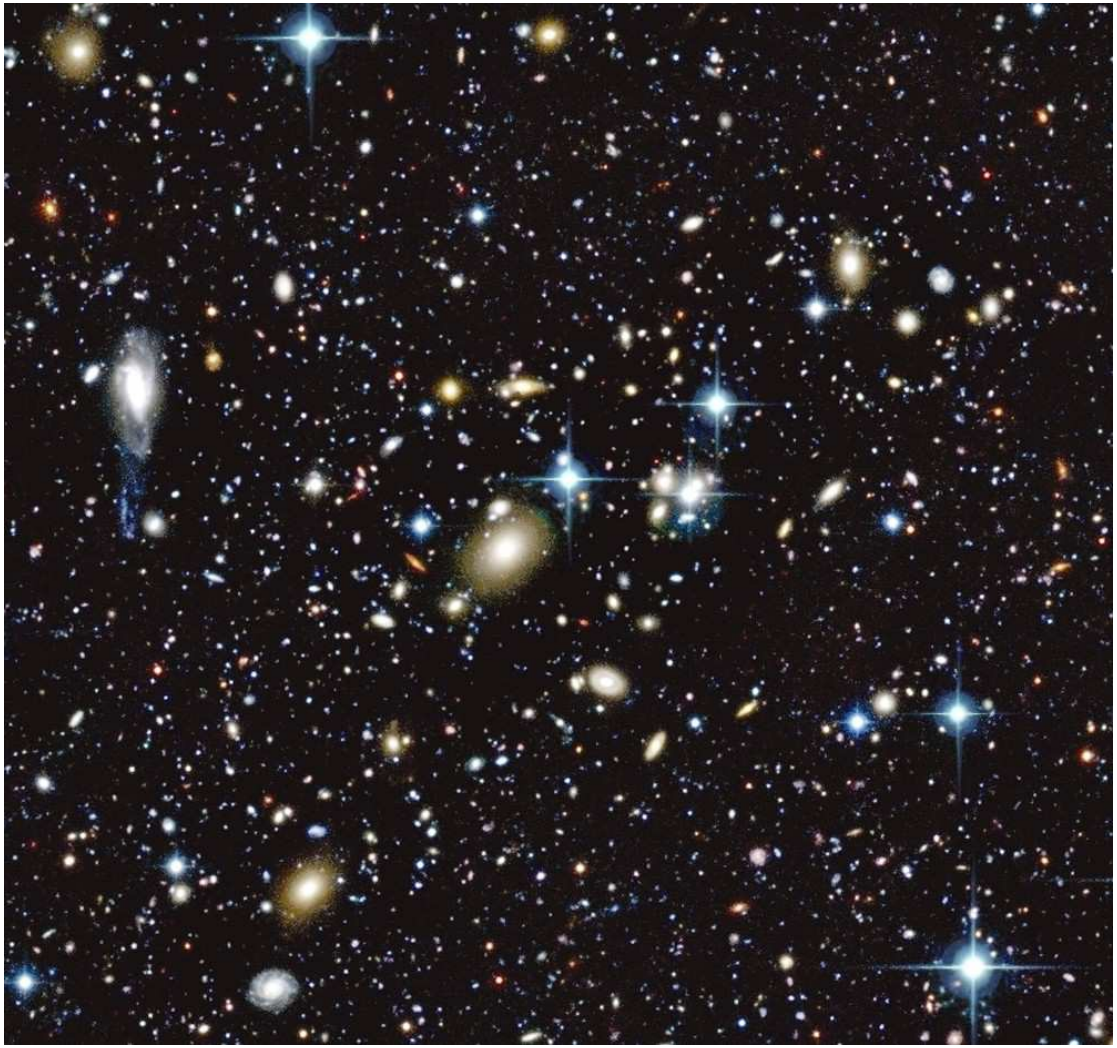
- $<\mu> \simeq 0.8$, from fit to numerical models
- $\frac{1}{\sigma_g} = \frac{5.3\,10^{20}}{Z'}\,\mathrm{cm}^{-2}$, for typical grain composition
- $\alpha\, G \simeq 1.5\,\frac{I_{UV}}{(n_{\mathrm{H}}/100\,\mathrm{cm}^{-3})}\,\frac{1}{1+\sqrt{2.64\,Z'}}$
- If balance between WNM and CNM, then $\frac{\alpha G}{2} \simeq 1.1$, so:

$$N_{1,tot} \simeq \frac{2.2\,10^{20}}{Z'}\,\mathrm{cm}^{-2}$$

Effects of metallicity



Expansion



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Expansion

From: "The Dawn of Chemistry",
D. Galli & F. Palla, ARA&A, 51, 163 (2013)

Expansion

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- Density (baryons):

$$n_b = 2.2\,10^{-7}\,(1+z)^3\ \mathrm{cm}^{-3}$$

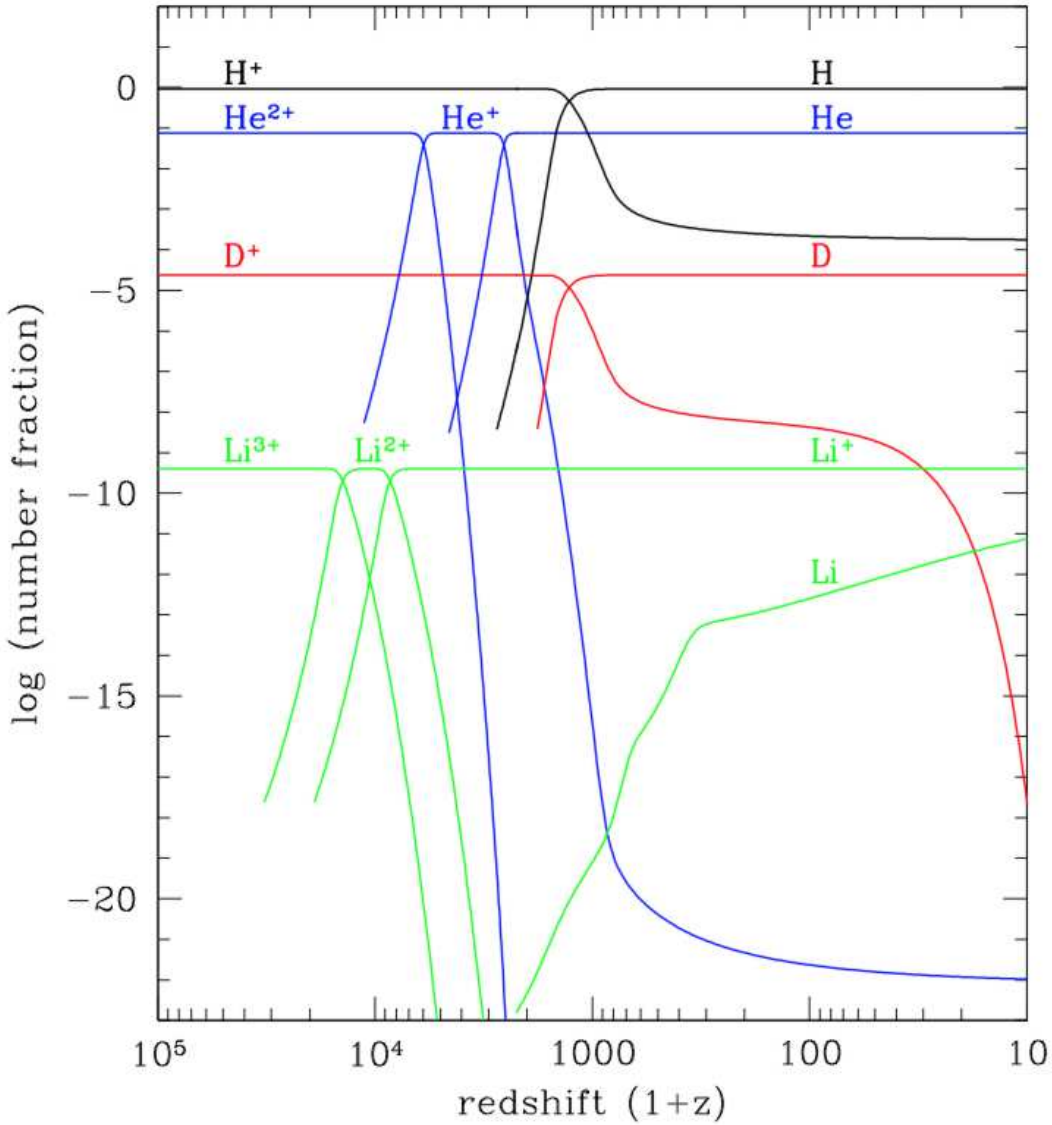
- Recombination: $z \sim 1000 \Rightarrow n_b \sim 220\,\mathrm{cm}^{-3}$
- CMB, $T_0 = 2.725\,\mathrm{K}$:

$$T_r = T_0\,(1+z)$$

- Gas temperature:

$$\begin{cases} T_g \simeq T_r\,; & z > 300 \\ T_g \simeq 0.02\,(1+z)^2\,; & z < 100 \end{cases}$$

Recombination



Abundances

H	He	D	Li
0.924	0.076	$2.38\,10^{-5}$	$4.04\,10^{-10}$

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- Full chemistry (with isotopes): ~ 250 reactions and ~ 30 species.
- Requires detailed balance of all main species (at least vibrational excitation for H_2 and H_2^+)
- Photo-destruction by CMB and non-thermal photons (e.g. Lyα) is important.
- But also new processes. E.g.

PHYSICAL REVIEW A **85**, 043411 (2012)

Resonances in photoionization: Cross sections for vibrationally excited H_2

J. Zs. Mezei,[1,2,*] I. F. Schneider,[1,†] E. Roueff,[3] and Ch. Jungen[2,‡]

Gas phase formation

- Radiative association:

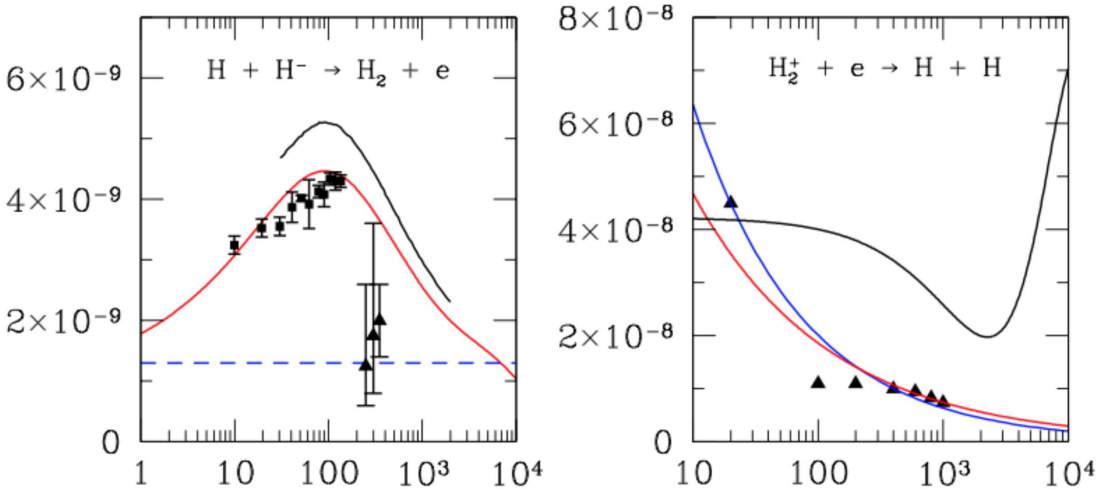
$$H + H^+ \rightarrow H_2^+ + h\nu$$

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

- H^- formation:

$$H + e^- \rightarrow H^- + h\nu$$

$$H^- + H \rightarrow H_2 + e^-$$



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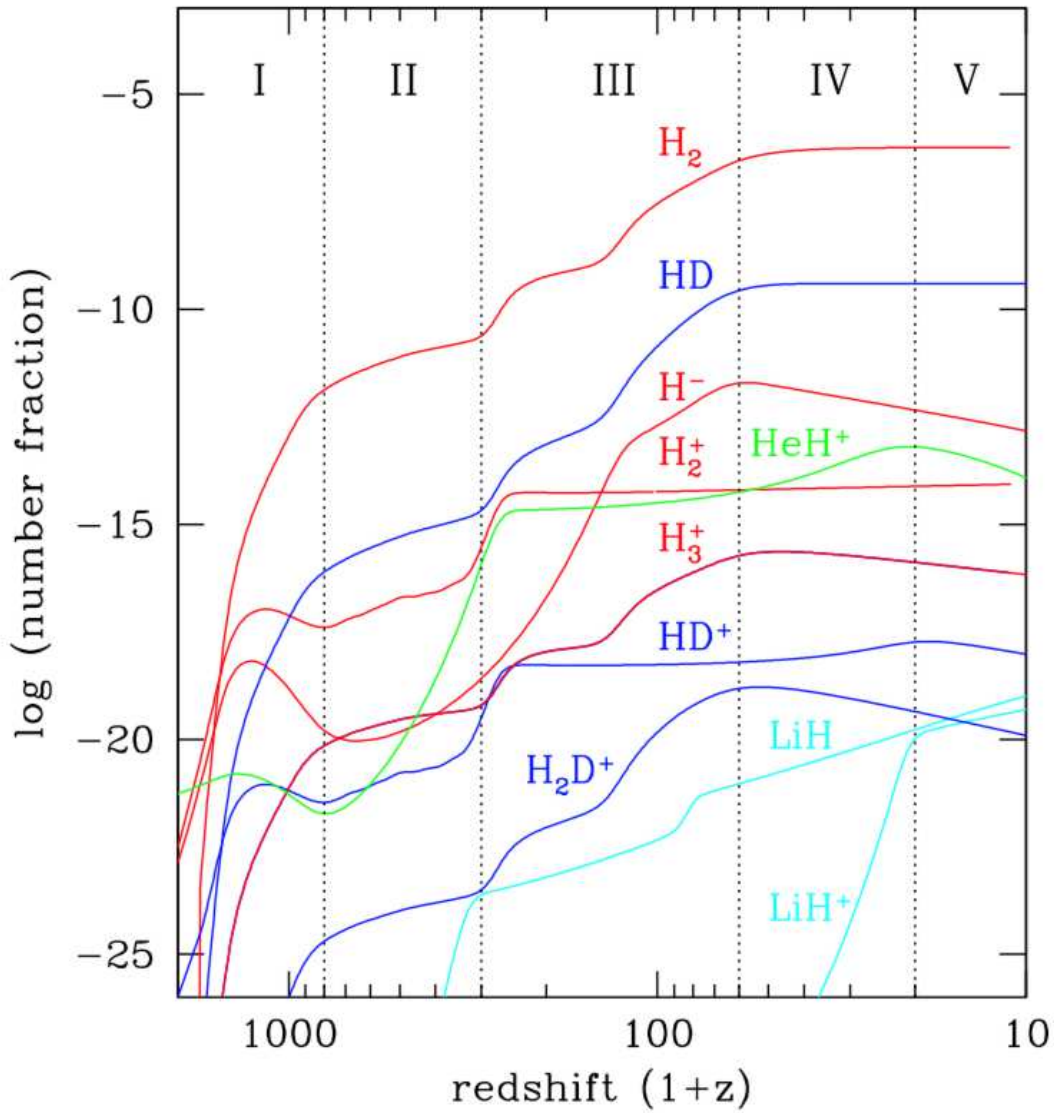


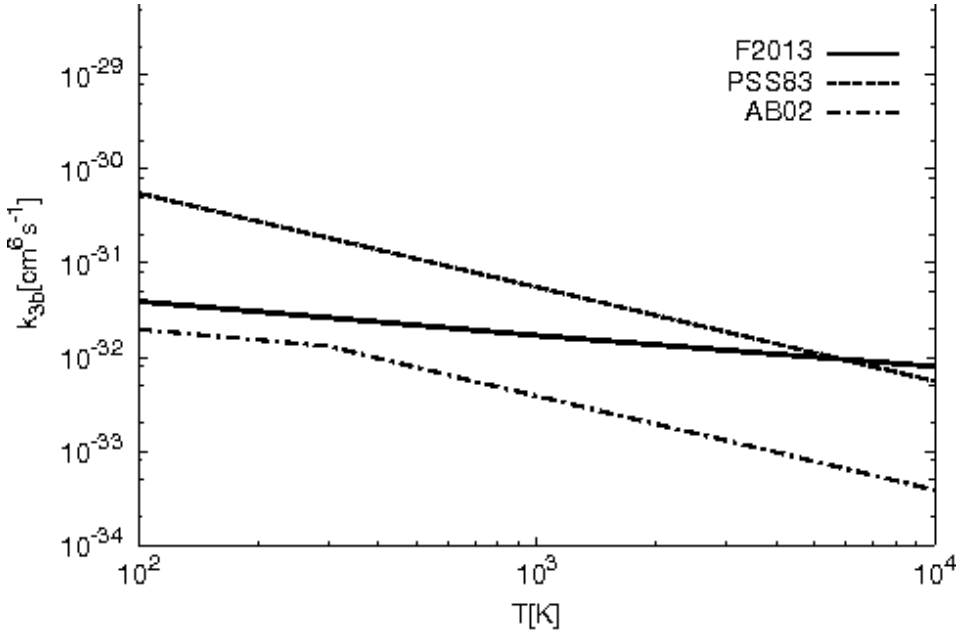
Gas phase formation

- 3 body reactions (in collapsing clouds above $10^9\,\mathrm{cm}^{-3}$):

$$\mathrm{H} + \mathrm{H} + \mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{H}$$

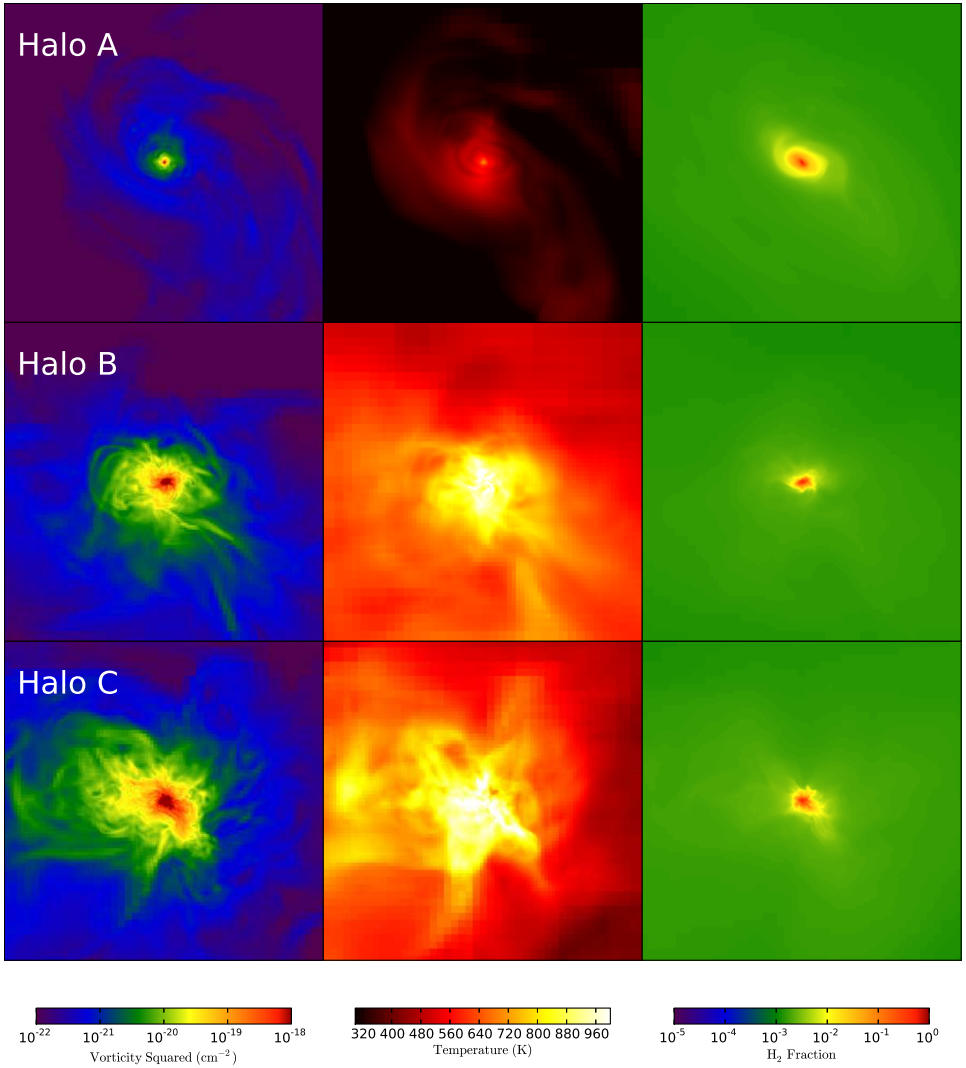
$$\mathrm{H} + \mathrm{H} + \mathrm{H}_2 \rightarrow \mathrm{H}_2 + \mathrm{H}_2$$

- Rates based on reverse reaction rate measurement (collisional dissociation)



First stars

Bovino et al., 2014, A&A, 561, 13



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- Three papers:
  - Bron, E. et al., 2014, A&A, 569, 100
  - Sternberg, A., Le Petit, F. et al., 2014, ApJ, 790, 10
  - Galli, D., Palla, F., 2013, ARA&A, 51, 163