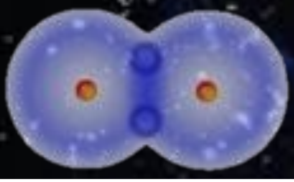
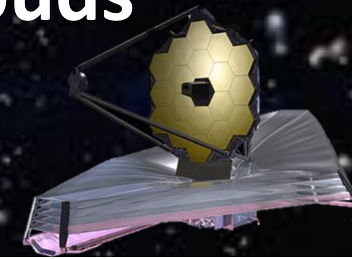
Workshop: The Physics of H_2 in space with the James Webb Space Telescope

Consequences of out-of-equilibrium H_2 on the chemistry of diffuse molecular clouds





<u>Outline</u>

① H_2 modelling in numerical simulations
② Multiphase ideal MHD simulations
③ Consequences of warm H_2: the CH^+ case

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Thanks to J. Le Bourlot

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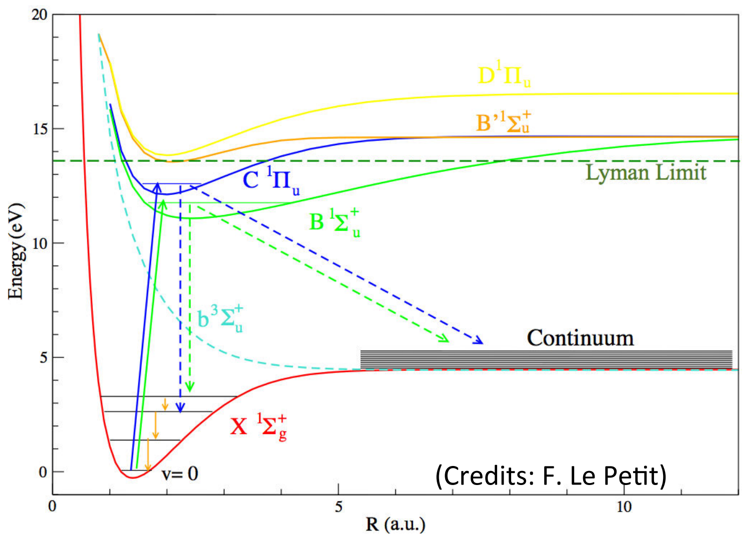
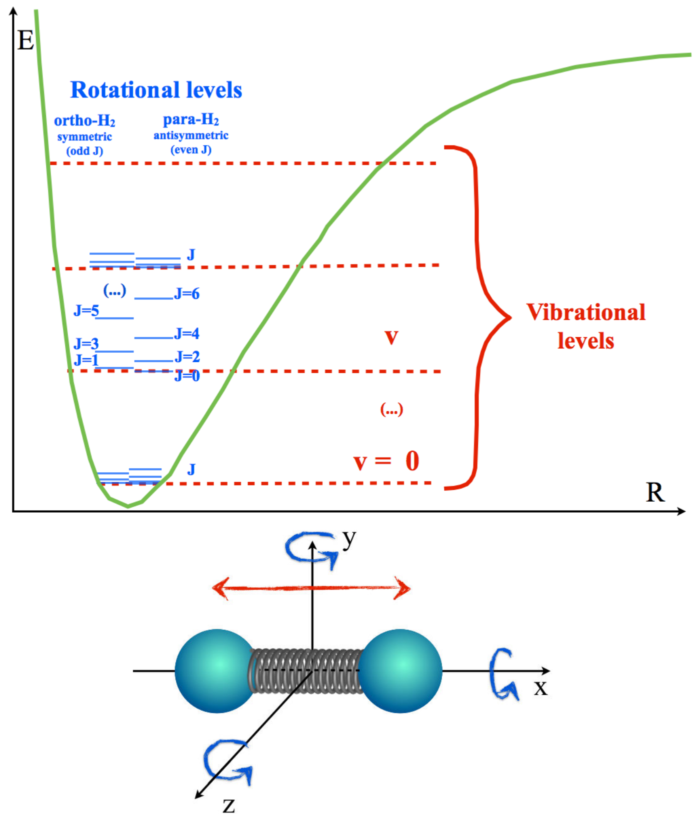
Introduction

Absorption:
UV Lyman and Werner bands
Copernicus, ORPHEUS, FUSE

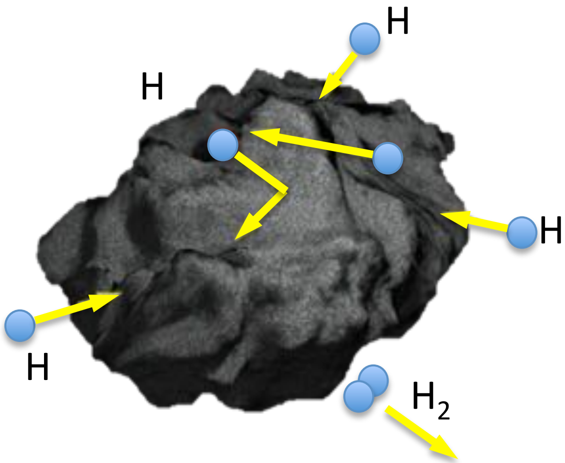
Emission:
mid-IR and NIR
ISO, Spitzer, JWST

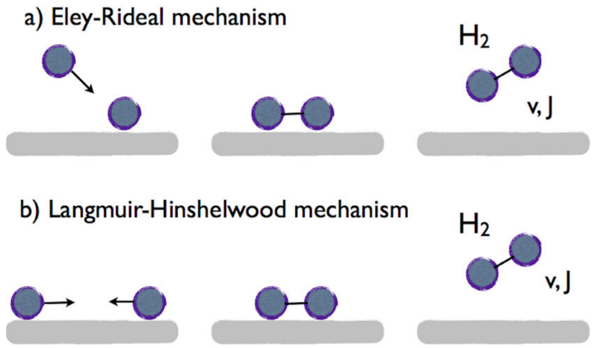




H_2 formation

H_2 formation on grain surfaces





$$k_{\rm form} = 3 \times 10^{-17} \times \sqrt{\frac{T}{100\ \rm K}} \times \frac{1}{1 + \left(\frac{T}{464\ \rm K}\right)^{1.5}}\ \rm cm^3 s^{-1}$$

k_0 (Jura 1974)

Sticking factor (Le Bourlot et al. 2012, Bron et al. 2014)

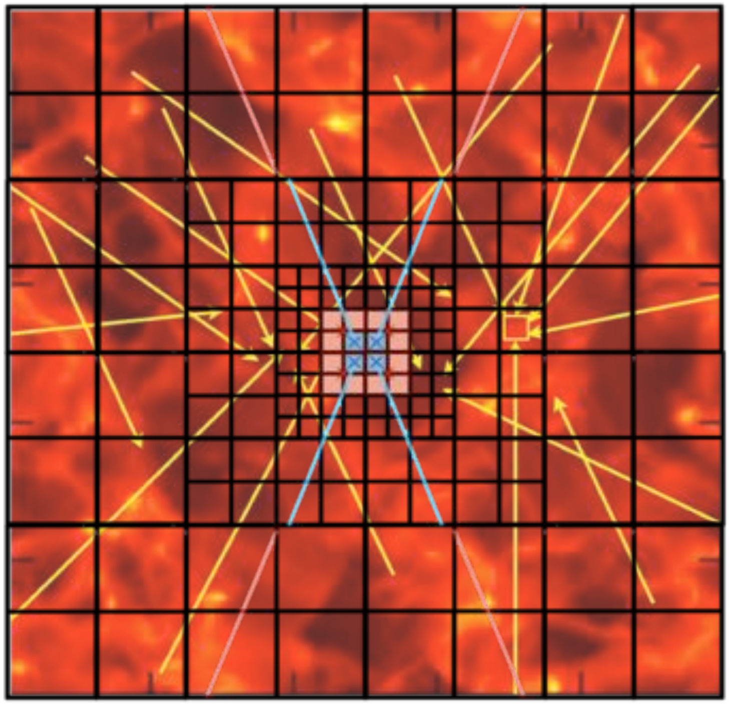
H_2 destruction

H_2 destruction by UV fluorescent photodissociation

$$k_{\mathrm{ph}} = 3.3 \times 10^{-11} \times G_0 < \underbrace{\mathrm{e}^{-\sigma_d \mathcal{N}}}_{\text{Dust shielding}} \times \underbrace{f_{\mathrm{shield}}(\mathcal{N}_{\mathrm{H}_2})}_{\text{Self-shielding}} > \ \mathrm{s}^{-1}$$

Dust shielding   Self-shielding (Draine & Bertoldi 1996)

UV photons



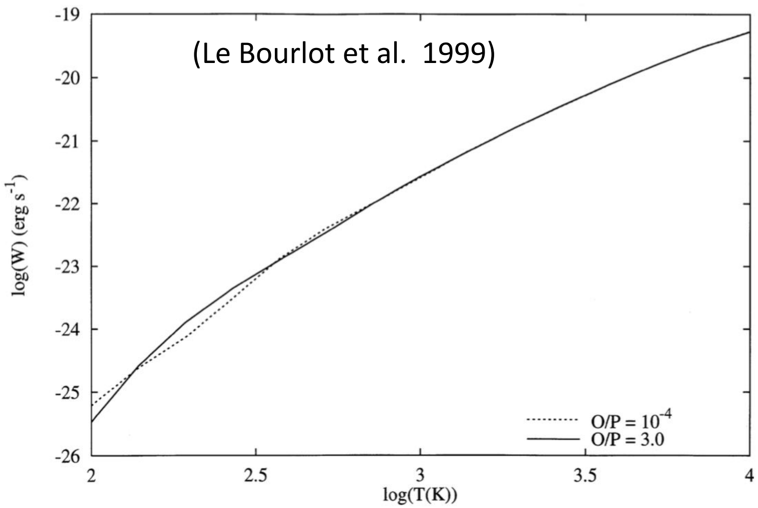
Tree-based method (Valdivia & Hennebelle, 2014)

H_2 Thermal feedback

Cooling:

- H_2 line emission: (Le Bourlot et al. 1999)

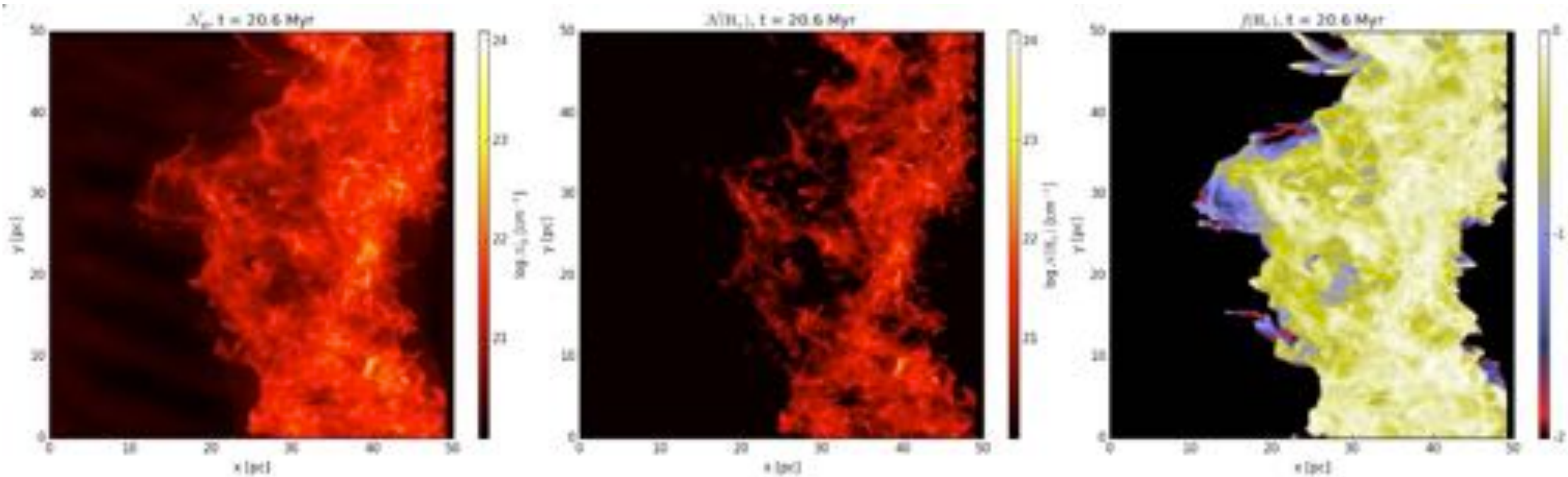
$$W(\mathrm{H}_2) = \frac{1}{n(\mathrm{H}_2)} \sum_{vJ,v'J'} (E_{vJ} - E_{v'J'})\, n_{vJ} A(vJ \rightarrow v'J')$$



Heating:

- H_2 formation: 1.5 eV
- H_2 destruction: 0.4 eV (Black & Dalgarno 1977, Glover & Mac Low 2007)

Ideal MHD multiphase simulation



RAMSES AMR code
(Teyssier 2002)

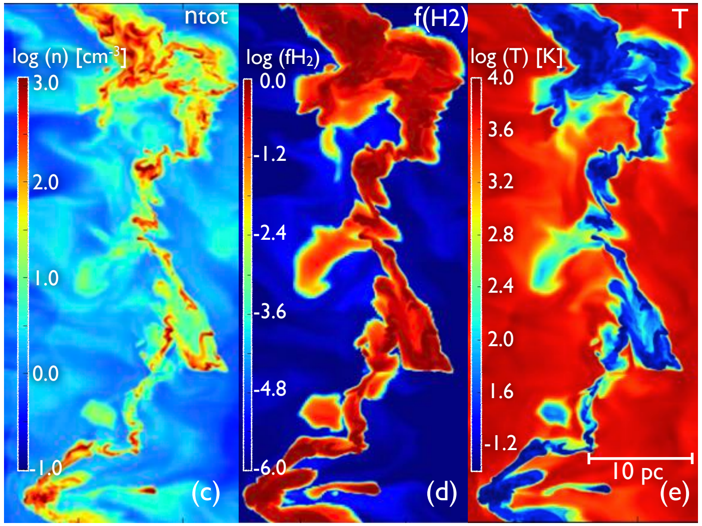
$L = 50$ pc
$N = 1$ cm^{-3}
$V_{in} = 15$ km s^{-1}
$B = 2.5$ μG
$dx_{min} = 0.05$ pc
$dx_{max} = 0.2$ pc

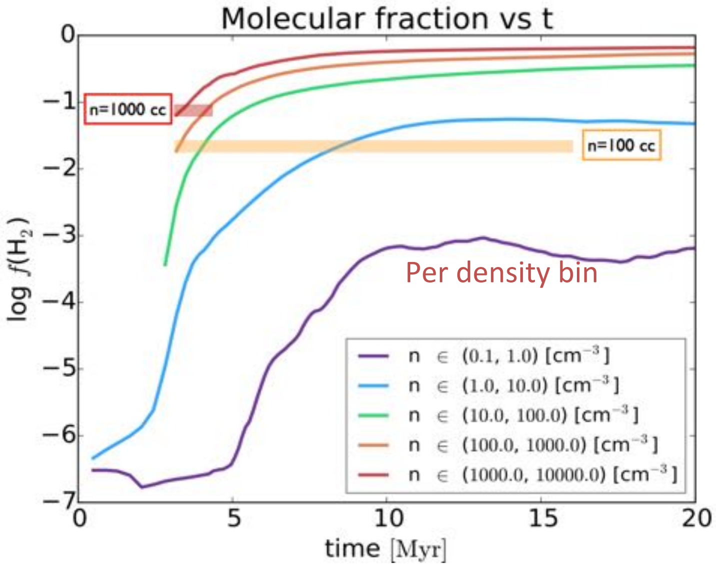
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0,$$
$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} - \boldsymbol{B}\boldsymbol{B}) + \nabla P = -\rho \nabla \phi,$$
$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + P)\boldsymbol{v} - \boldsymbol{B}(\boldsymbol{B}\boldsymbol{v})] = -\rho \mathcal{L},$$
$$\frac{\partial \boldsymbol{B}}{\partial t} + \nabla \cdot (\boldsymbol{v}\boldsymbol{B} - \boldsymbol{B}\boldsymbol{v}) = 0,$$
$$\nabla^2 \phi = 4\pi G \rho,$$

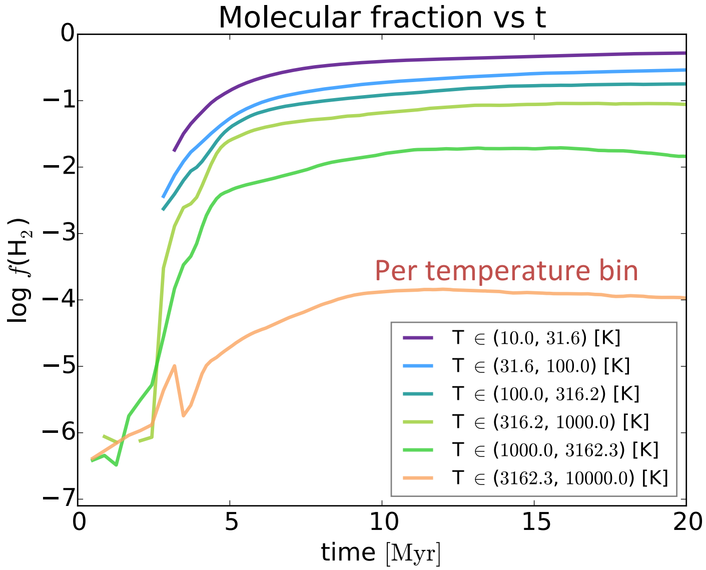
(Valdivia et al. 2016)

$$\frac{\partial n_{H_2}}{\partial t} + \nabla \cdot (n_{H_2} \boldsymbol{v}) = k_{form} n (n - 2n_{H_2}) - k_{ph} n_{H_2}$$

H_2 fraction evolution

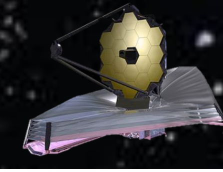


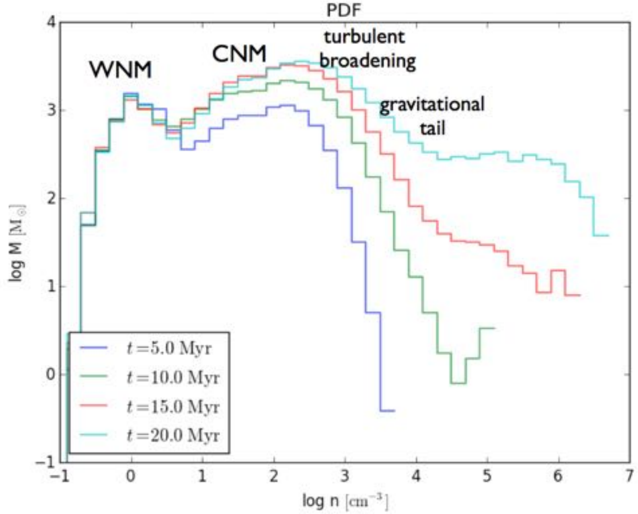




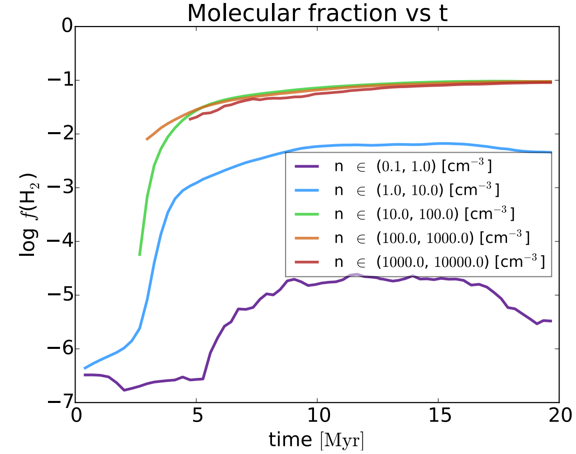
(Valdivia et al. 2016)

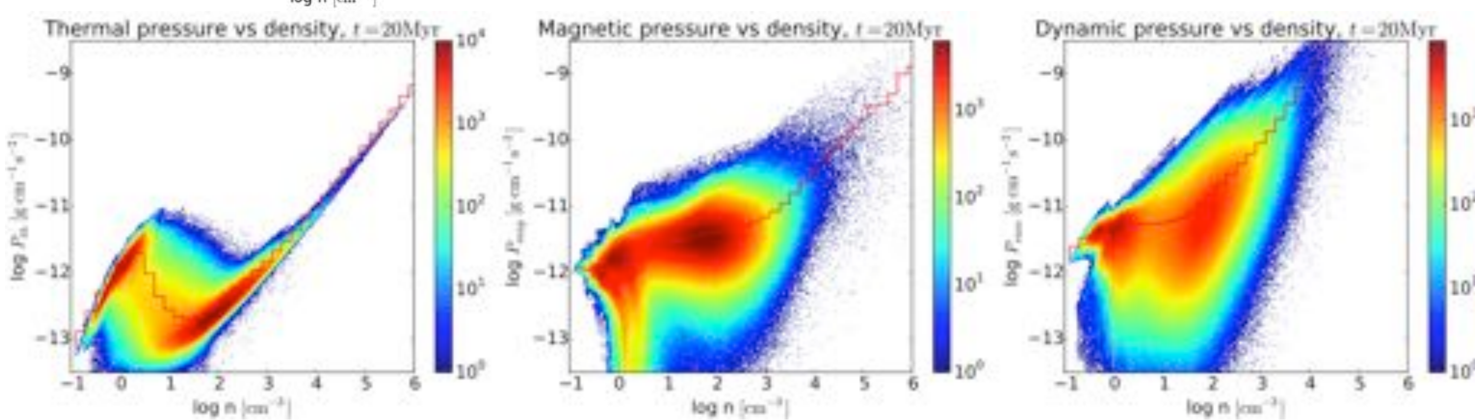
Origin of warm H_2





H_2 formation suppressed for $n_{thresh} \geq 100$ cm^{-3}

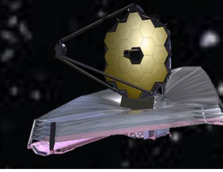


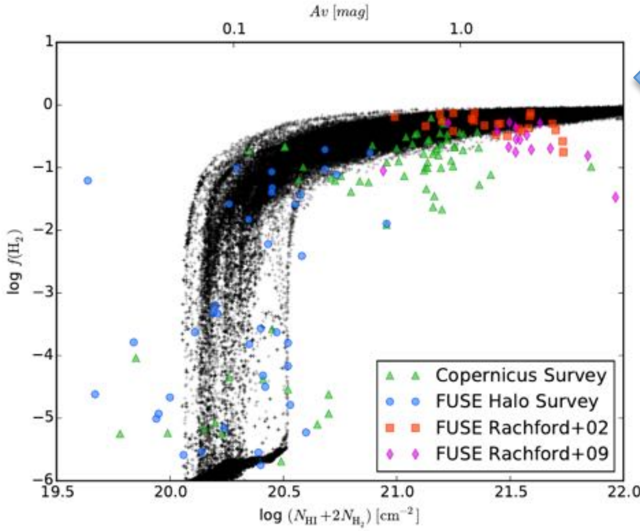


(Valdivia et al. 2016)

- Clumps are dominated by the **turbulent pressure** => **Transient** structures
- H_2 can be **transported** from cold and dense regions towards **warm and diluted** environments, where it survives due to the shielding provided by the **multiphase structure**

Good match with FUV observations



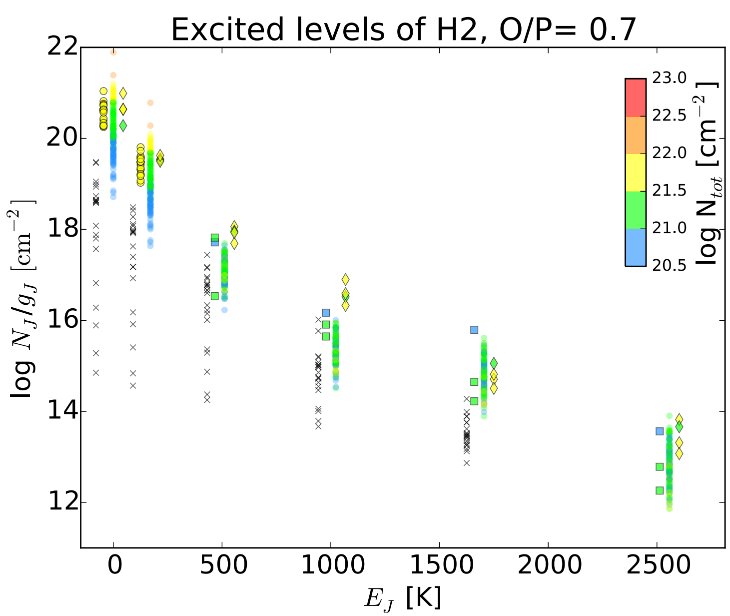


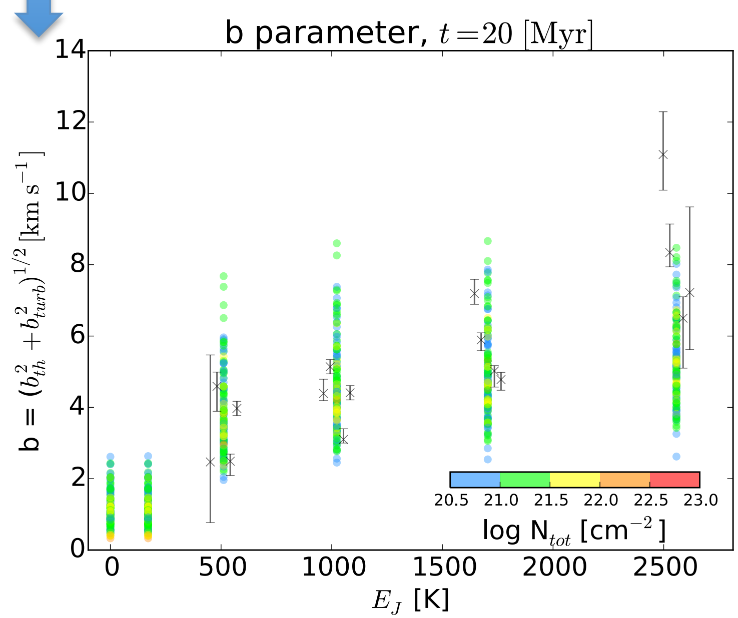
HI-to-H_2 transition

Left: Excited populations
Right: b Doppler parameter

Data:

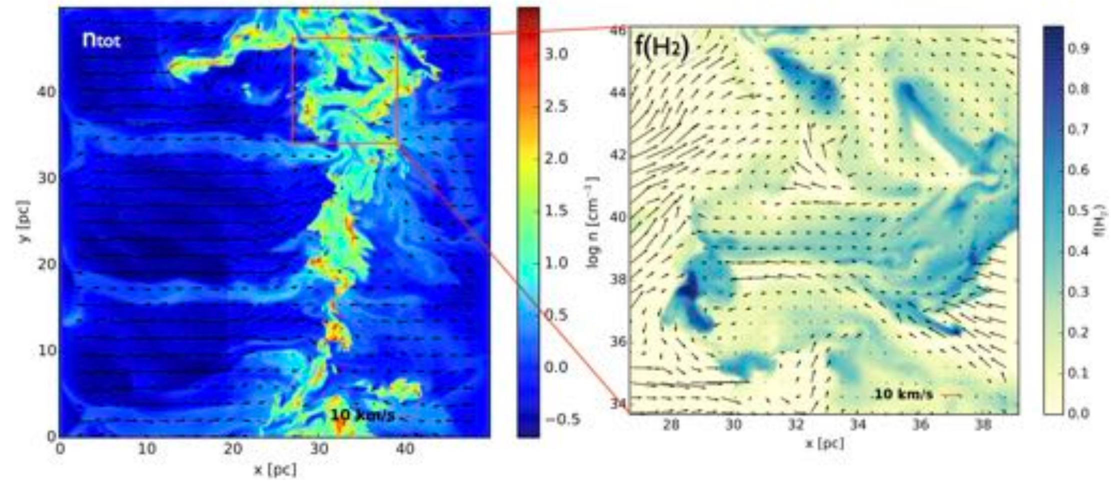
✖	Wakker 2006	*(Copernicus)*
○	Rachford et al. 2002	*(FUSE)*
□	Gry et al 2002	*(FUSE)*
◇	Lacour et al. 2005	*(FUSE)*

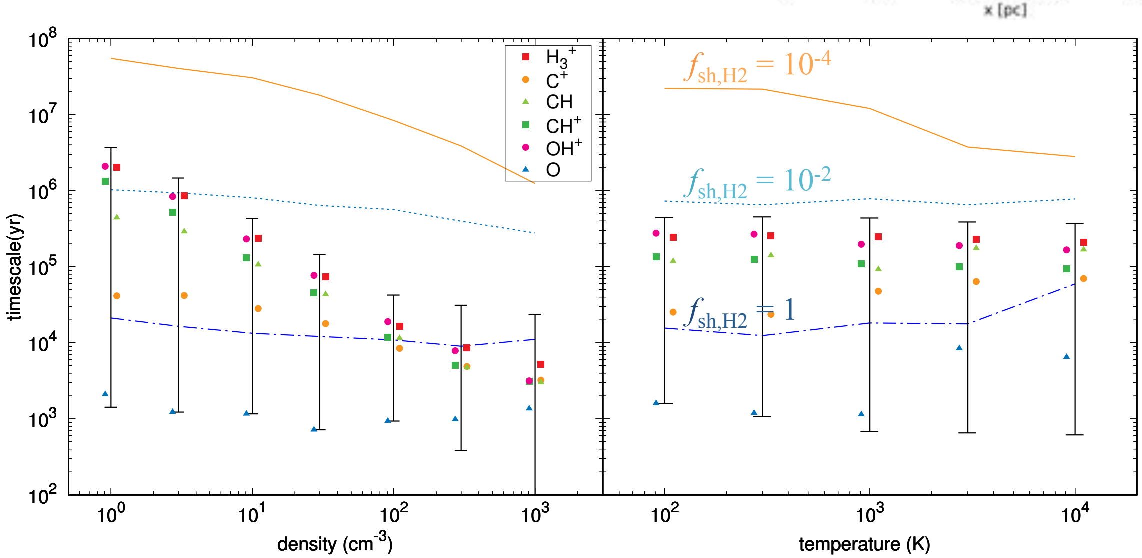


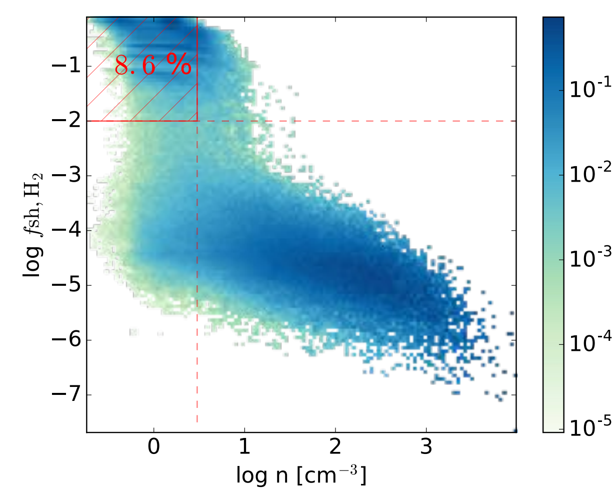


Hybrid approach for the chemistry

- H_2 is a **bottleneck** for the chemistry
- We calculate the equilibrium abundances for all the species (besides H_2 and HI)







Left: Timescales required to reach the equilibrium abundance.
Right: Mass distribution in the simulation

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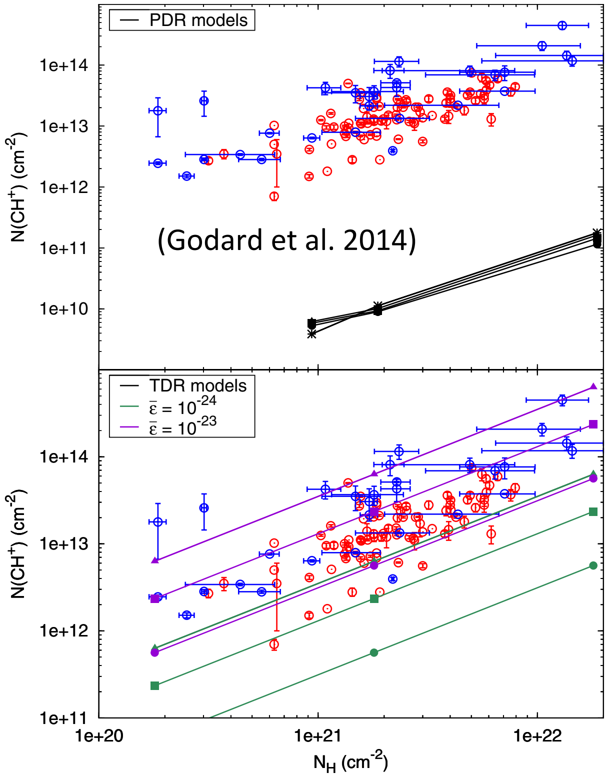
Warm chemistry of the diffuse ISM

Highly endothermic reactions require warm reactants to occur efficiently.

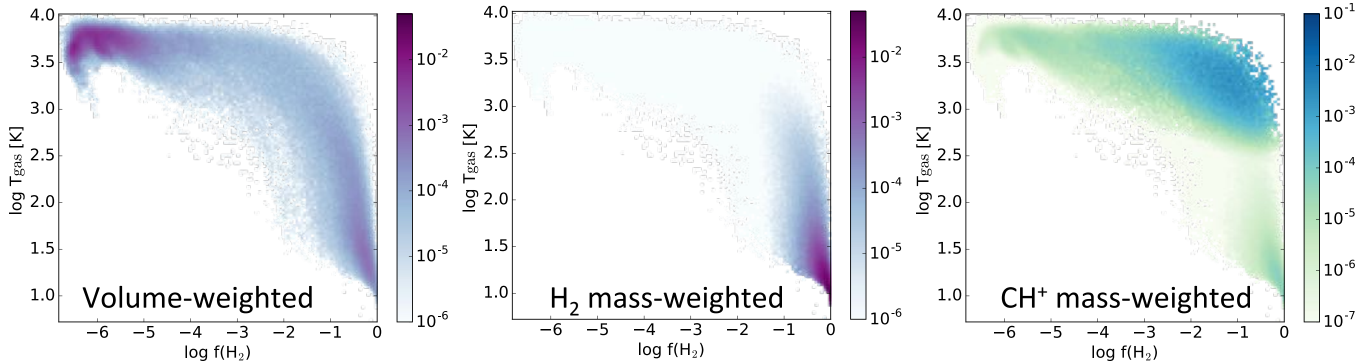
- CH^+ **requires H_2** to be formed efficiently in the diffuse ISM.
- The main reaction path is **highly endothermic**.

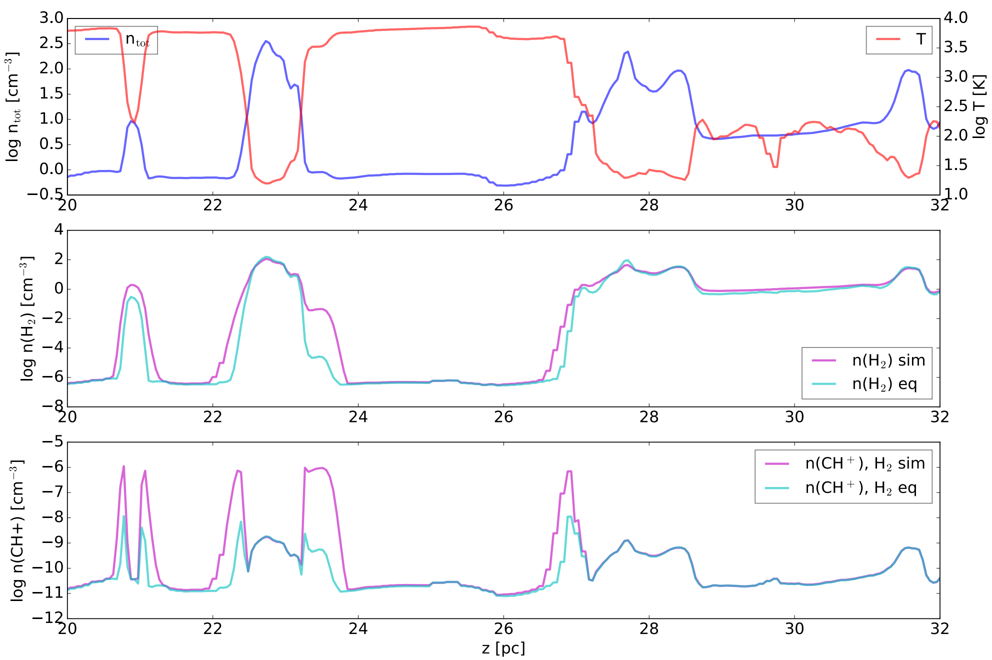
$$C^+ + H_2 \rightarrow CH^+ + H \qquad (\Delta E/k = -4300\ K).$$

- CH^+ is easily **destroyed**.
- PDR models **failed** at explaining its abundance.

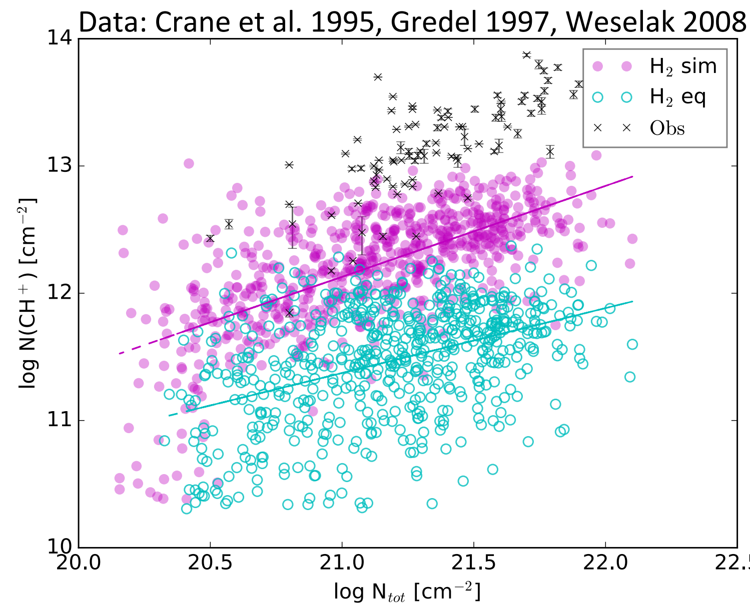


Consequences of warm H_2 on CH^+





Line-of-sight showing the local physical conditions and abundances

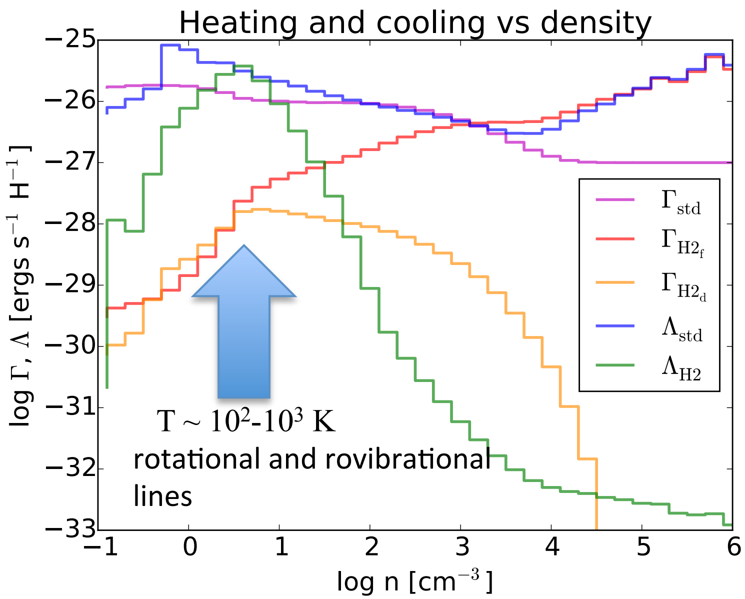


$N(CH^+)$ vs $N(H_{tot})$

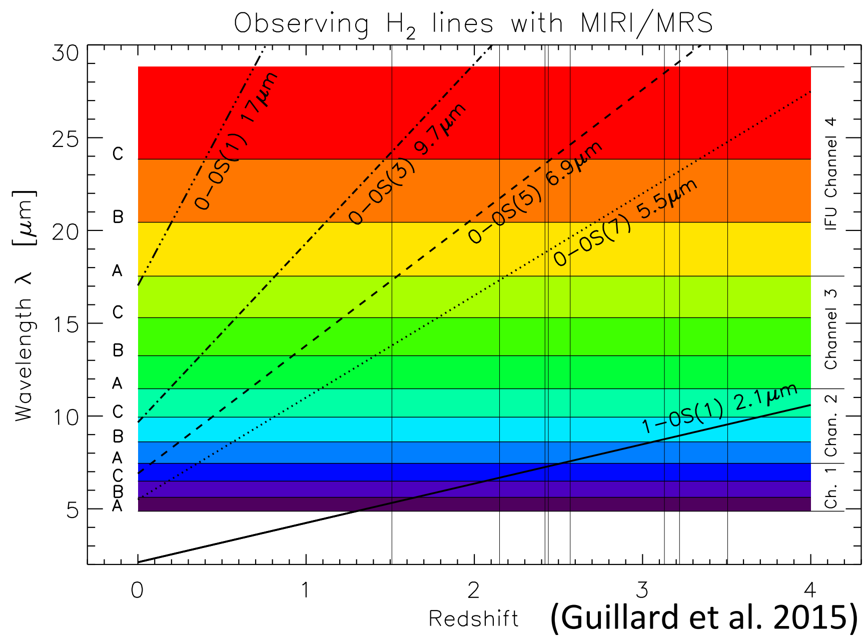
(Valdivia et al. submitted)

Summary

- **Long lived molecules**, such as H_2, can be transported by turbulent motions towards warm environments.
- Once H_2 is present, the chemistry can proceed **much faster**.
- **Out-of-equilibrium H_2** plays a significant role in the abundance of CH^+, nevertheless other physical processes, such as the **dissipation of turbulence**, are needed to explain the observed abundances.
- The **JWST** will provide crucial information about the **warm H_2** through rotational and rovibrational lines.



(Valdivia et al. 2016)



(Guillard et al. 2015)