

# H<sub>2</sub> FORMATION : EFFECT OF DUST GRAIN TEMPERATURE FLUCTUATIONS

# E. BRON, J. LE BOURLOT, F. LE PETIT

### PROBLEM

H<sub>2</sub> **formation** in the interstellar medium occurs through **surface reaction on dust grains**.

The standard mechanism involving physisorption of H atoms and random hopping across the surface (Langmuir-Hinshelwood mechanism) is only efficient at low dust temperatures. But PDR observations have found efficient formation despite hot grains [1].

Several explanations have been proposed: stronger binding energies (surface roughness) [2], **Eley-Rideal mechanism** on chemisorption sites [3],...

# MECHANISM



However, small grains in strongly illuminated environments (PDRs) exhibit strong temperature fluctuations. These stochastic excursions in the high temperature regime affect the formation rate in a way that is not equivalent to a calculation at the mean temperature.

The work presented here computes this effect on the Eley-Rideal formation rate.

#### METHOD

We aim to compute the **adsorbed H atom population fluctuations coupled to the grain temperature fluctuations**. This will then allow us to compute the formation rate.

We use a **master equation approach**, but instead of solving the main master equation in two variables ( $T_{grain}$  and  $n_{ads}$ ), we take advantage of a simplification.

As the **temperature fluctuations** are governed by **only photon interactions**, they obey a **reduced master equation** for the PDF in only one variable,  $f_T(T)$ .

#### RESULTS

As expected, we obtain a **reduction of the formation rate**, which is **stronger for smaller grains** (up to 2 nm) and **for stronger radiation fields**.



This **reduction of the formation rate** with illumination intensity is **stronger for lower gas density**, as the adsorption timescale is longer, giving more importance to the temperature fluctuations.



Then, averaging the main master equation over  $n_{ads}$  gives a simpler equation in  $< n_{ads} > (T)$ , which is enough for us to compute the formation rate.

Both equations are **eigenvector equations for integral operators** of the shape :

 $f(x) = \int_0^{+\infty} dy \, K(x, y) \, f(y)$ 

We solve them numerically using iterative methods.

## **OUT OF EQUILIBRIUM**



# FULL CLOUD SIMULATION WITH THE MEUDON PDR CODE

We coupled this formation rate computation to the **Meudon PDR Code** [4], for a cloud with  $\chi = 100$  and  $P = 1 \cdot 10^6$  K.cm<sup>-3</sup>.

The H/H<sub>2</sub> transition is deeper in the cloud resulting in slightly reduced H<sub>2</sub> lines (less than



25%). The C+/C/CO transition is also modified, with a **quicker C+/C transition** (resulting in **C lines increased by a factor of 2**), but a **later C/CO transition** (resulting in **CO lines reduced by a factor of 2** for J=5-8).



#### References

- [1] E. Habart, F. Boulanger, L. Verstraete, C. M. Walmsley, G. Pineau des Forêts, A&A, 414, 531, 2004
- [2] Q. Chang, H. M. Cuppen, E. Herbst, A&A, 434, 599, 2005
- [3] J. Le Bourlot, F. Le Petit, C. Pinto, E. Roueff, F. Roy, A&A, 541, A76, 2012
- [4] F. Le Petit, C. Nehmé, J. Le Bourlot, E. Roueff, ApJS, 164, 506, 2006

# CONCLUSIONS

Temperature fluctuations significantly reduce the Eley-Rideal formation rate for small grain sizes, strong radiation fields. The effect is further enhanced by low gas density.
The minimal size in the dust size distribution controls the strength of this effect.
It leads to modifications of observable quantities by up to a factor of 4.