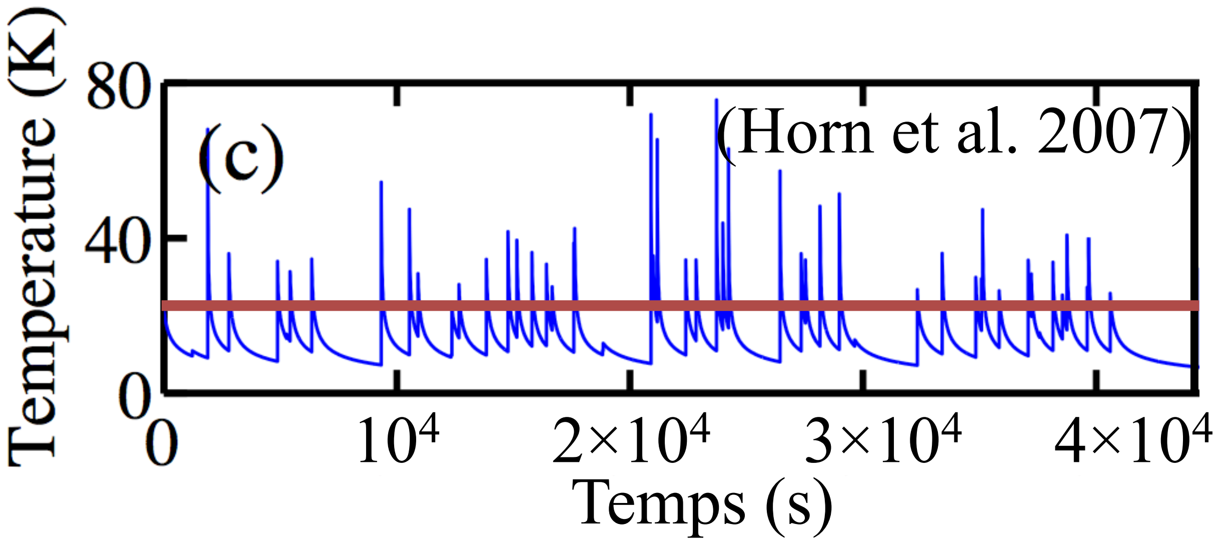
My current post-doc position is funded by the NANOCOSMOS ERC-SyG-2013 project, Grant Agreement number 610256

H_2 OPR in the ISM : the role of dust grains

Emeric Bron[1,2], Jacques Le Bourlot[2,3], Franck Le Petit[2]

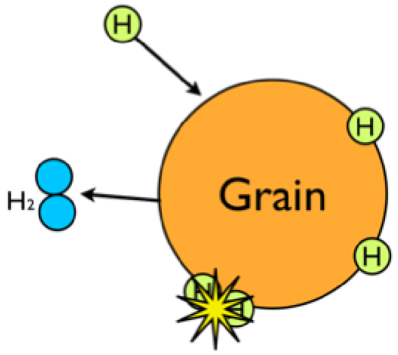
[1] ICMM, CSIC, Madrid, Spain
[2] LERMA, Observatoire de Paris, PSL Research University, CNRS, UMR8112, Paris, France
[3] Université Paris Diderot, Paris, France

Surface processes and dust temperatures :

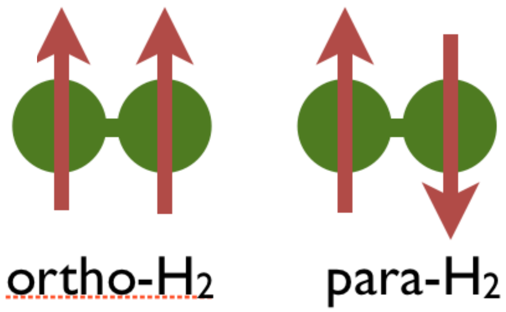


- crucial for the formation of molecules (from H_2 to COMs)
- very sensitive to surface temperature (thermal desorption and migration)
- ISM grains subject to temperature fluctuations (UV photons, cosmic rays and secondary UV photons)
- equilibrium chemistry at constant grain temperature not sufficient

Models for H_2-related processes :



- H_2 formation (Bron et al. 2014)
- Ortho/para conversion of H_2 (Bron et al. 2016)

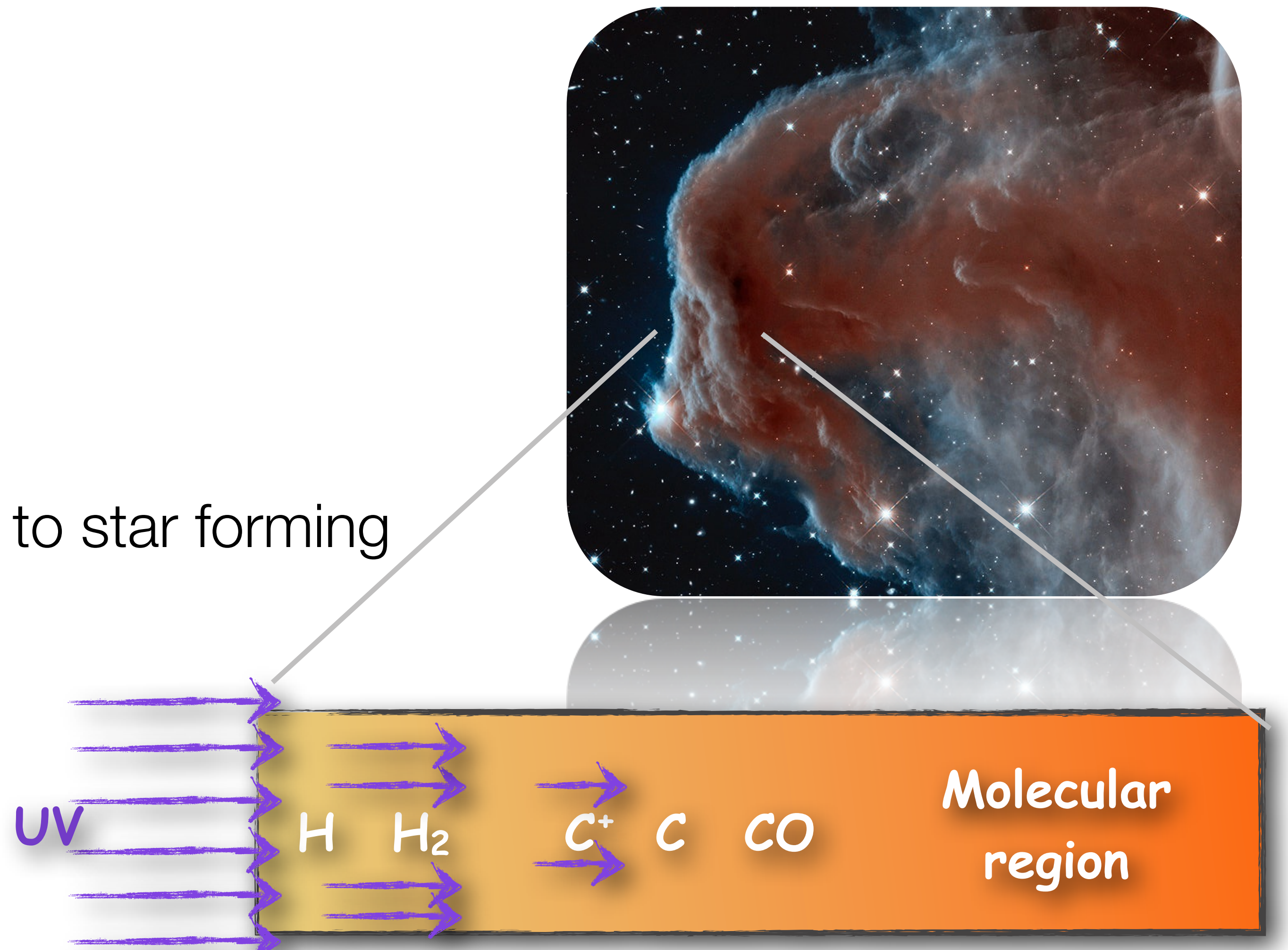


Photodissociation Regions (PDR)

Molecular cloud exposed to UV radiation

- warm molecular gas
- numerous tracers in emission
- same physics/chemistry from diffuse clouds to star forming regions, and proplyds.

→ Ideal to study the processes at play !

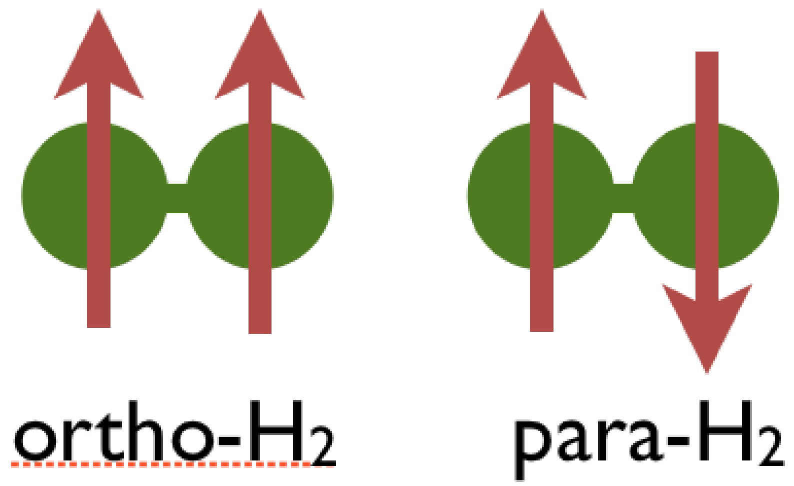


H_2, a central molecule

- First step of interstellar chemistry
- Atomic to molecular transition
- Tracer of warm molecular gas

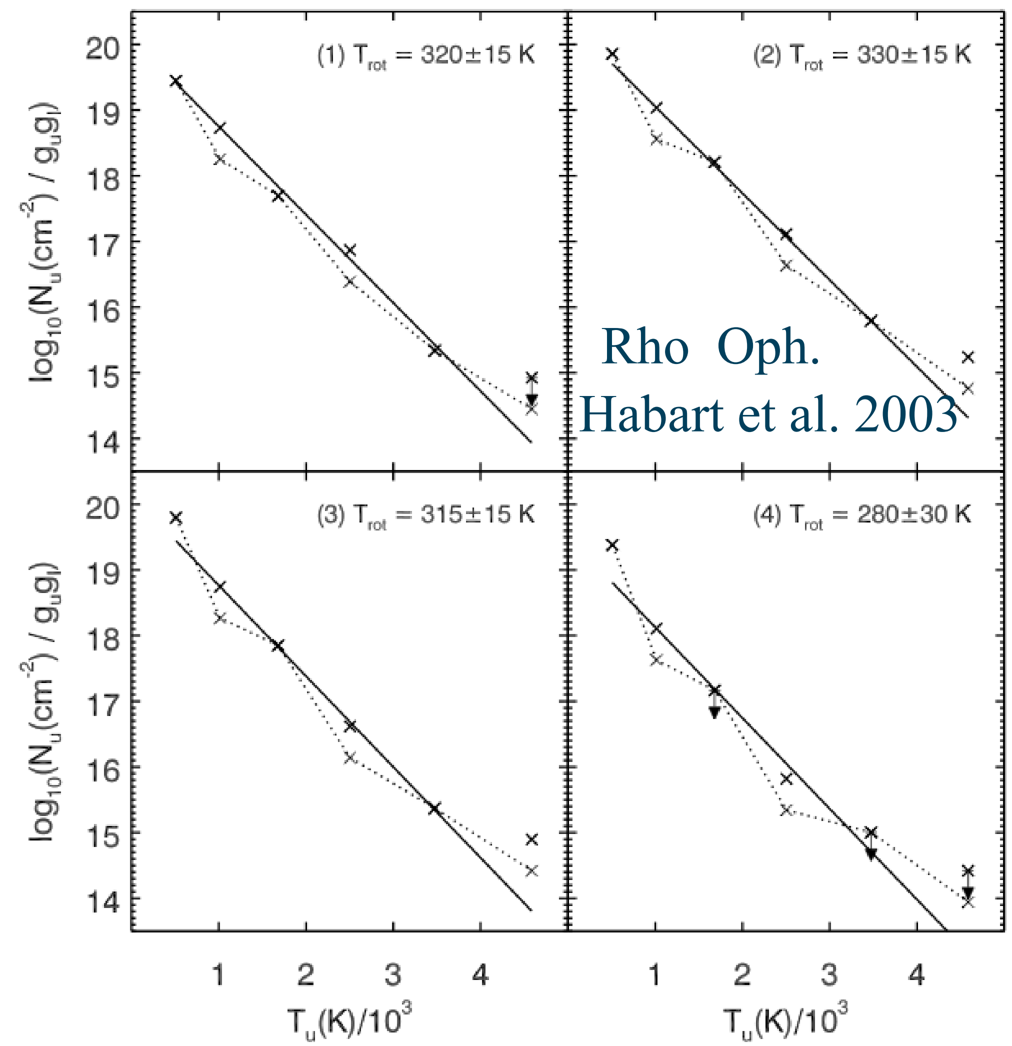
➛ ideal tracer of stellar feedback on molecular clouds with JWST

The ortho-para ratio (OPR) :



- two spin isomers
- nitrogen and deuterium chemistry
  (Dislaire et al. 2012, Flower et al. 2006)
- affects the equation of state
  (Vaytet et al. 2014)

- thermodynamical value at >200K : 3
- observations in PDRs (warm gas) :
  ~1 (ISO/Spitzer)
  (Habart et al. 2011)



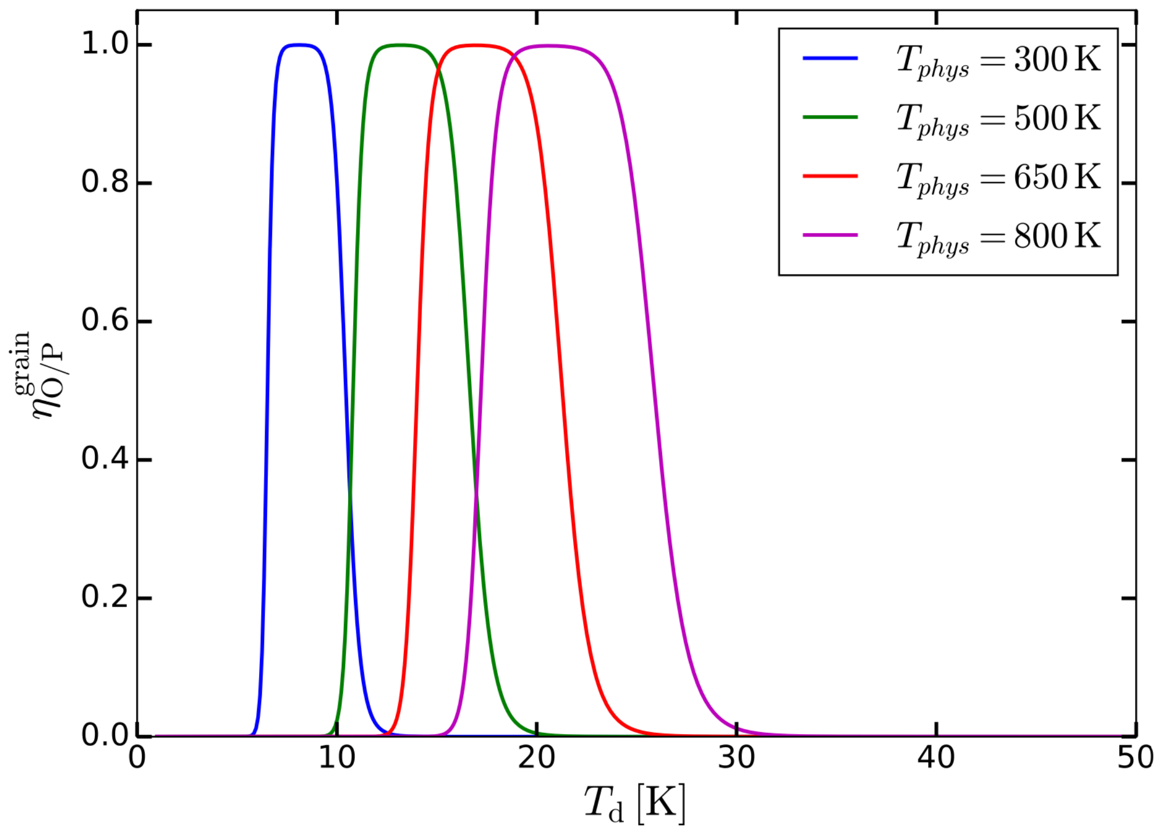
Control mechanisms for the OPR :

- reactive collisions (H, H^+, H_3^+)
  ➢ thermalization to gas temperature, but slow process
- competition with surface conversion
  ➢ thermalization to dust temperature
- before H/H_2 transition, formation/destruction cycling dominates (OPR locally >3)

Ortho-para conversion on grains :

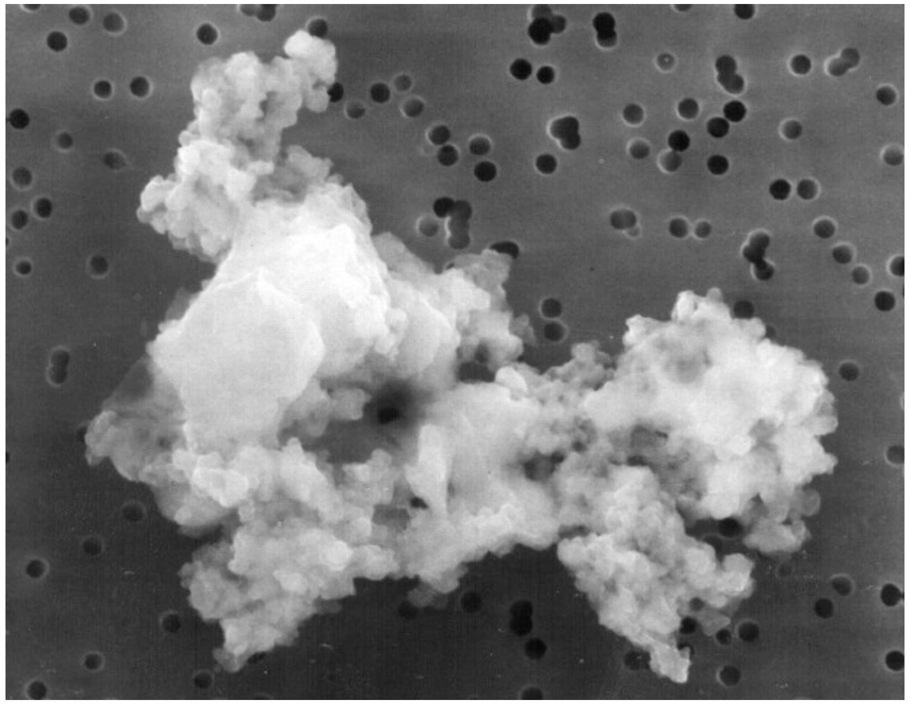
- Few experiments, mostly on ice surfaces (Fukutani & Sugimoto 2013)
- Experiments
  ➢ efficient only on cold surfaces (<25K)

    ➢ inefficient in PDRs ?



but, Le Bourlot et al. 2000, Sheffer et al. 2001 : if efficient, explains observations very well

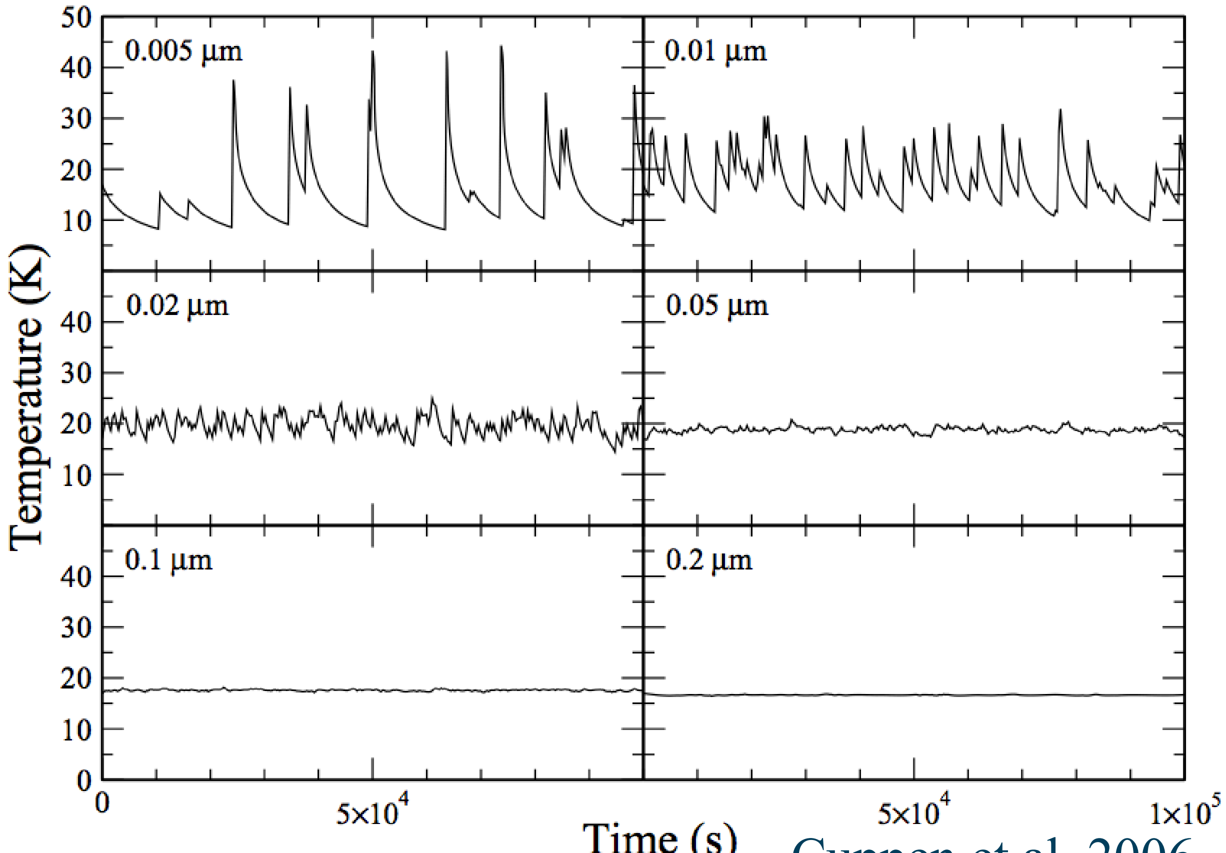
Introduction



- Dust grains absorb UV photons, re-emit in IR
- Discrete radiative processes
- Small grains → small heat capacities → large temperature fluctuations
- Short peaks / long cold phases

- Average rate ≠ rate at average temperature
- IR emission: dominant during the temperature peaks

➛ How do we estimate the average efficiency of chemical surface processes ?



Cuppen et al. 2006

- Coupled fluctuations of the dust temperature and of the surface chemical state
- Interested in average rates (formation, conversion)
- Statistical state of the grain : PDF $f(T,n)$ (temperature, surface population)
- Obeys a Master equation :

$$\int dY\, p_{Y\to X}\, f(Y) = f(X) \int dY\, p_{X\to Y}$$

statistical equilibrium : departure rate = arrival rate for each state.

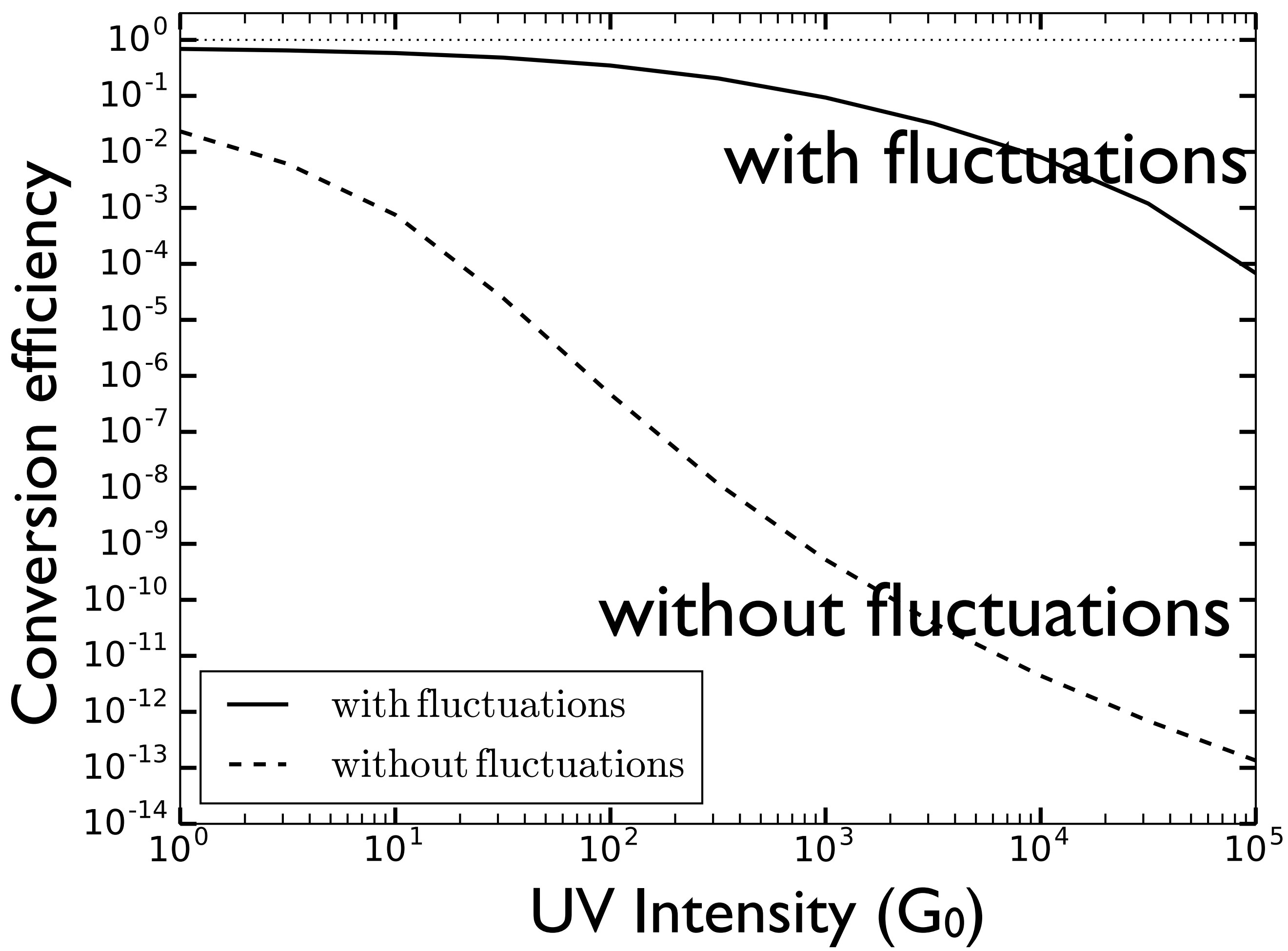
- Integral equation $\longrightarrow$ solved numerically
- Average rates :

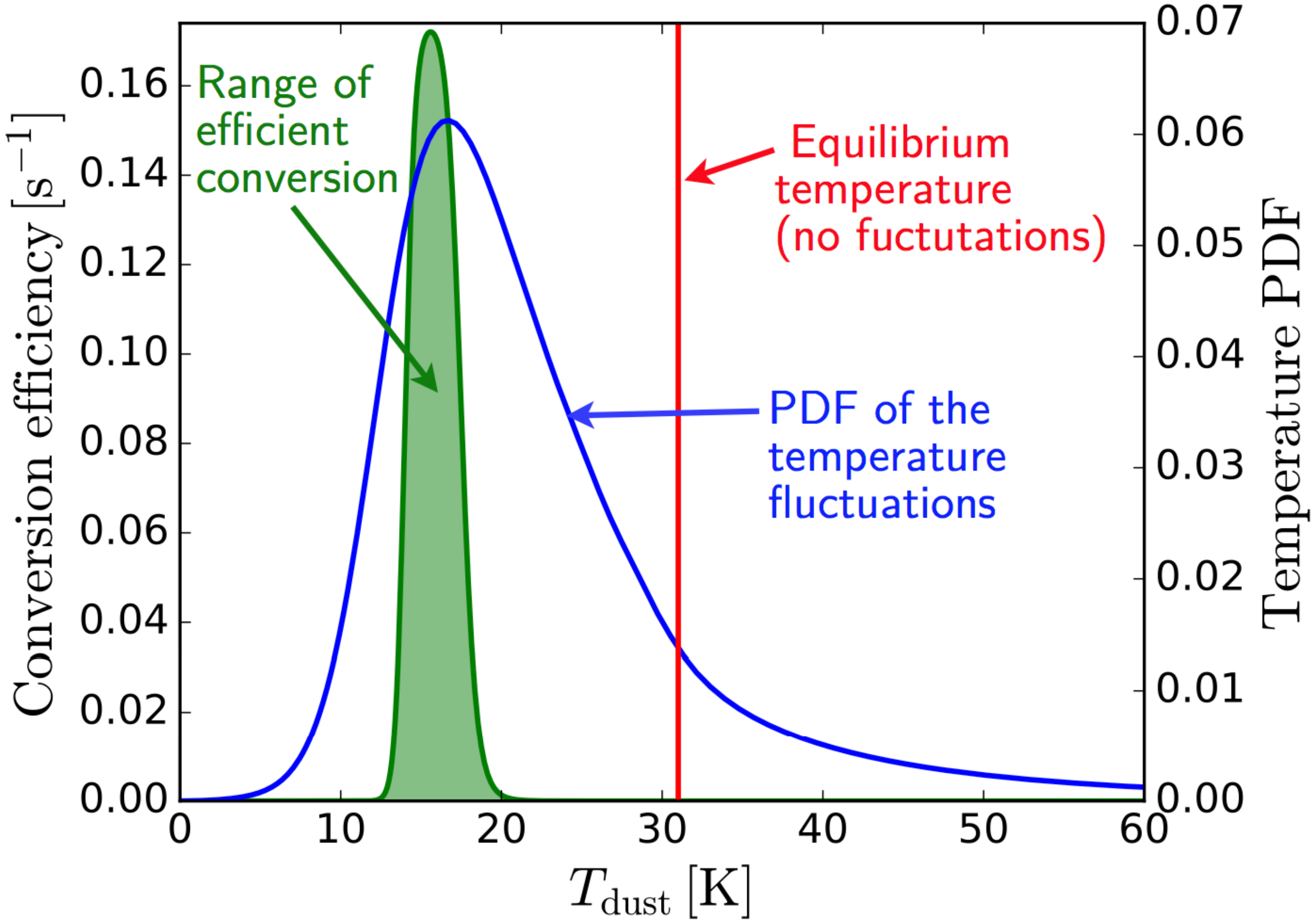
$$\langle k \rangle = \int dX\, f(X)\, k(X)$$

➛ Bron et al. 2014, 2016

Results

Ortho/para conversion





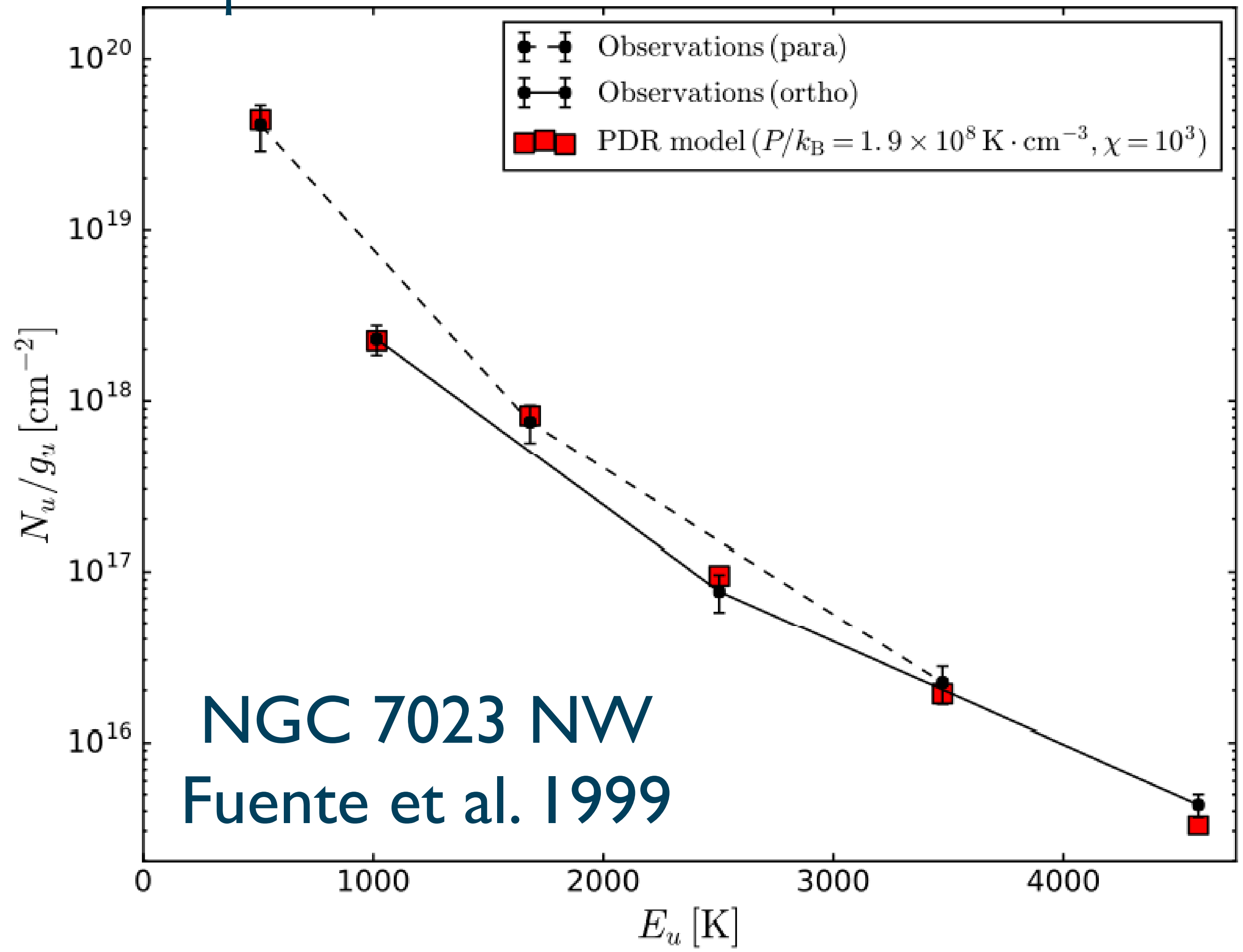
- Efficient conversion on UV-exposed grains (several % up to $G_0 \simeq 10^4$)
- Small grains spend most of their time at low temperature between spikes
  ➛ equilibrium or average temperature are not relevant !

Bron et al. 2016

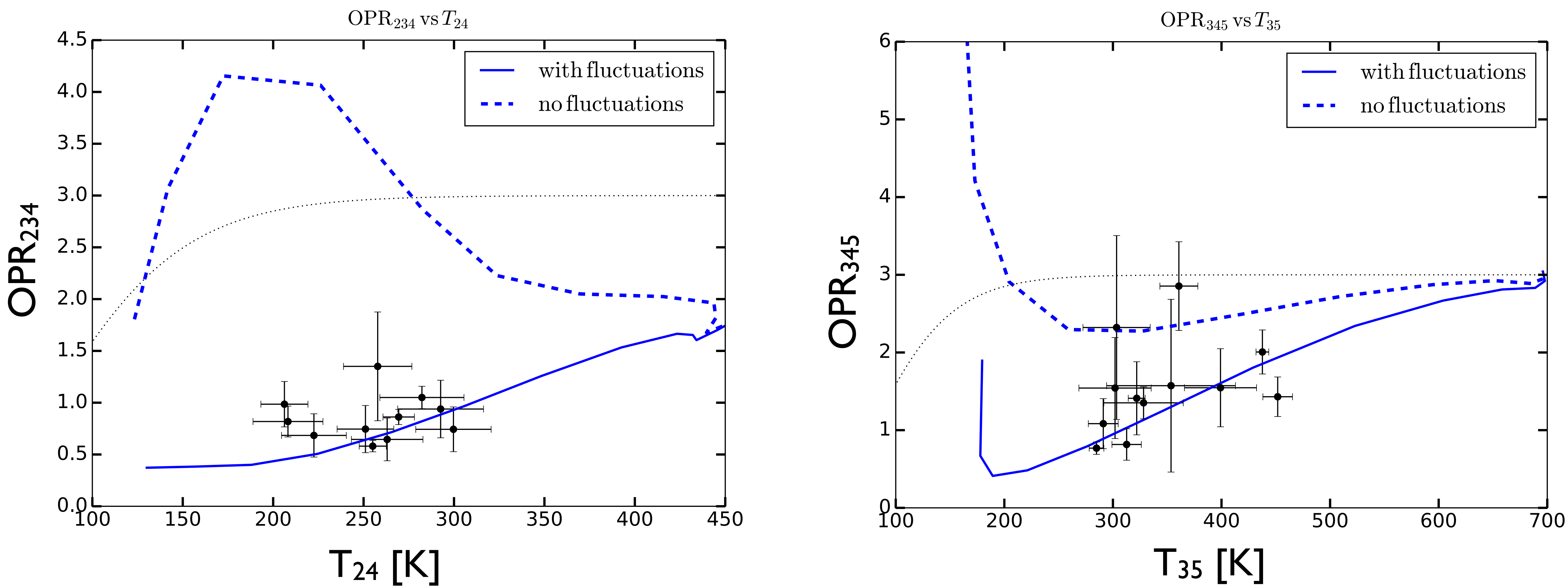
Observing the OPR :

- Emission ➛ we only see excited levels
- In dense PDRs, low rotational levels dominated by collisions.
- PDR ➛ Strong temperature gradient
- OPR deduced from offset between ortho and para states

- Each triplet of rotational lines ➛ OPR value + excitation temperature
- Probe evolution of the OPR across the PDR + variation with gas temperature



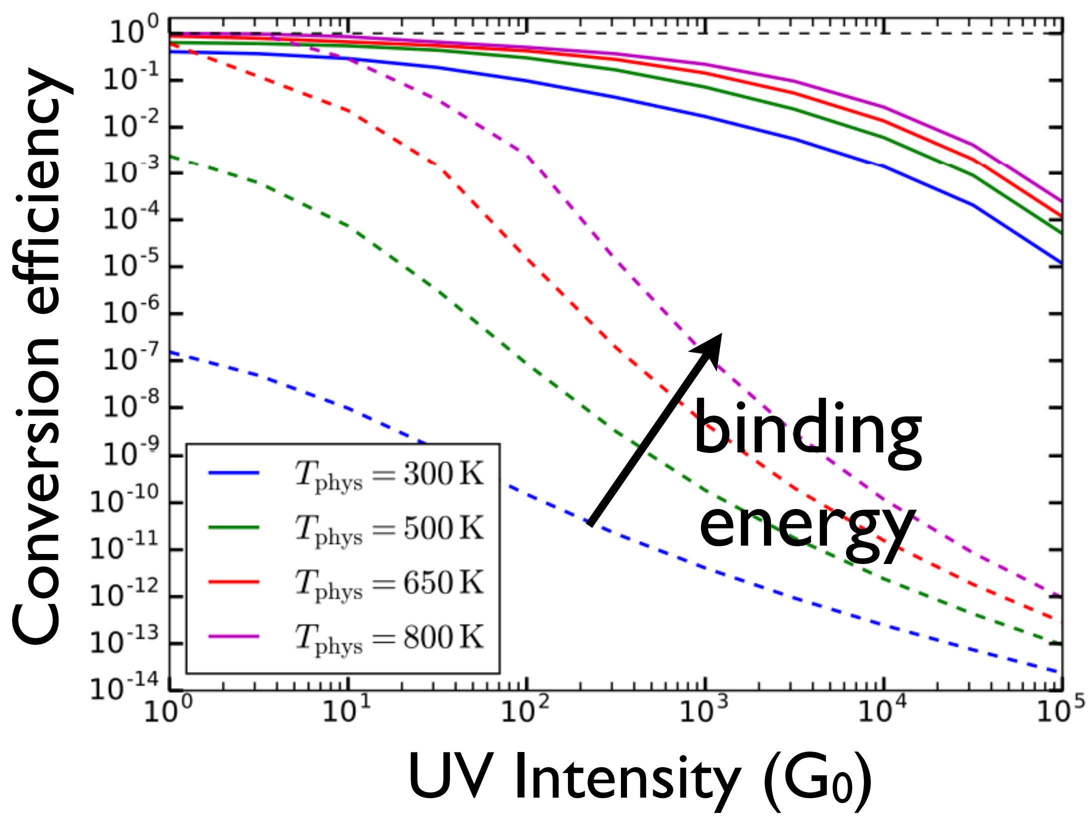
Comparison to PDR observations :

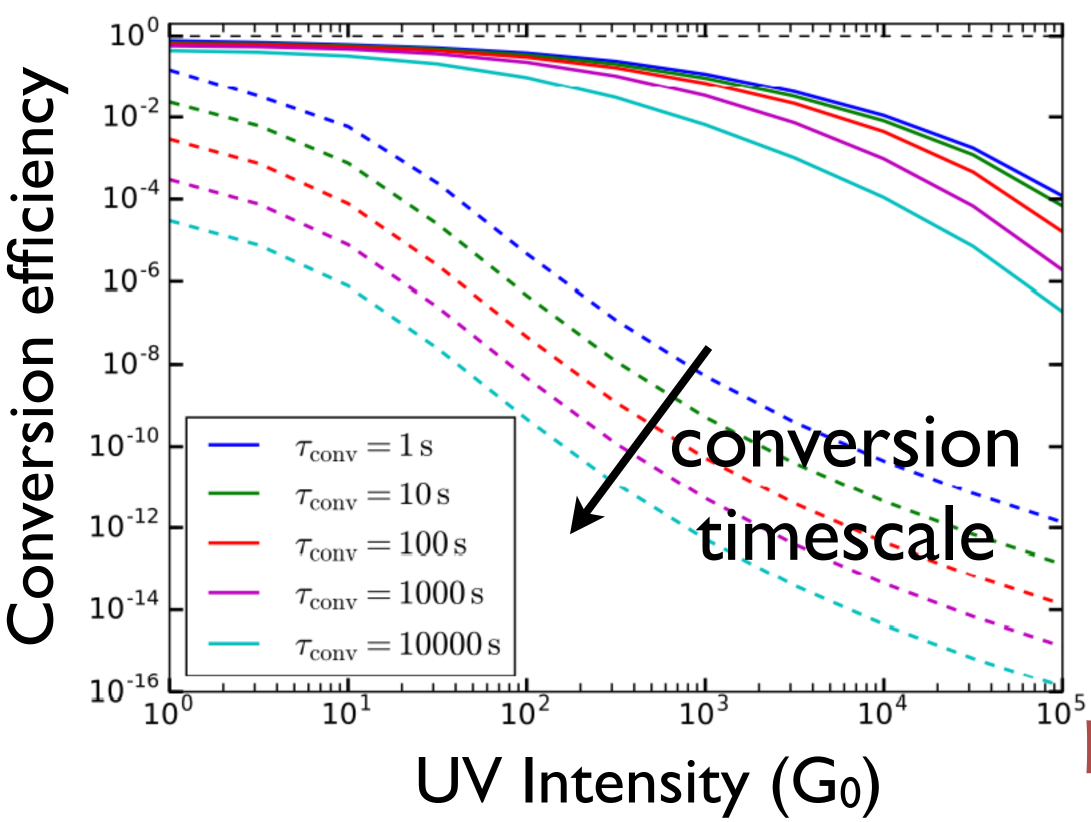


- Observations show efficient conversion
- Including the fluctuations allow sufficient conversion efficiency

Bron et al. 2016

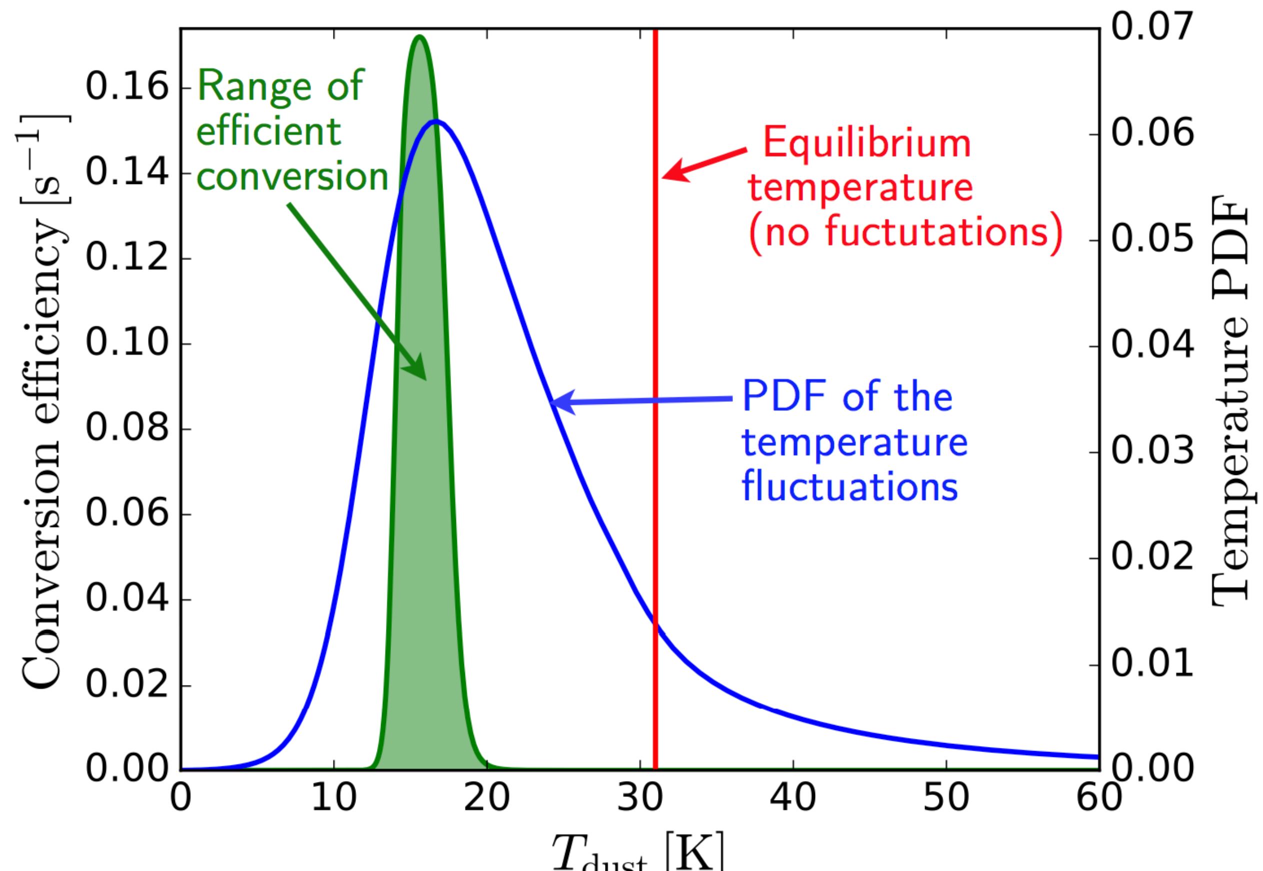
Results | Sensitivity to uncertainties





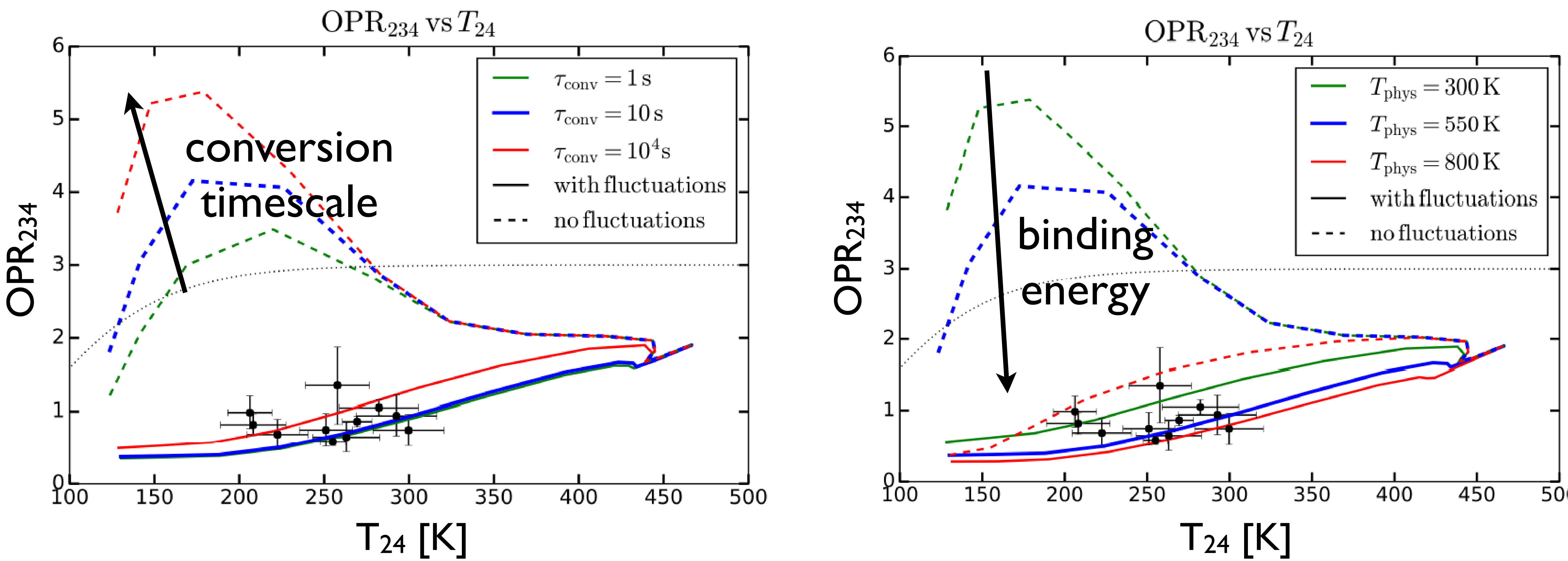
Sensitivity to microphysical parameters :

- Strong impact without fluctuations / weak impact with fluctuations !
- Temperature distribution smoothes the variations



Bron et al. 2016

Uncertainties on microphysical parameters :



- Strong impact of the uncertainties when neglecting fluctuations
- Low sensitivity when including temperature fluctuations

Bron et al. 2016

Conclusions

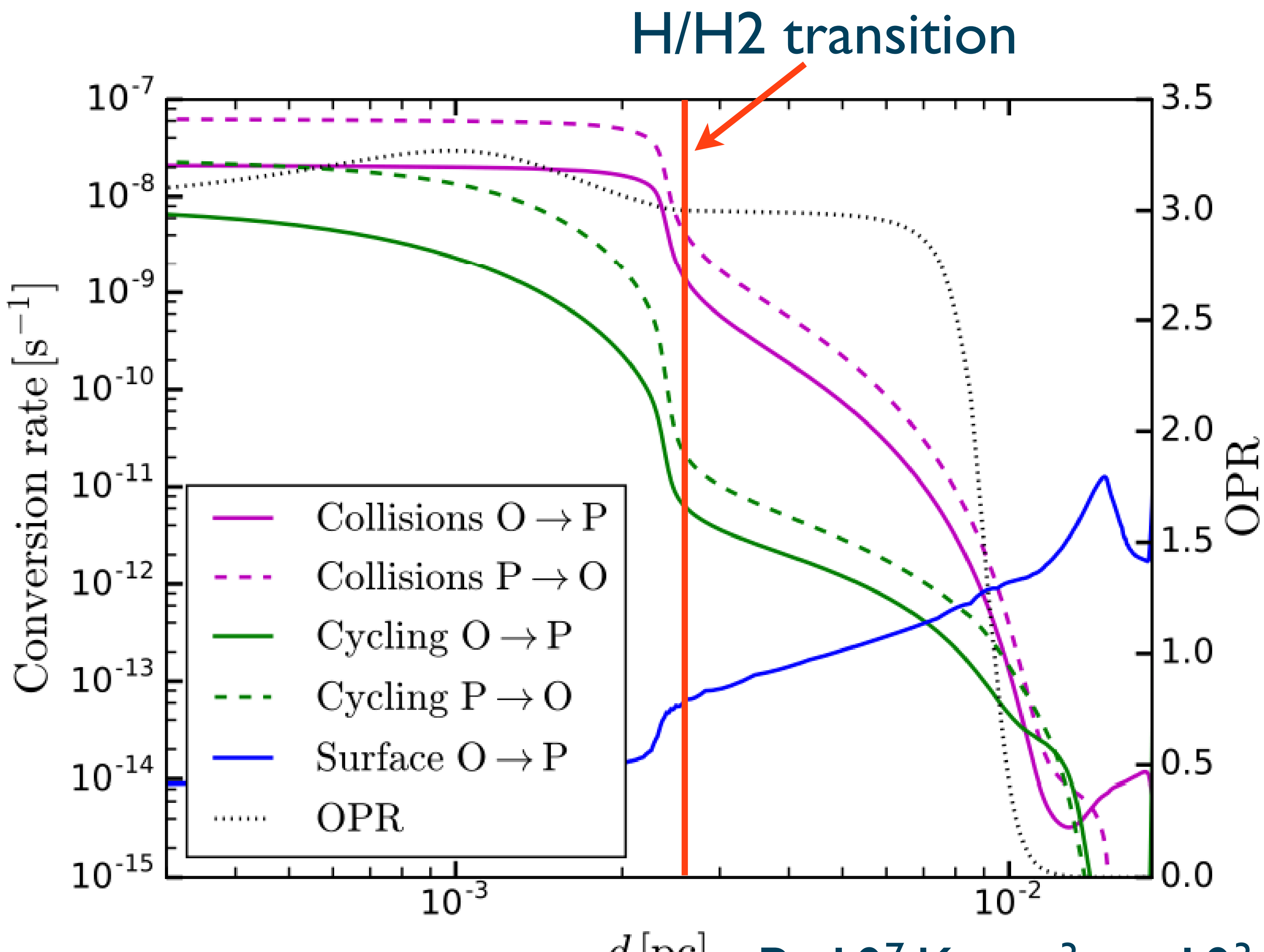
- Without dust temperature fluctuations : conversion only on cold grains
- H_2 observations in PDR indicate efficient conversion
- Conversion efficiency explained by temp. fluctuations for small grains
- Fluctuations reduces sensitivity to microphysical parameters (binding energy, etc...)

Temperature fluctuations can have a strong impact on surface processes

Thank you for your attention !

Results

Conversion timescales



$P=10^7$ K cm^{-3}, $\chi=10^3$

Bron et al. 2016

Results

H_2 emission zone