Molecule formation in the early Universe

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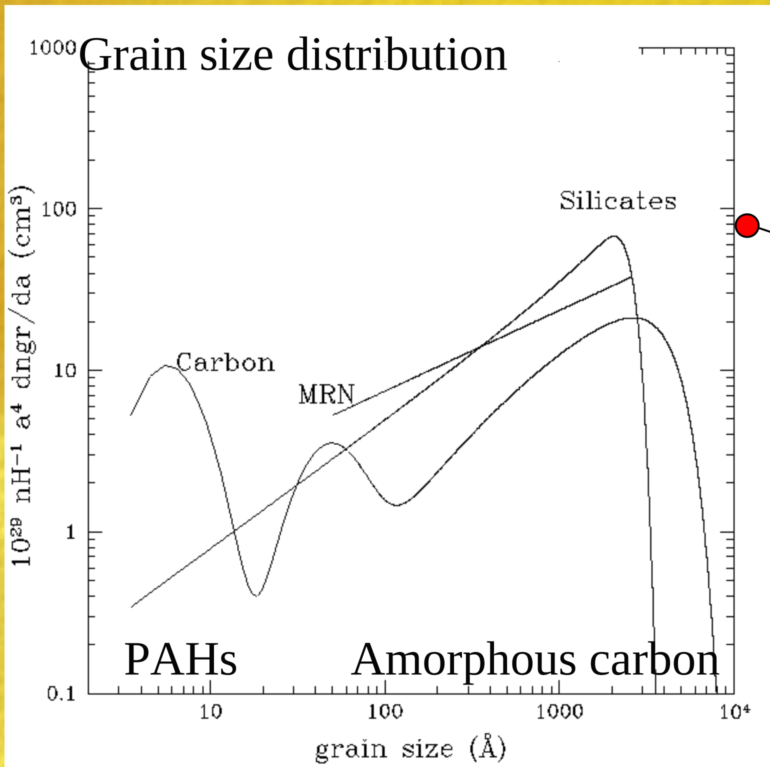
Molecules and **Du**st at **lo**w metallicity

11th March 2010

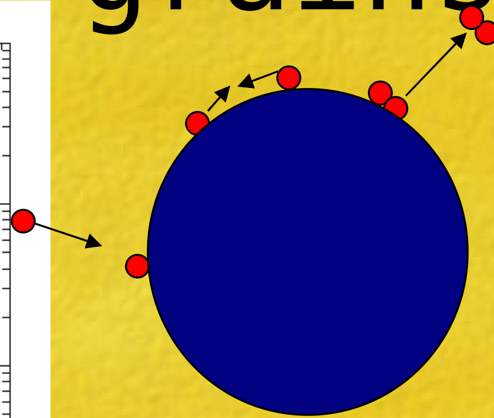
Introduction

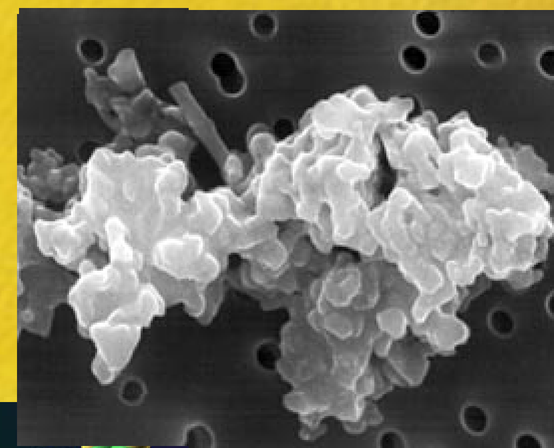
- Stars formation = cloud collapse (**gas + dust**)
- **Molecules** such as CO, O_2, H_2O, **cool** the gas *(Neufeld et al. 1995)*
- **Metal poor** environments $\rightarrow$ **H_2 & HD** are important coolants.
- Formation of the **first stars** of the Universe = **H_2** *(Bromm 2002).*
- Molecules form in **gas & on dust**.
- Formation routes of molecules VS **metallicity**?

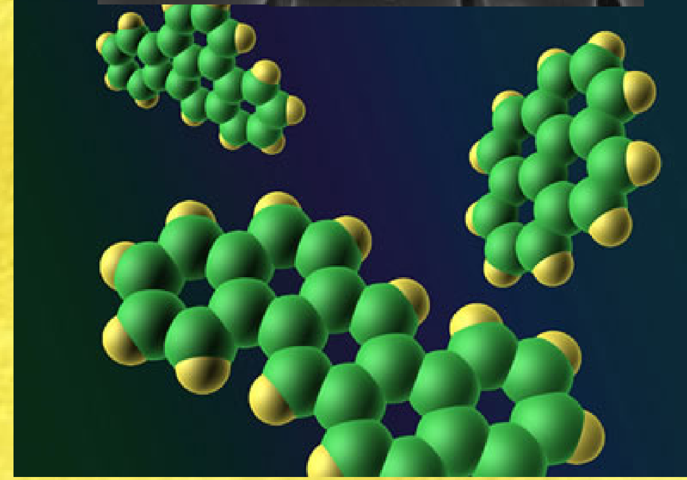
Interstellar dust grains



Weingartner & Draine 2001
Mathis, Rumpl & Nordsieck 1977







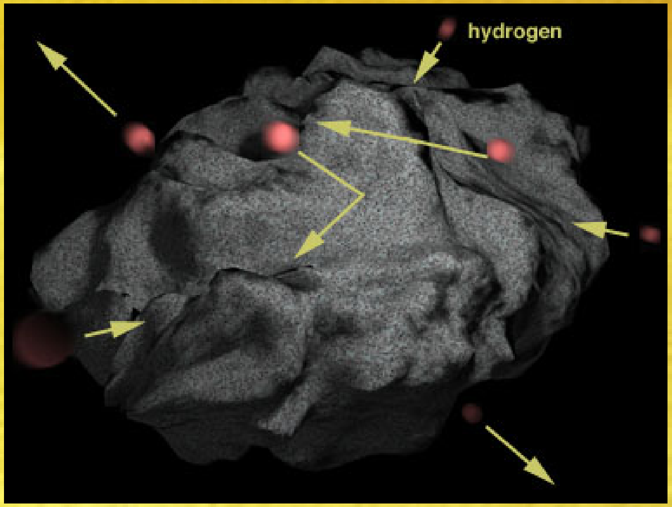
How does H_2 (HD and D_2) form on interstellar dust grains?

Does the formation of H_2 (HD and D_2) change with the size of dust grains?

H_2 (HD) formation on interstellar dust

Process studied by several authors:

Hollenbach & Salpeter 1971, Duley 1996, Katz et al. 1999, Morisset 2004, Cuppen & Herbst 2005, Cuppen & Hornekaer 2008



Our model:

- Interactions atom/surface:
  - Experiments: TPD
  - ab initio calculations

➡ Mobility atoms on the surface.

Rate equations and Monte carlo simulations

Comparison with observations

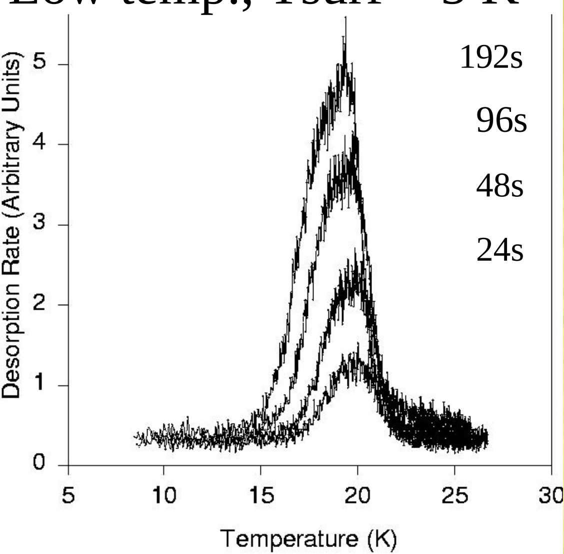
Interaction atom/surface: experiments

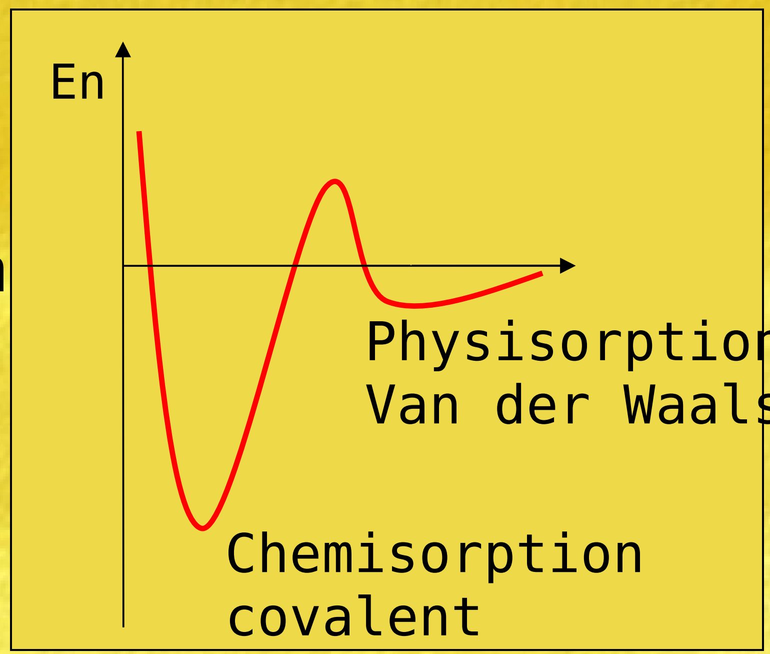
Experiments on graphite, amorphous carbon, silicates

Pirronello et al. 1997, 1999, Zecho et al. 2002, Perets et al. 2007, Vidali et al. 2007

Amorphous Carbon

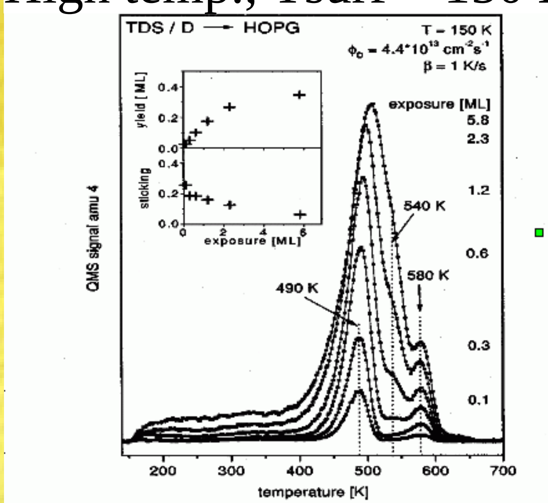
Low temp., Tsurf = 5 K



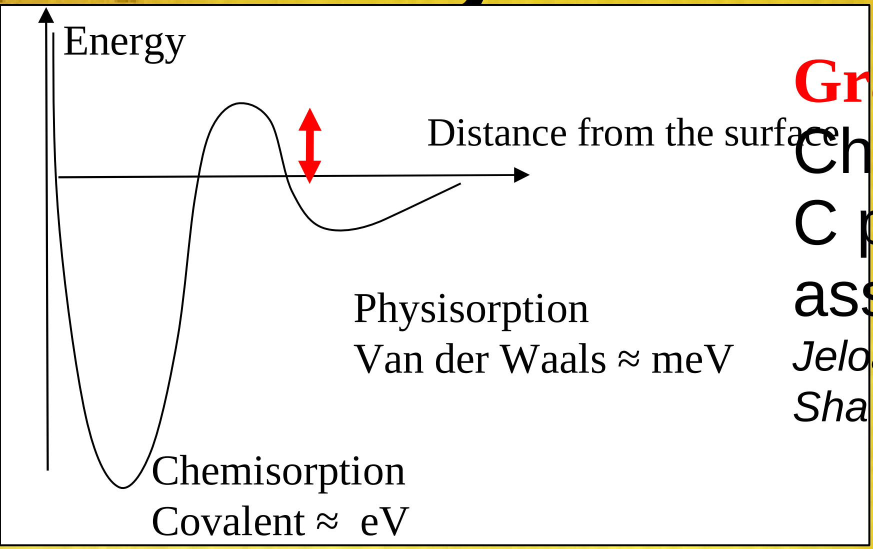


Graphite

High temp., Tsurf = 150 K



Interaction atom/surface: Density functional theory (DFT)



Graphite:

Chemisorption of H

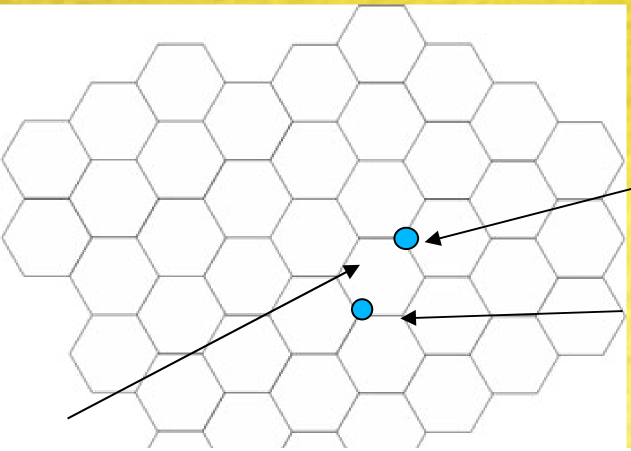
C puckered out of the basal plane

associated with barrier ~ 0.2 eV.

Jeloaica & Sidis 1999

Sha & Jackson 2002

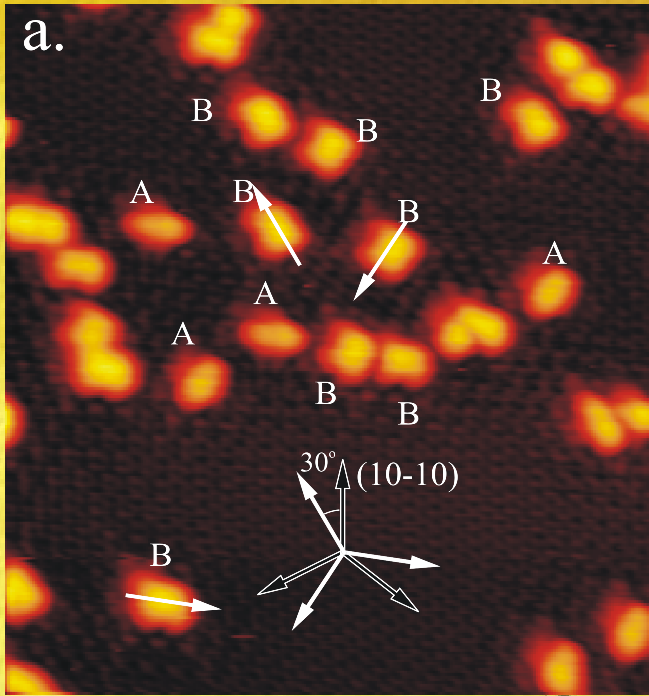
Recent studies: Hoernekær et al. 2006, Rougeau et al. 2006, Bachellerie et al. 2007



1^{st} H → barrier

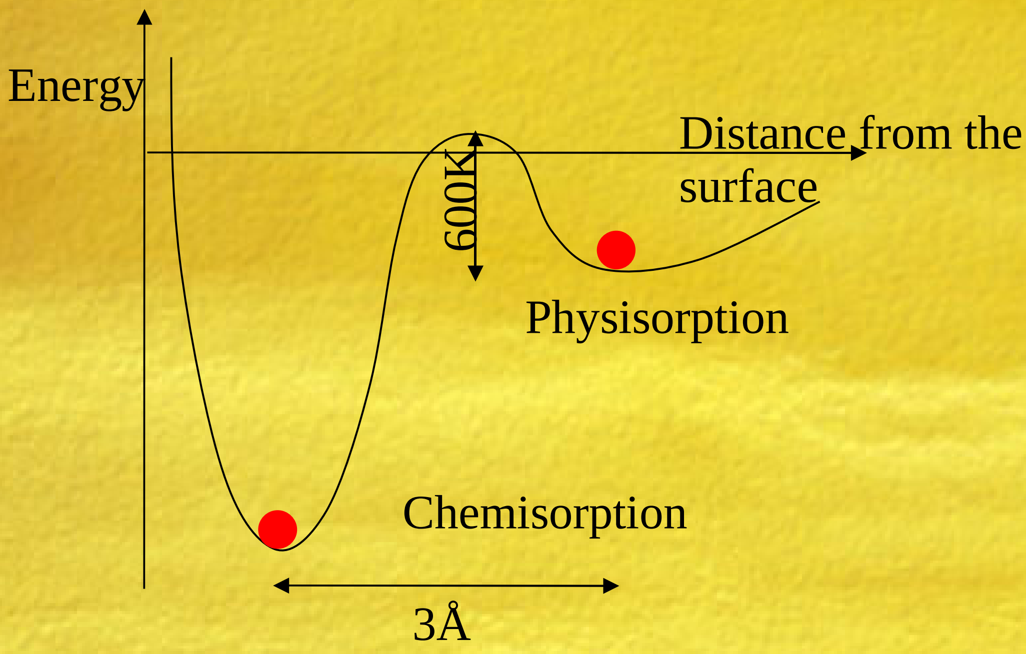
2^{nd} H → no barrier to enter para site if spin opposite to 1^{st} H

● 3^{rd} atom → no barrier to form H_2



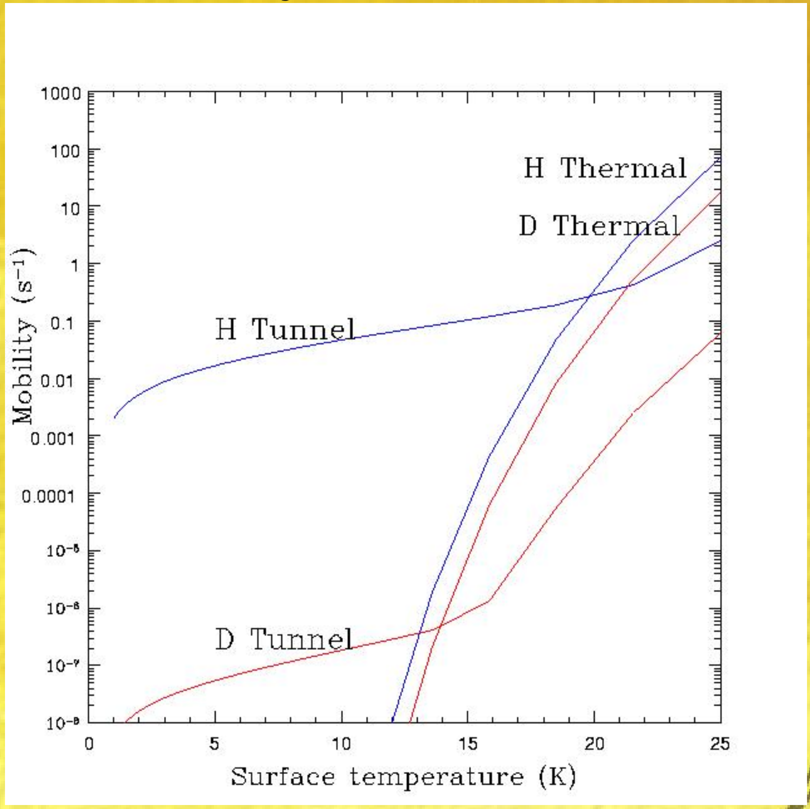
STM @ 170K

Model: Interaction and mobility



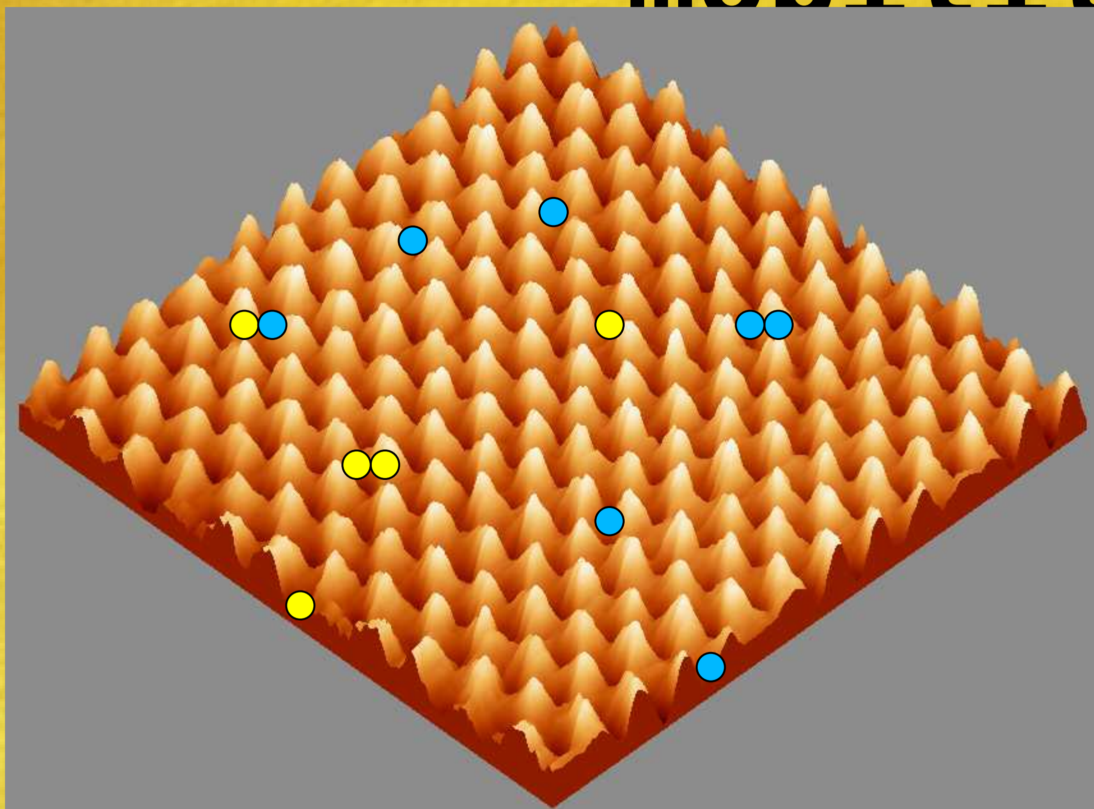
Transmission coefficient of the barriers

・ mobility of H and D atoms



- Physisorption + chemisorption
- tunnel + thermal hopping

Model: Interaction and mobility



physisorbed H atoms

physisorbed D atoms

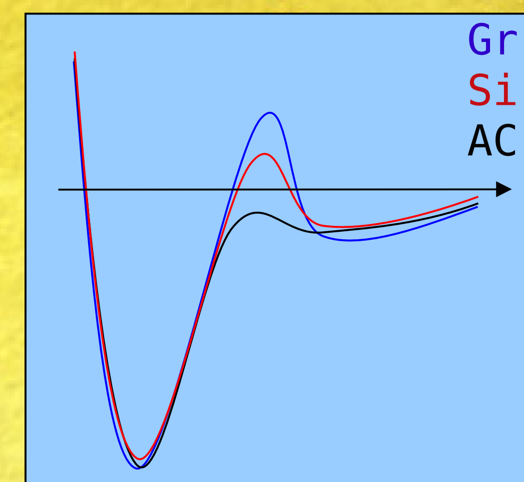
chemisorbed H atoms

chemisorbed D atoms

H_2

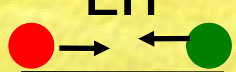
HD

D_2

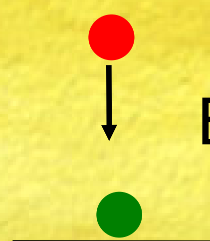


Mechanisms:

LH



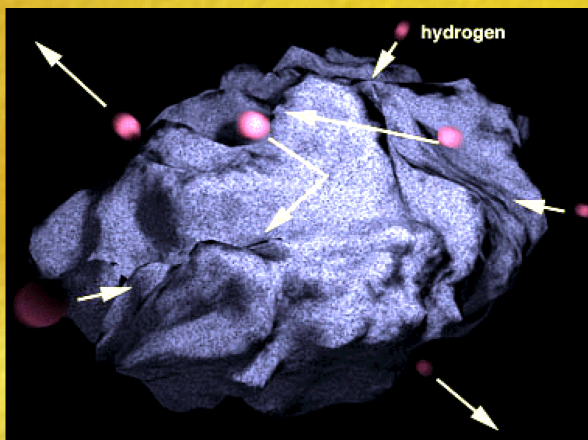
ER

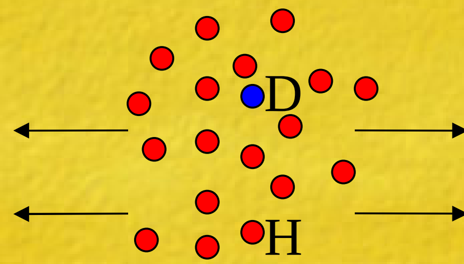


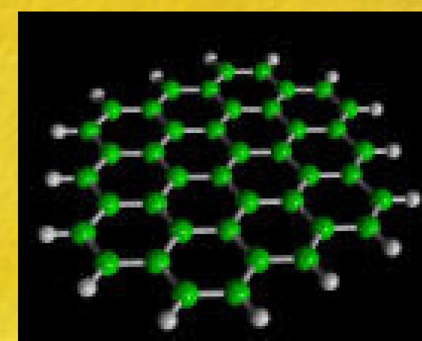
Rate equations and Monte Carlo simulations.

Rate equations

Monte Carlo



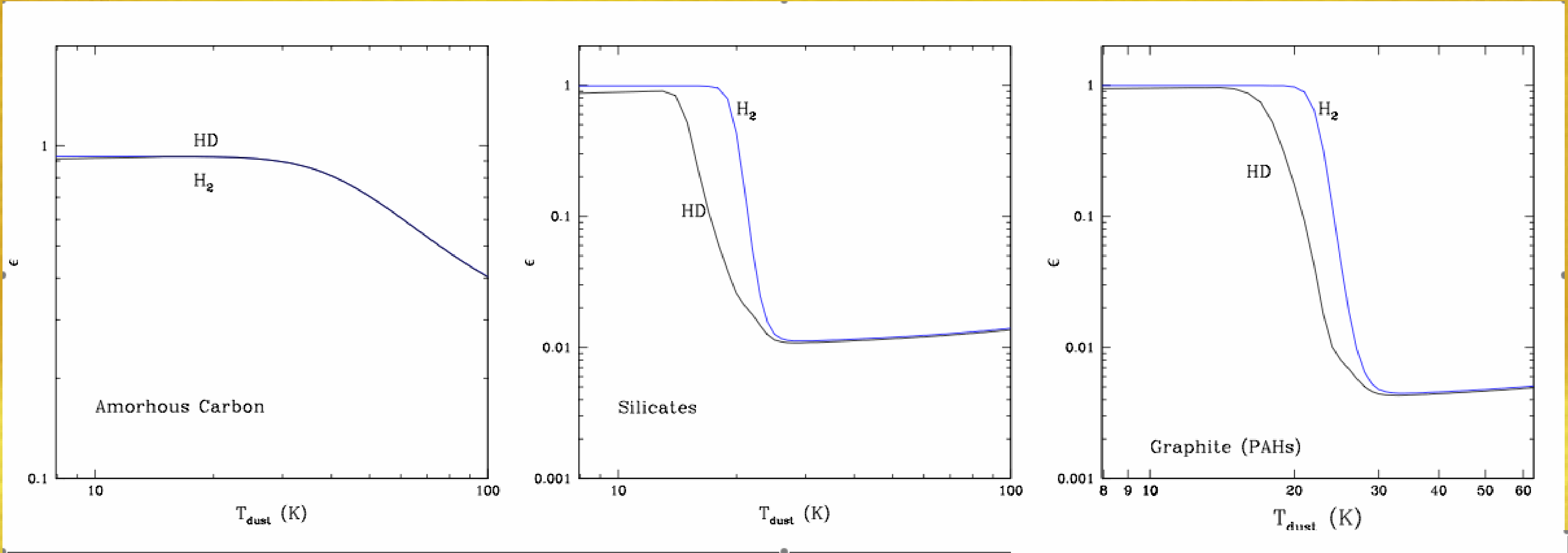




Follow populations
Big grains → always 1 species

Follow each species
small grains
random accretion and random walk
detail characteristic of the surface → para sites

Results



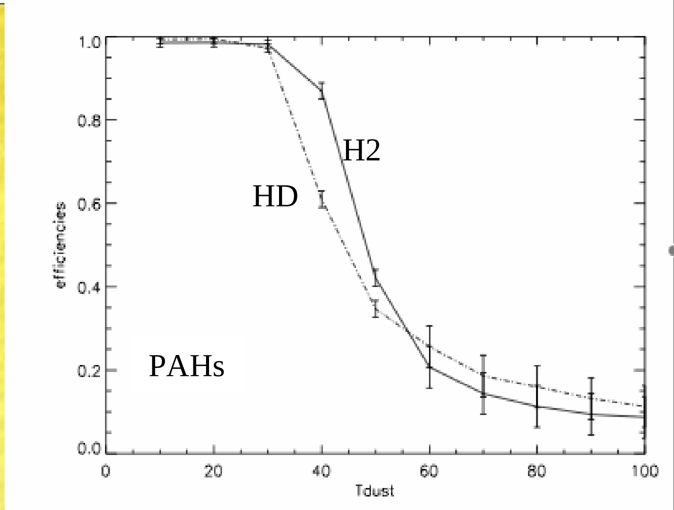
Formation of H2 and HD

→ physisorbed atoms @ low T_{dust}

→chemisorbed atoms @ high T_{dust}.

Inclusion para sites

→ Increase the efficiency >1 mag

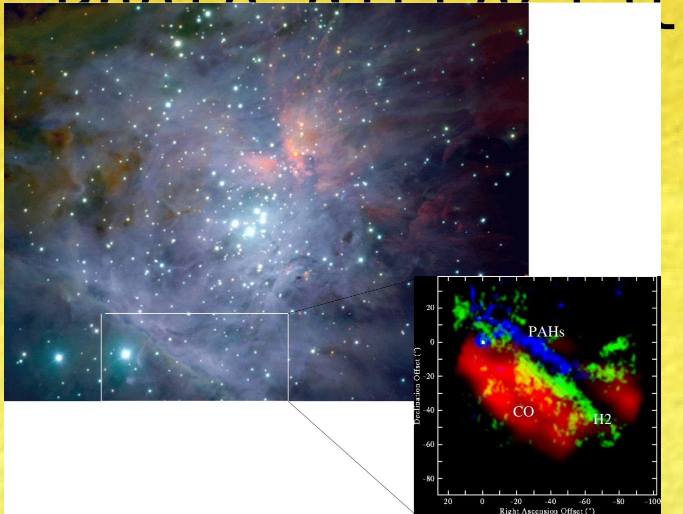


H_2 formation rate in the ISM

$$R(H_2)=(1/2)\ n_H\ v_H\ \sigma\ n_d\ S_H\ \underline{\boldsymbol{\varepsilon}}$$

- n_H number density of H atoms
- v_H speed of H atoms in the gas phase
- $\boldsymbol{\sigma}$ area of the grain
- n_d number density of dust grain
- S_H sticking coefficient of the H atoms on the grain
- $\boldsymbol{\varepsilon}$ H_2 recombination efficiency

Photo dissociation regions



H_2 formation rate: Photo-dissociation Regions

Observations of several PDRs
(*Abergel et al. 1996; Habart et al. 2003)*

T_{dust}= 15 - 90K

T_{gas}= 60 - 620K

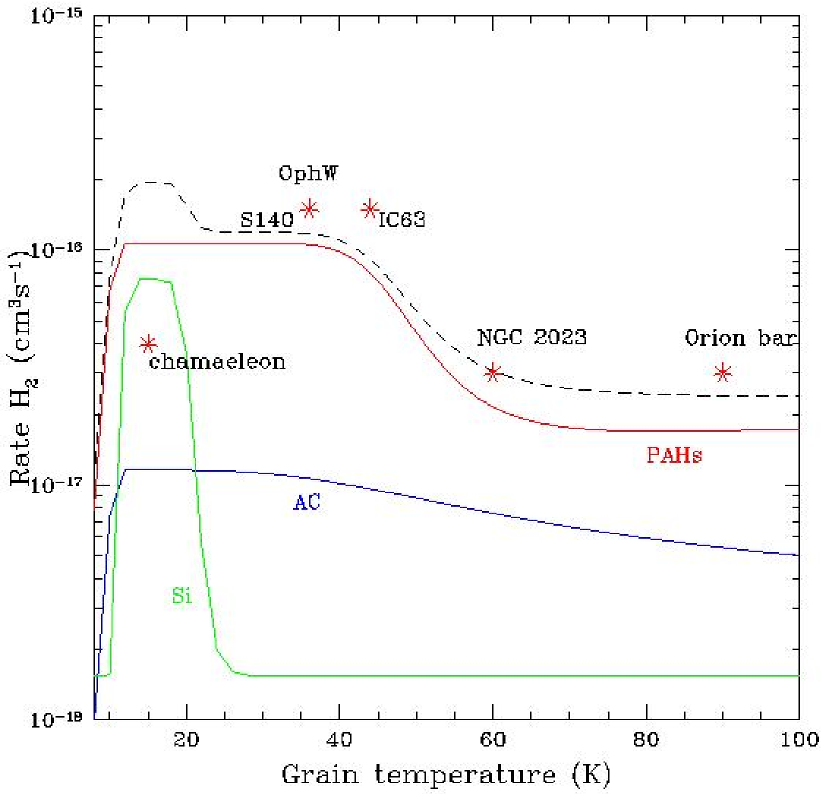
$R(H_2)$= 3 10^{-17} - 1.5 10^{-16} cm^3s^{-1}

H_2 formation @ high Tdust and Tgas → para sites properties

Other factors: **$R(H_2)=(1/2)\ n_H\ v_H\ \sigma\ n_d$**

Observations of PDRs → H_2 forms efficiently on cold and warm dust grains.

The inclusions of the barrier-less route to form H_2 on PAHs (para sites) is necessary to reproduce the observations of PDRs.



Gry et al. 2002
Habart et al. 2004

H_2 and HD in the early Universe

- **First stars** (pop III) are cooled by $\mathbf{H_2}$ (quadrupolar transitions)

- H_2 cools until 200K → **very massive** star ~100$M_{\odot}$ *(Abel et al. 2000, 2007, Bromm et al. 2002, Omukai & Palla 2003, Jappsen et al. 2007)*

- First stars ionize the Universe → **next generation** can form in a **HD** cooled gas (dipolar transitions, cool until few ×10K) → star of **few × 10$M_{\odot}$** *(Johnson & Bromm 2006, Yoshida et al. 2007, Mc Greer & Bryan 2008)*

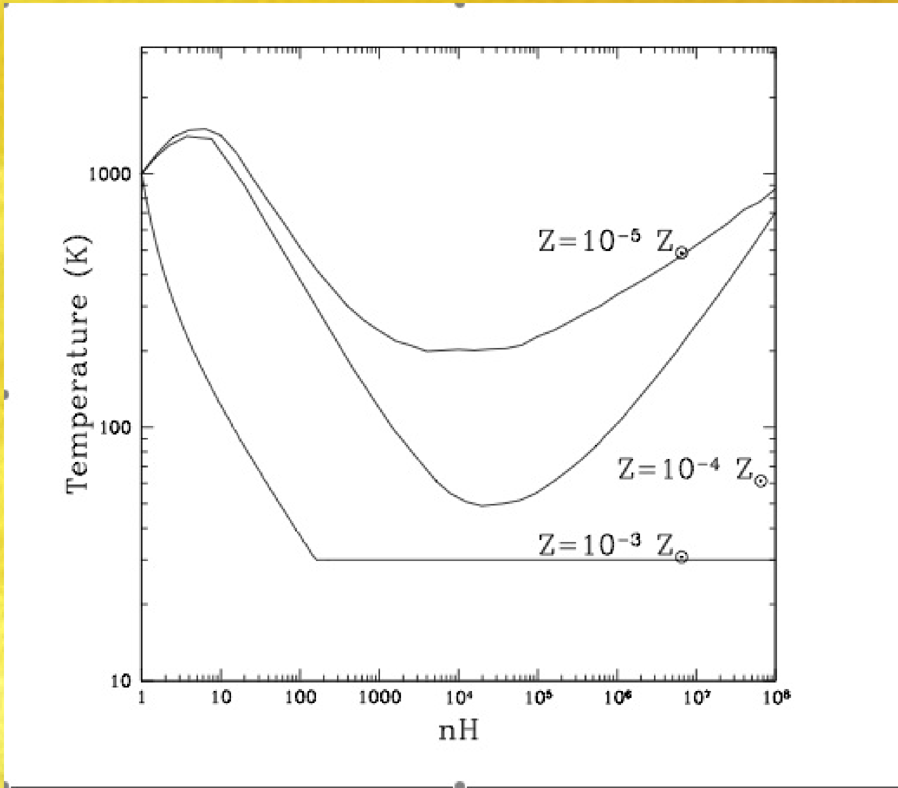
- **Chemical** composition of **collapsing clouds** → which coolants dominate → resulting star

H_2 and HD in the early Universe

- Model: **gas cloud** with uniform metallicity undergoes **gravitational collapse** at the free fall rate.
- Chemistry **dust + gas** phase (*Glover & Savin 2008, Galli & Palla 1998*). Which formation routes dominate:
  - For H_2
    - Grain surface
    - H^- + H route
  - For HD
    - Grain surface
    - D^+ + H_2 route
- **Grain size distribution** linear to *Weingartner & Draine 2001*

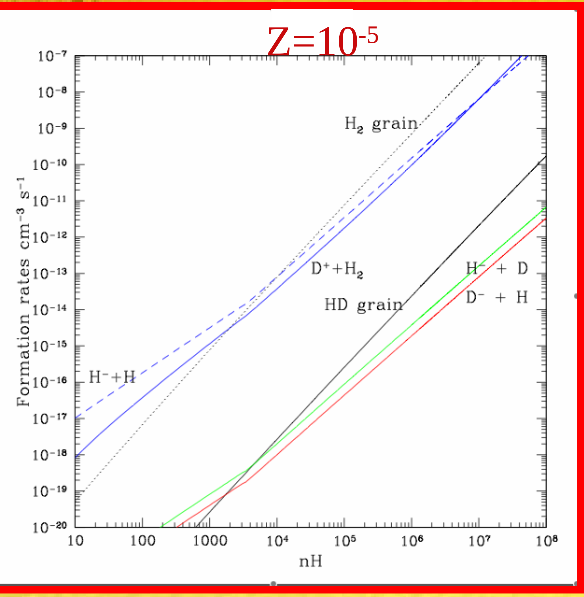
H_2 and HD in the early Universe

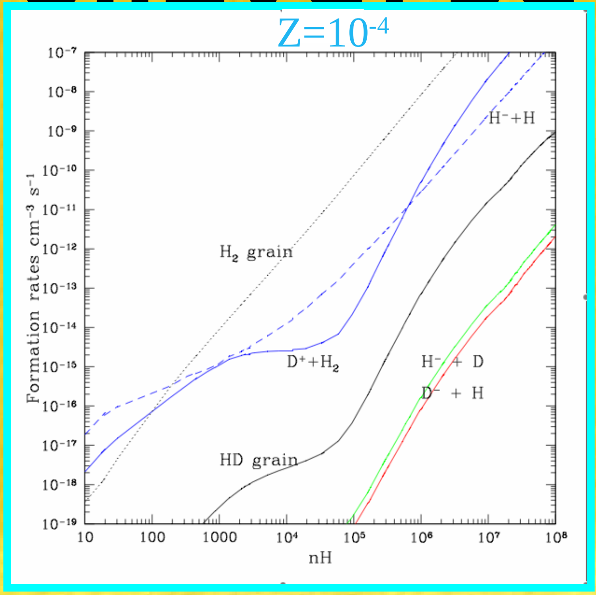
- Clouds collapse @ z = 10; nH = 1 cm-3
- Temperatures profiles depend on
  - Adiabatic heating
  - Cooling by H_2 and HD (when no metals, *Glover & Abel 2008*)
  - Cooling by fine structure lines (*Meijerink & Spaans 2005*)

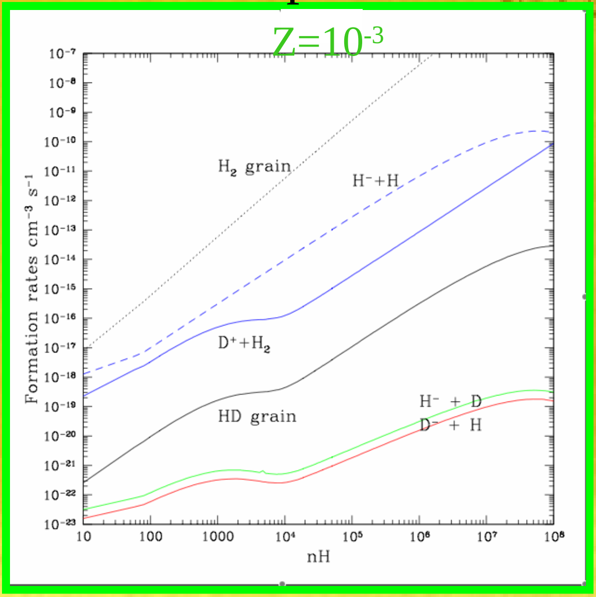


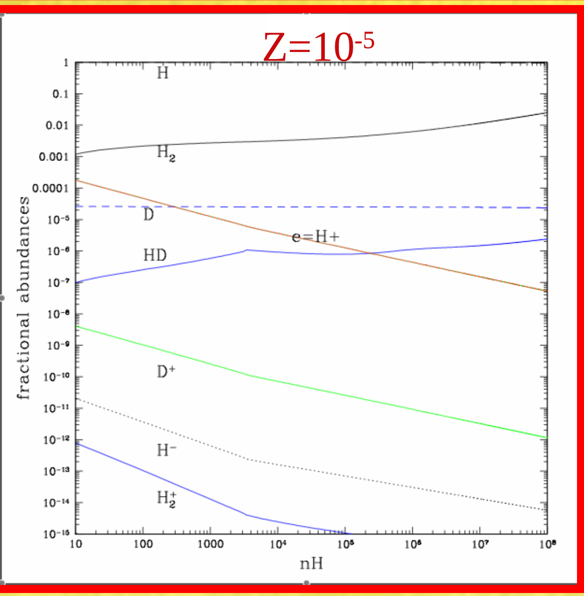
H_2 and HD in the early Universe

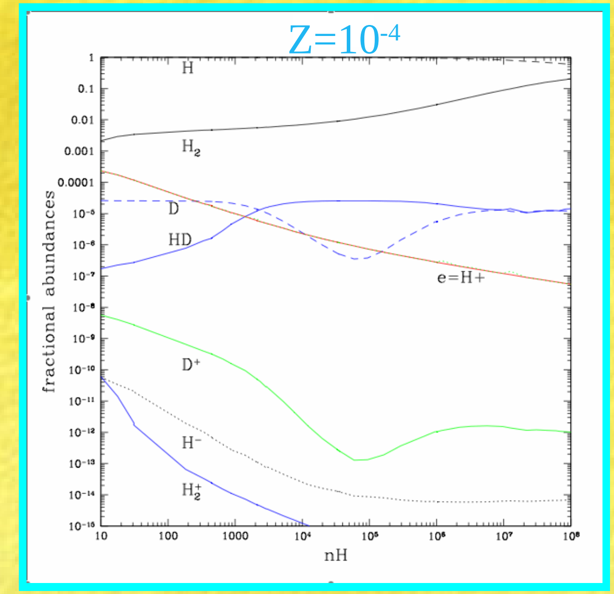
Cazaux & Spaans 2009

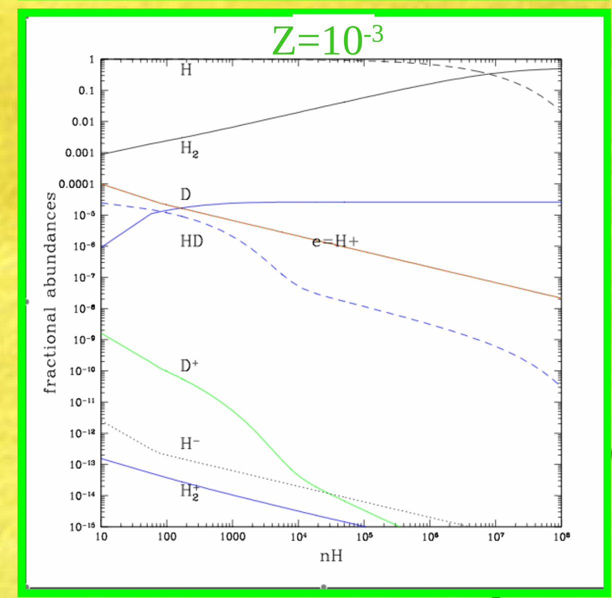












H_2 and HD in the early Universe: Conclusions

- **Small fraction of dust** $\rightarrow$ formation of **H_2 on dust** grain the most efficient route.

- **H_2** enhanced $\rightarrow$ **HD** enhanced through $D^+ + H_2$. HD formation on dust never dominates.

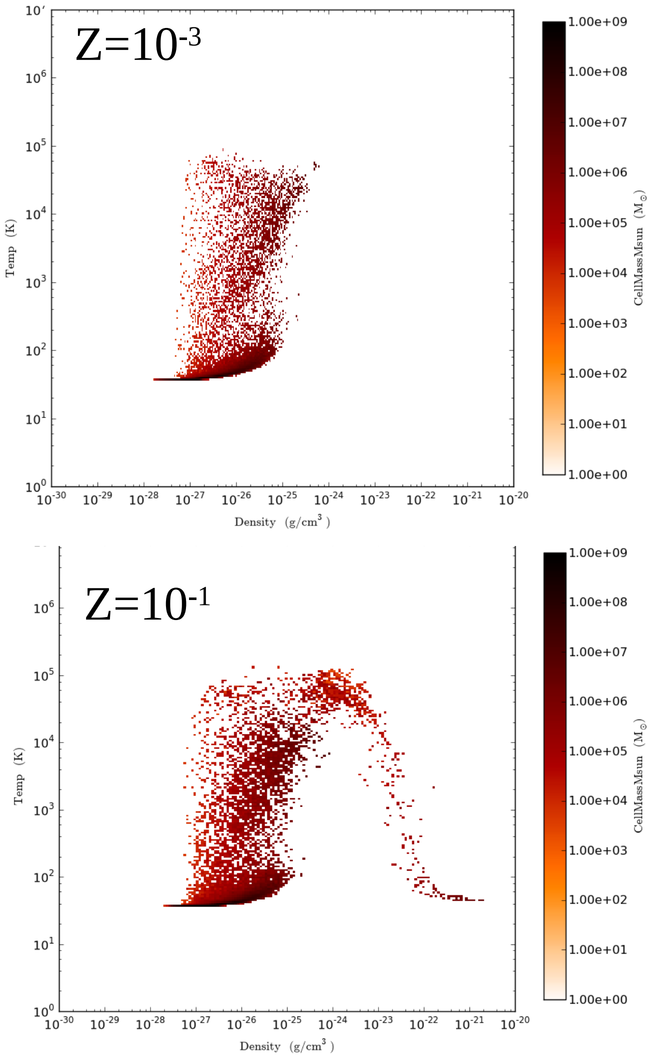
- Impact of this chemistry on **star formation** (*Aykutalp & Spaans*)

Star formation VS metallicity

- Follow formation and evolution of primordial clouds $\rightarrow$ hydrodynamic code (ENZO)
- Simulations start with cloud of 8 Mpc, and focus on minihalo of 50 kpc.
- Changing metallicity $\rightarrow$ impact on ISM and star formation of the minihalo.
- This code includes chemistry on dust for H_2 and HD
- Next step $\rightarrow$ formation of other species on dust.

Star formation VS metallicity

Density-temperature profile



Redshift z=12

ISM metal rich →

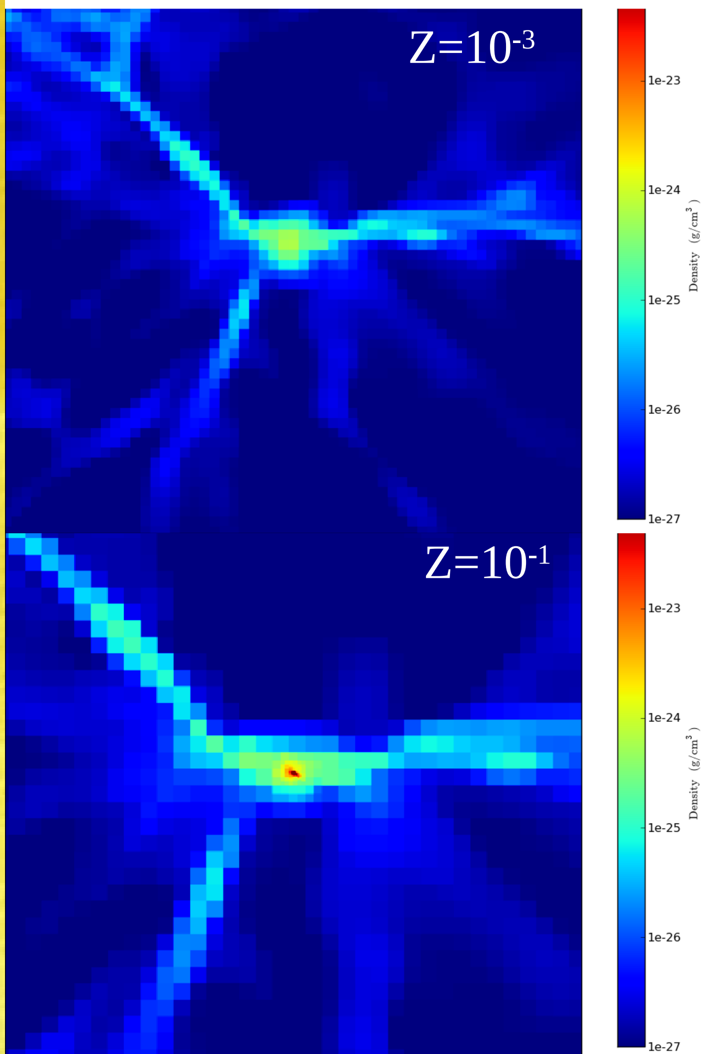
gas cools better →

Dense & cold region

minihalo evolve fast

and more compact

Density profile



Other species

Chemical network:

H_2, HD, D_2, OH, OD, O_2, H_2O, HDO, D_2O, O_3, HO_2, DO_2, H_2O_2, HDO_2, D_2O_2

On bare grains: reaction → product released in the gas phase.

Depend on: binding energy and enthalpy of reaction.

$H + O \rightarrow OH$	36%
$OH + H \rightarrow H_2O$	15 %
$H_2 + O \rightarrow OH + H$	4%
$H_2 + OH \rightarrow H_2O + H$	0.8%
O + O → O2	36%
O + O2 → O3	0.2%

Water formed in a molecular or atomic environment →

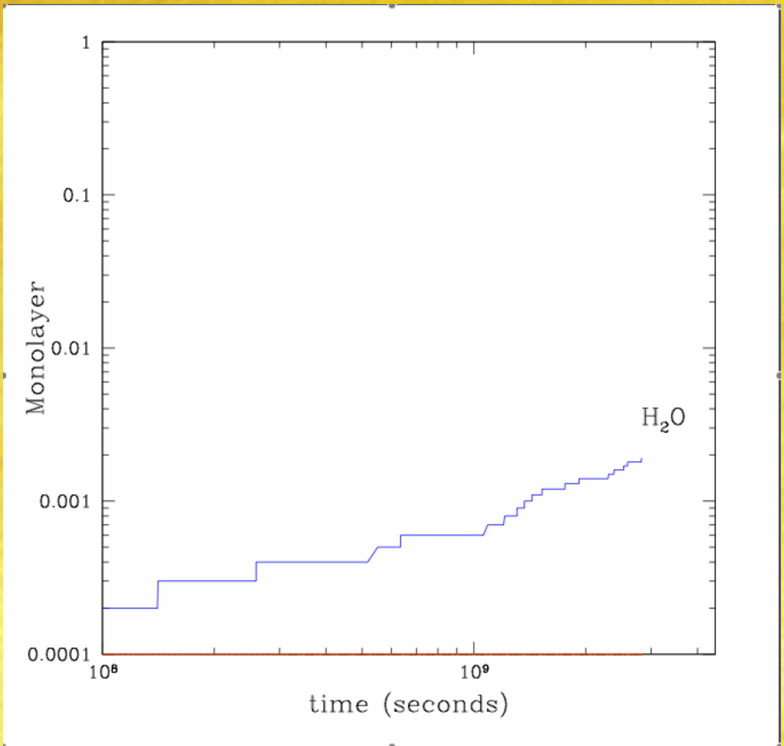
≠ impacts on gas phase

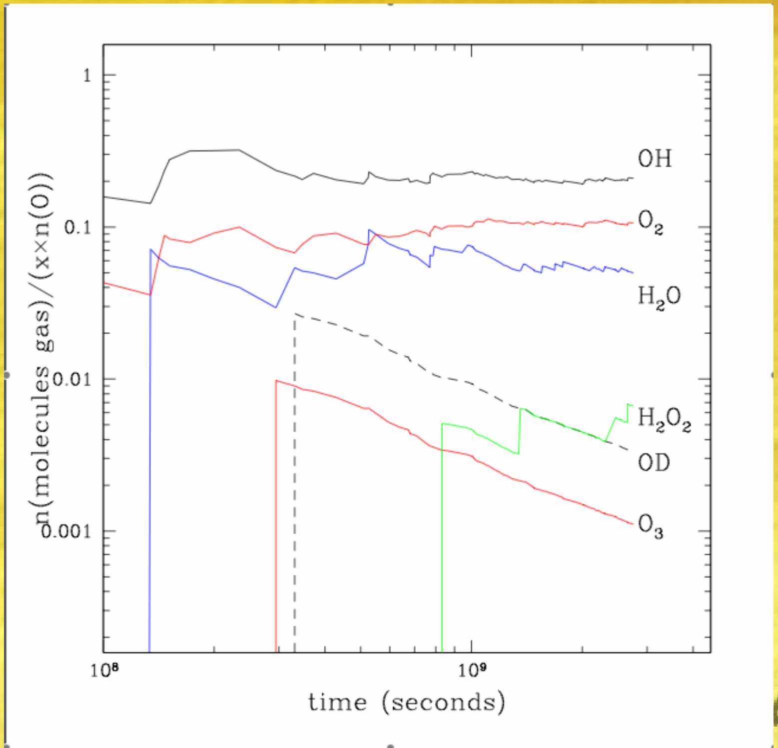
Photo-dissociation regions

H molecular, T_{dust}=30K, T_{gas}=30K,

$G_0=10^3$, Av=5

nH=1000 cm^{-3}, O/H =3 10^{-4}, D/H=2 10^{-5}





Summary and Conclusions

- **H_2 forms efficiently** for a wide range of physical conditions. To understand the formation of H_2 on cold and warm dust:
  - **2 interactions** atom/surface: physisorption and chemisorption.
  - **Mobility** = tunnelling and thermal

- To reproduce the observations of PDRs $\rightarrow$ **barrier-less route** to form H_2 (para sites).

- In the early Universe, **traces of dust** boost the formation of **H_2** $\rightarrow$ drives the formation of HD in the gas ($D^+ + H_2$).

- **Metals** allow the gas to **cool faster** $\rightarrow$ISM with cold and dense regions $\rightarrow$ more **compact mini halo**.

- Formation of **other species** on dust $\rightarrow$ added in models $\rightarrow$ **impact on star formation**