Impact of dust on interstellar gas

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Overview

Interstellar **dust** grains

The simplest molecule: **H_2**

- **Model**: Rate equations and Monte Carlo simulations
- Comparison with **observations**

Formation of **water** (and deuterated forms) on dust

- **Model**: Monte Carlo simulations
- Impact of grain surface chemistry on **interstellar gas**

The **first layer of ice**: impact for the freeze out of water on dust

- The snow border

Conclusions

Future work

Impact of interstellar dust.

Simplest molecule: H_2

Gas phase reactions do not explain the observed abundance of H_2 in the Milky Way.

$H + e^- \rightarrow H^- + h\nu$ and $H^- + H \rightarrow H_2 + e^-$

Grain surface chemistry: Gould & Salpeter 1963

In the MW, H_2 formation on dust grains dominates by many order of magnitude.

Complex molecules:

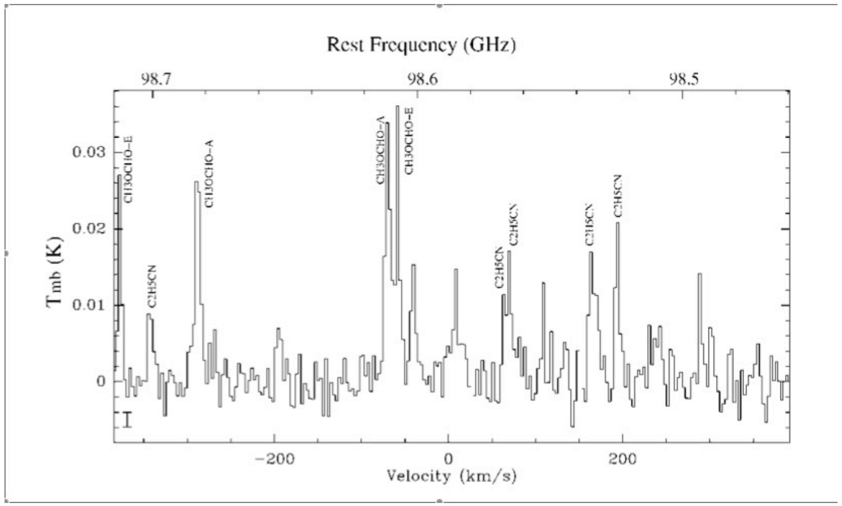
Hot Cores, Hot Corinos

This complex chemistry is a result of the evaporation of ices that covered dust grains.

High degree of deuteration:

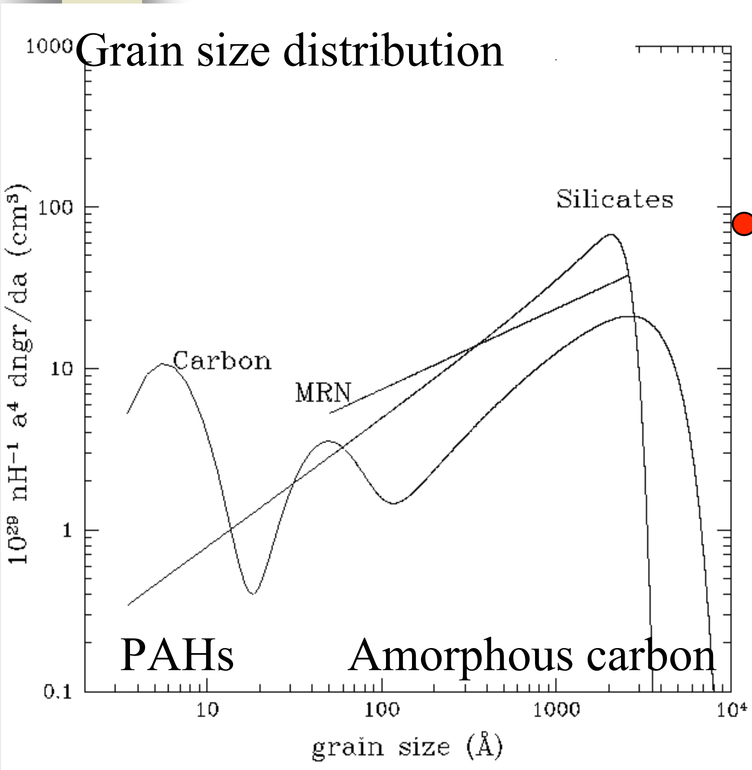
$D_2CO/H_2CO \sim 0.05$ while $D/H=10^{-5}$

(Ceccarelli et al. 1998)

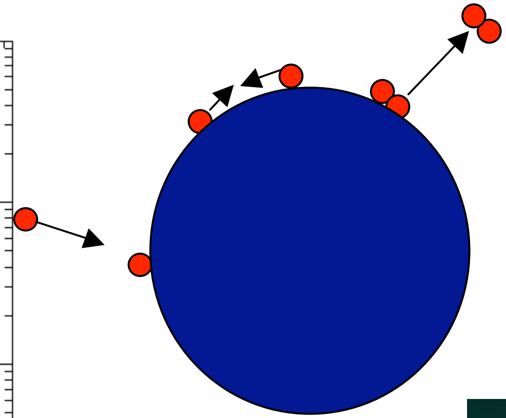


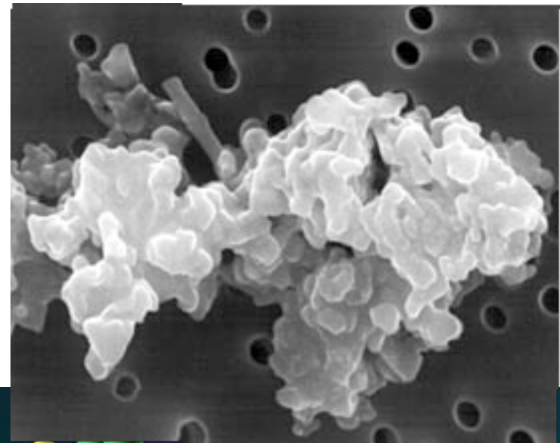
Iras16293; Cazaux et al. 2003

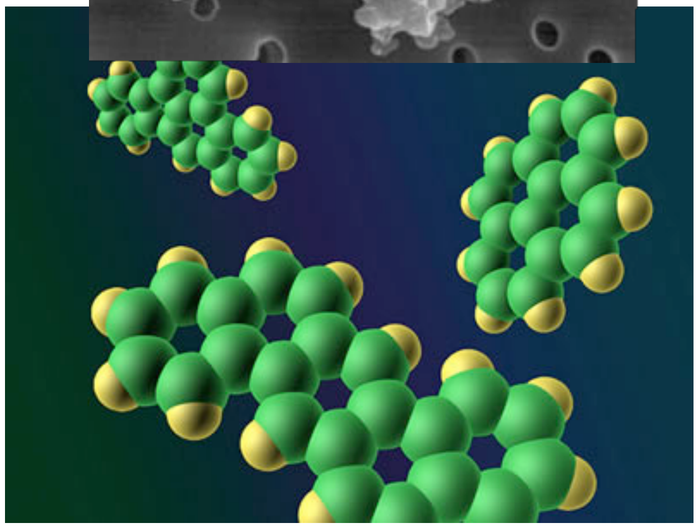
Interstellar dust grains



Weingartner & Draine 2001
Mathis, Rumpl & Nordsieck 1977







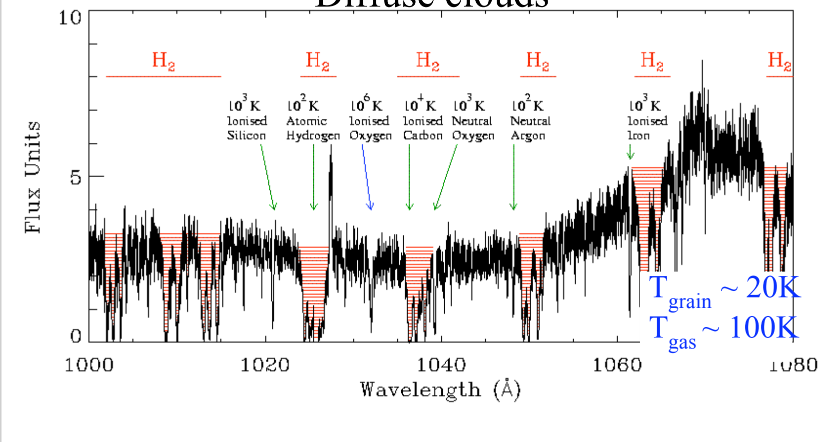
How does H_2 (HD and D_2) form on interstellar dust grains?
How does water forms on dust?
What is the impact of such a chemistry on interstellar gas?

Importance of H_2 (HD)

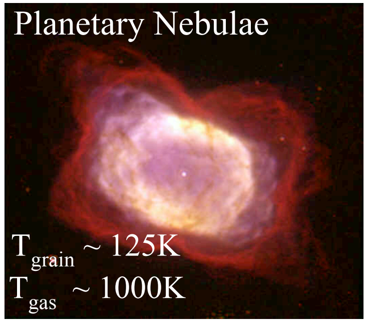
- Most abundant molecule in the universe
  $M(H_2) \sim 5.10^9$ M⊙ in the Milky Way
- Formation of the first stars of the Universe: H_2 is the only coolant available (Bromm 2002).
- Key species for the formation of other chemical species
- HD can be an important coolant in the early Universe because of its small dipole moment (Nagakura & Omukai 2005)

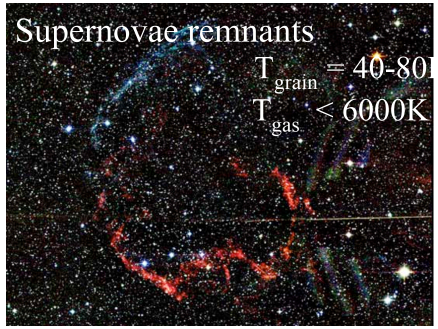
H_2 observations in astrophysical environments

Diffuse clouds

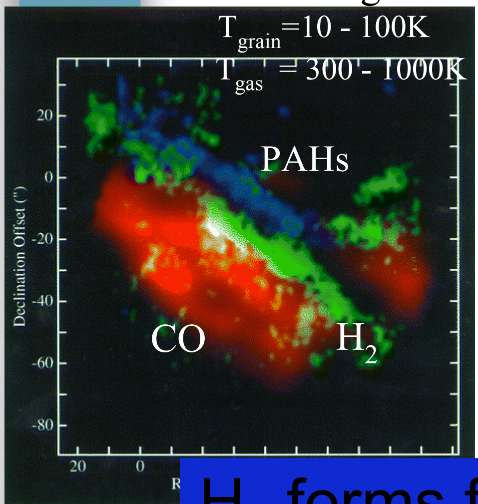


Dying stars

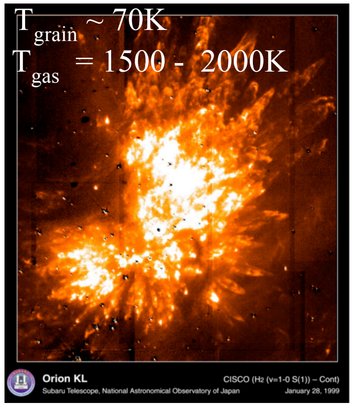




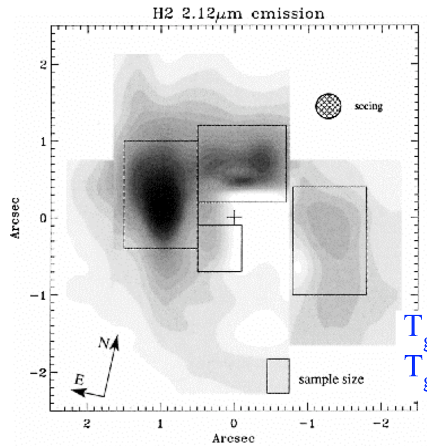
Photodissociation Regions



Newly born stars



Active galactic nuclei



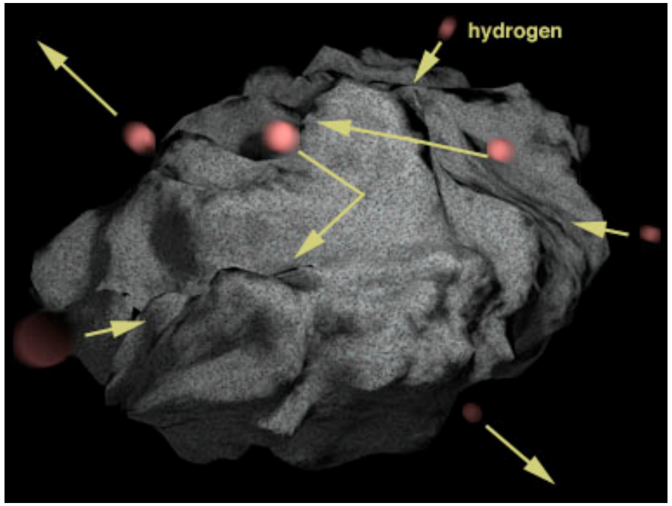
T grain = 15- 70K
T gazs ~ 2000K

H_2 forms for a wide range of physical conditions

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.

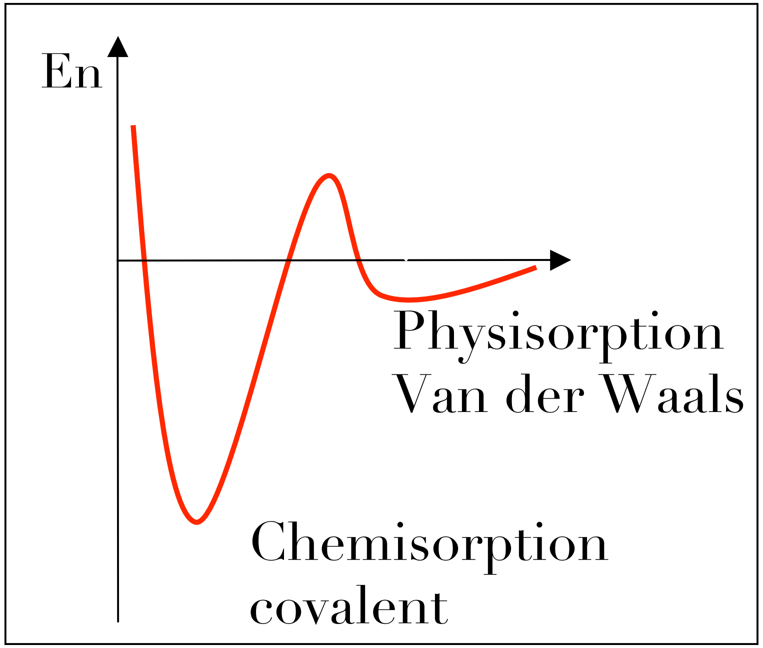
Rate equations and Monte carlo simulations

Comparison with observations

Interaction atom/surface: experiments

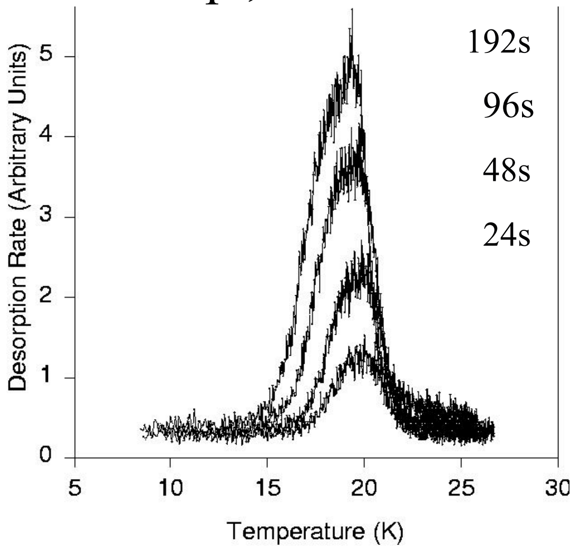
Experiments on graphite, amorphous carbon, silicates

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



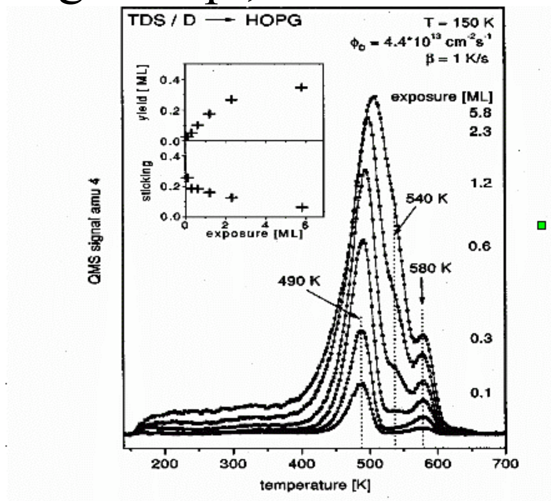
Amorphous Carbon

Low temp., Tsurf = 5 K

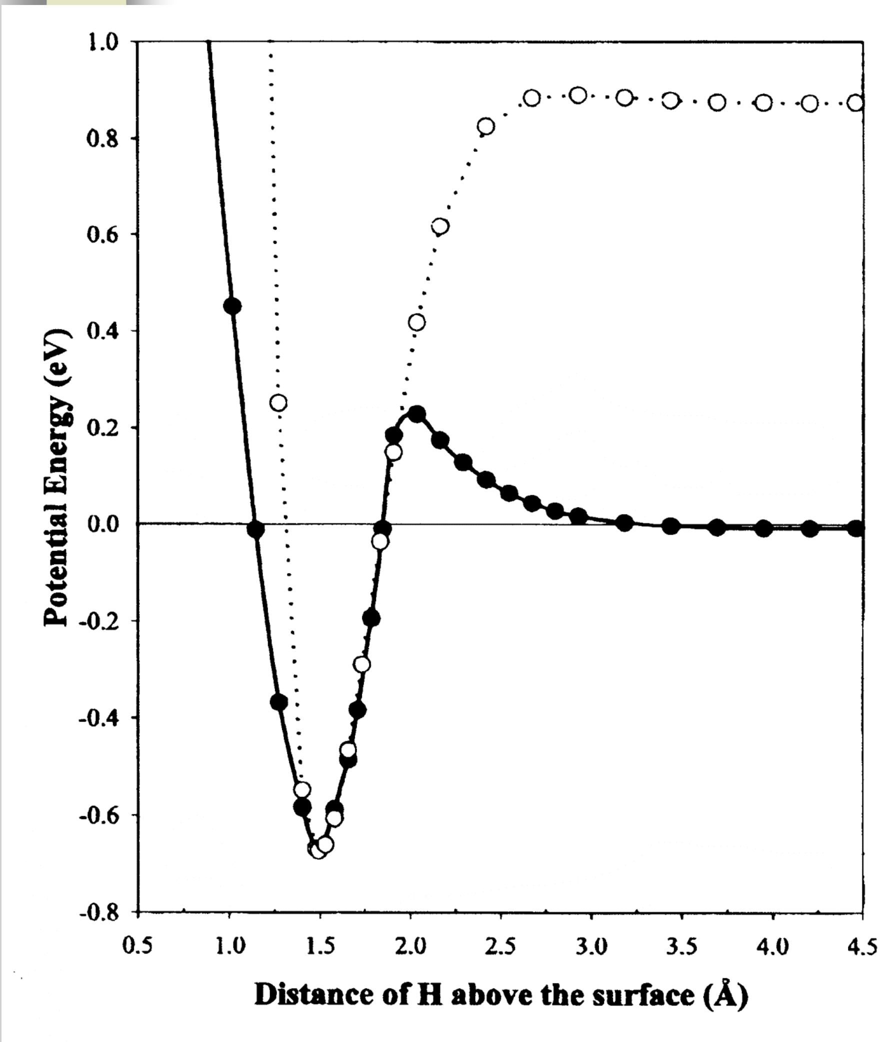


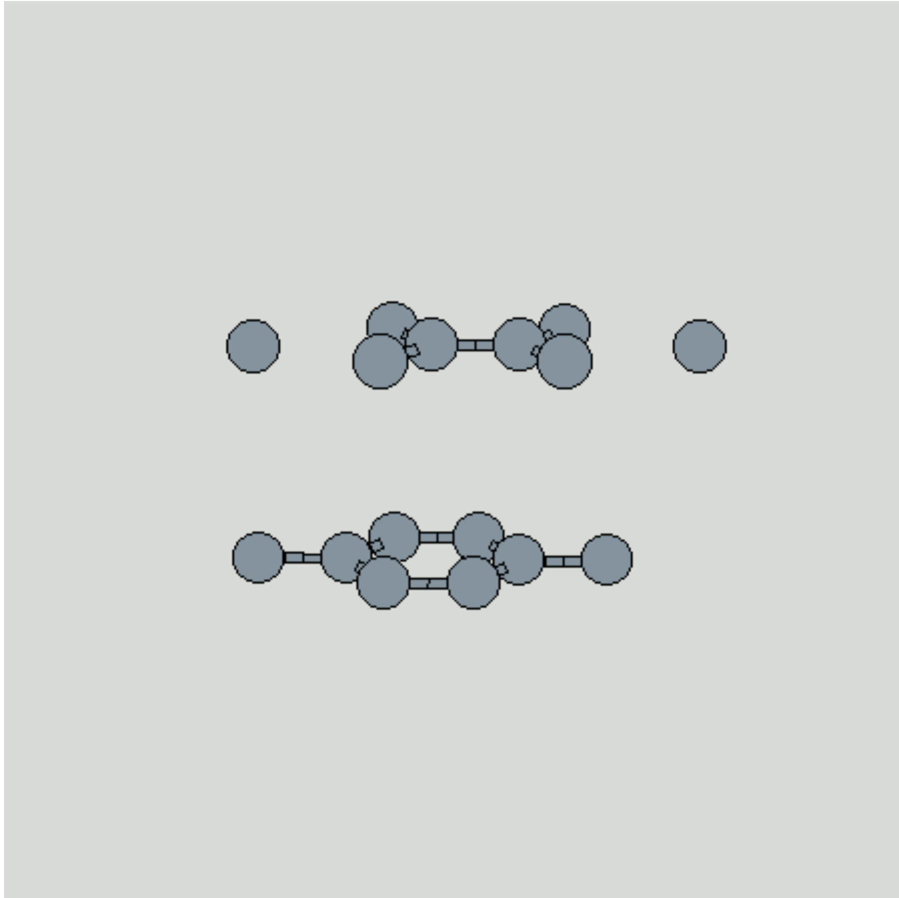
Graphite

High temp., Tsurf = 150 K



Interaction atom/surface: Density functional theory (DFT)

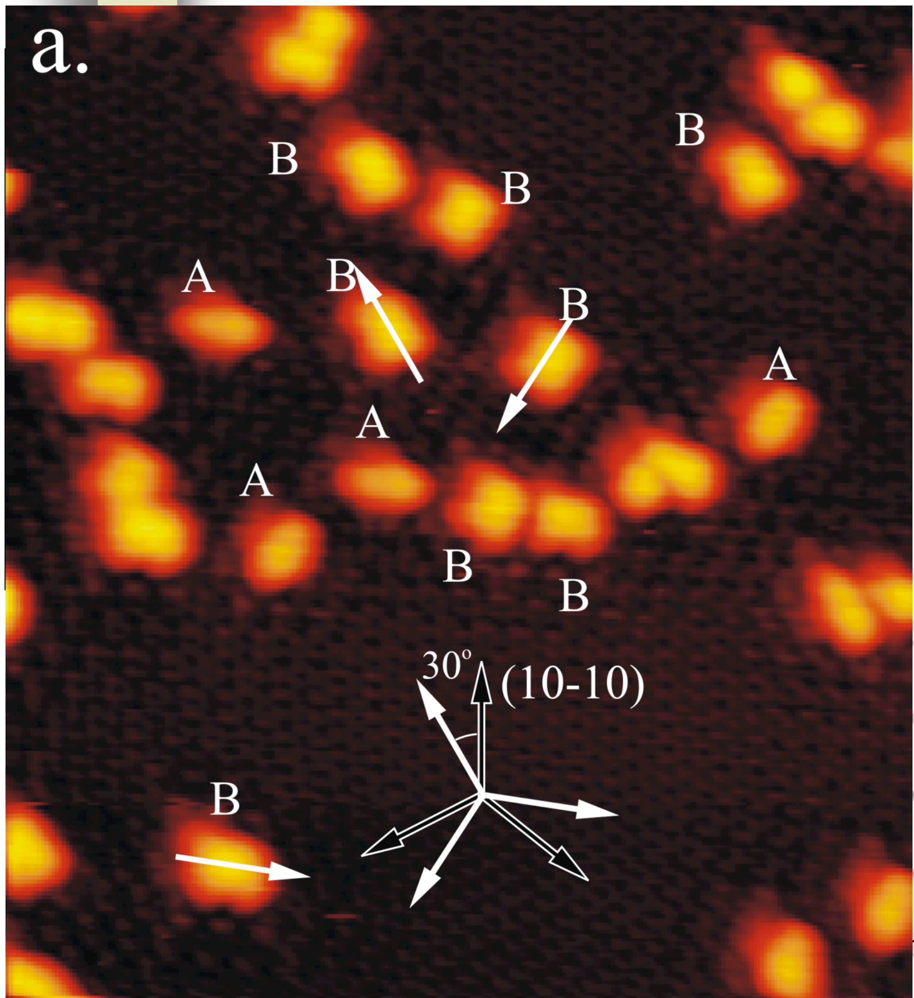




Eva Rauls

Sha et al, Surface Science 496, 318 (2002)

Interaction atom/surface: Density functional theory (DFT)



STM @ 170K

Ho r et al. 2006

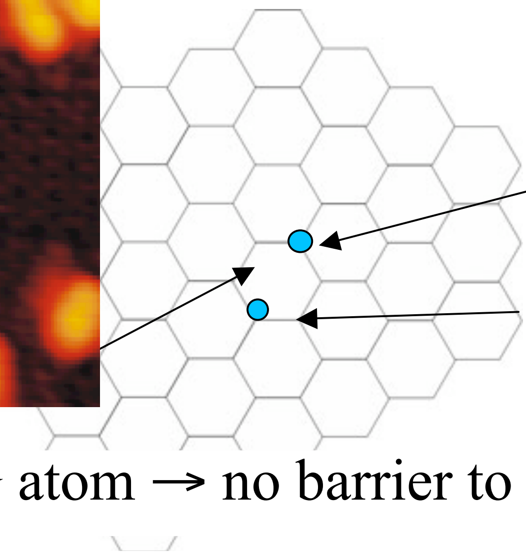
Graphite:

Chemisorption of H

C puckered out of the basal plane associated with barrier ~ 0.2 eV.

Jeloaica & Sidis 1999

Sha & Jackson 2002

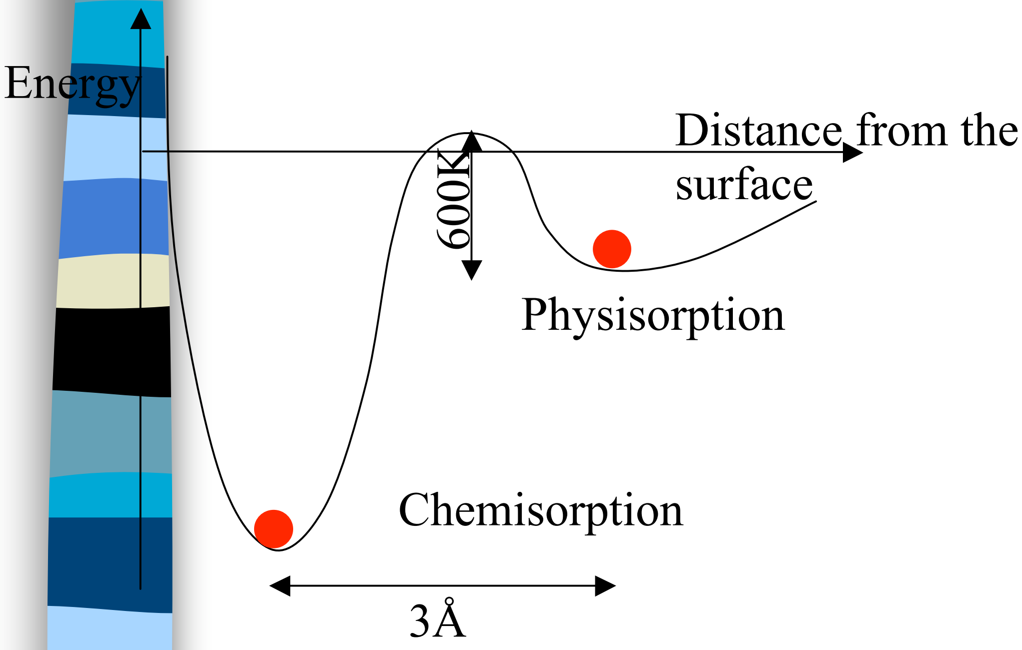


1^{st} H→ barrier

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

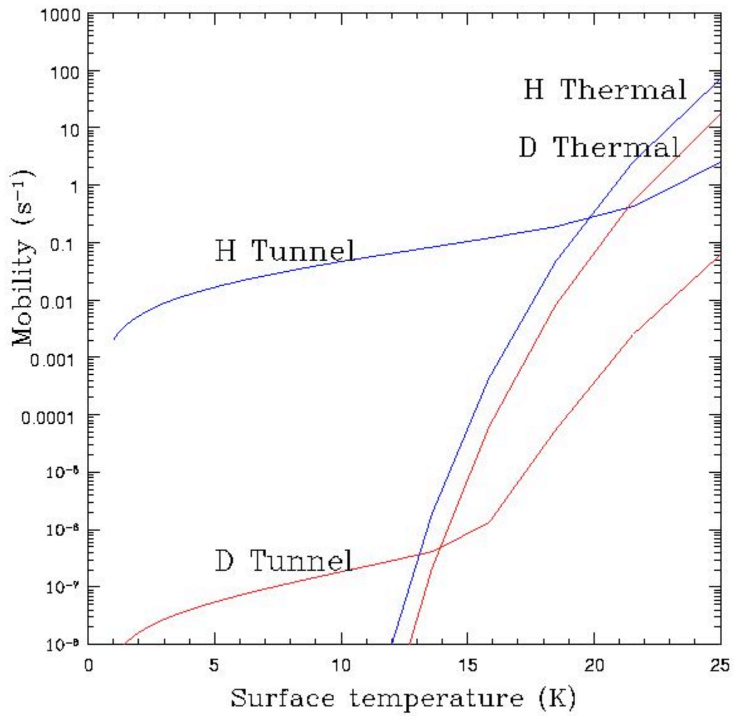
3^{rd} atom → no barrier to form H_2

Model: Interaction and mobility



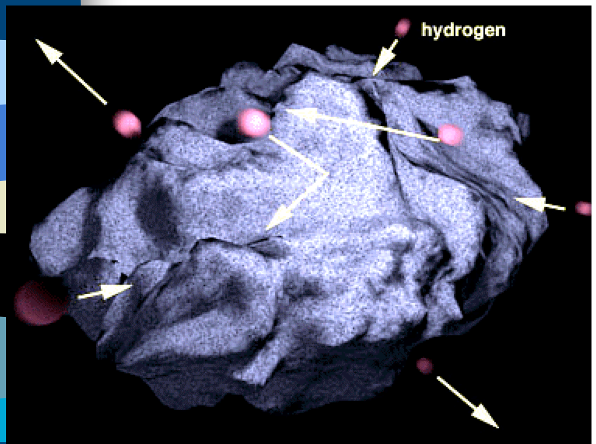
- Physisorption + chemisorption
- tunnel + thermal hopping

Transmission coefficient of the barriers
- mobility of H and D atoms

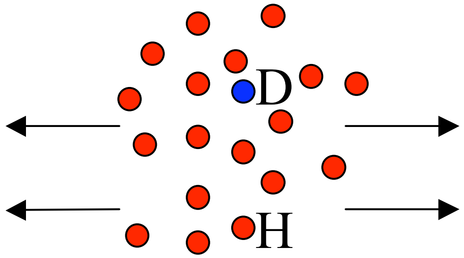


Rate equations and Monte Carlo simulations.

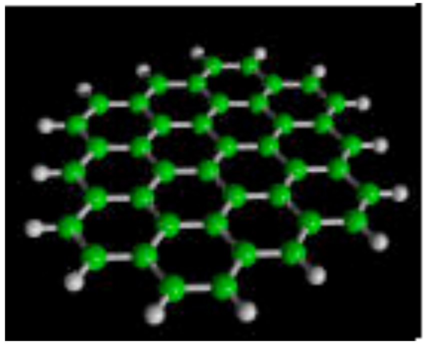
Rate equations



Follow populations
Big grains → always 1 species

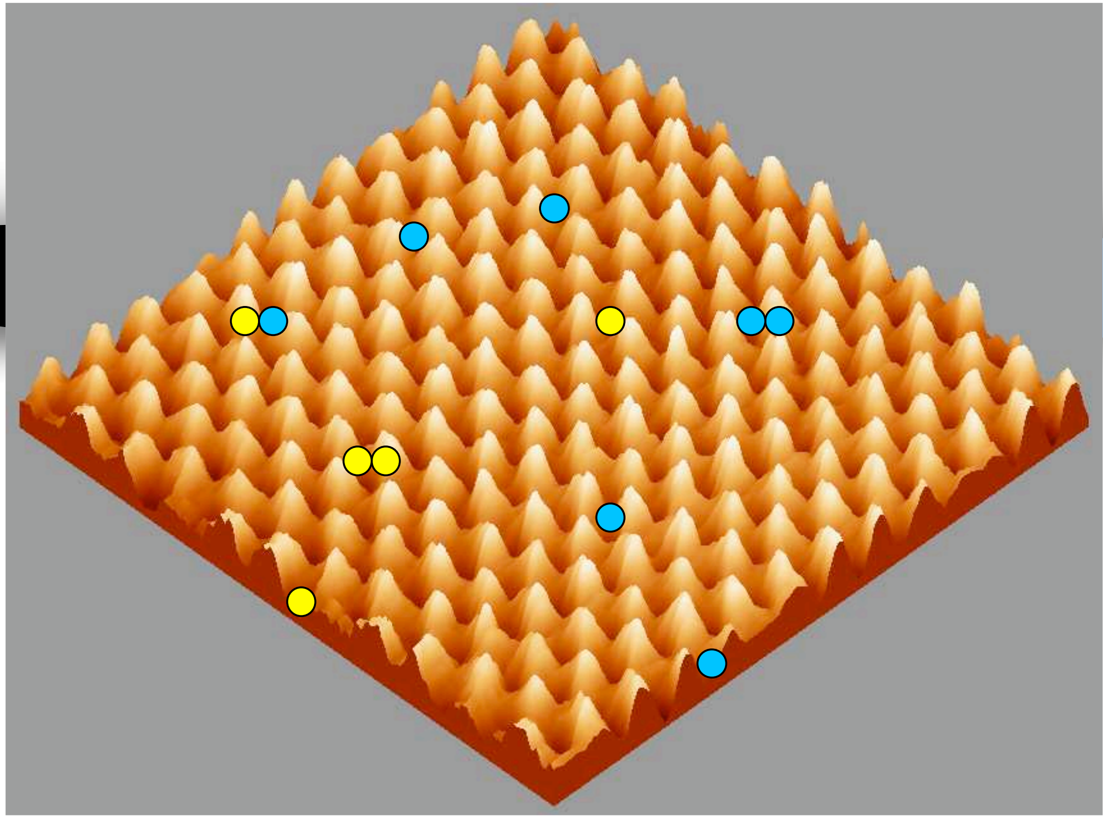


Monte Carlo



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

Model:
Interaction and mobility



physisorbed H atoms

physisorbed D atoms

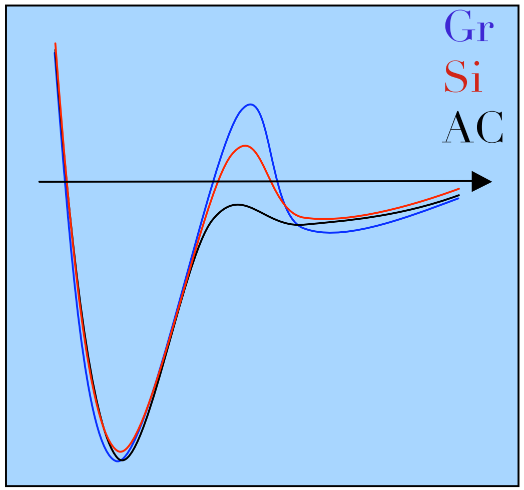
chemisorbed H atoms

chemisorbed D[redacted]oms

H2

HD

D2



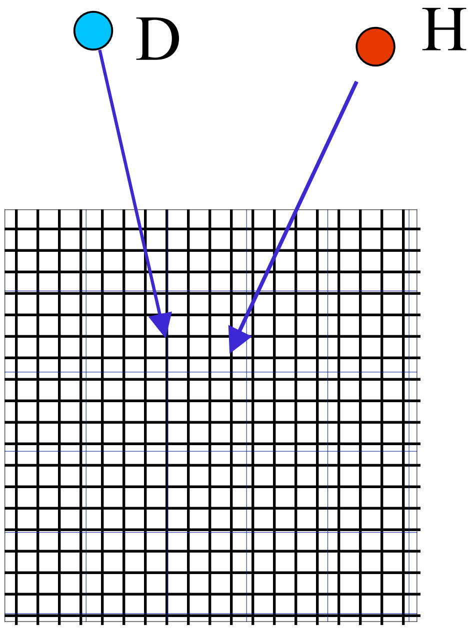
Mechanisms:

Monte Carlo simulations

chemistry on small grains
detailed characteristics of the surface (graphite, incusion of para sites properties)

grid sizes vary from few Å to 0.1 μm

Atoms arrive randomly on the grain
and have a random walk
Each point of the grid is a site:
physisorbed and chemisorbed



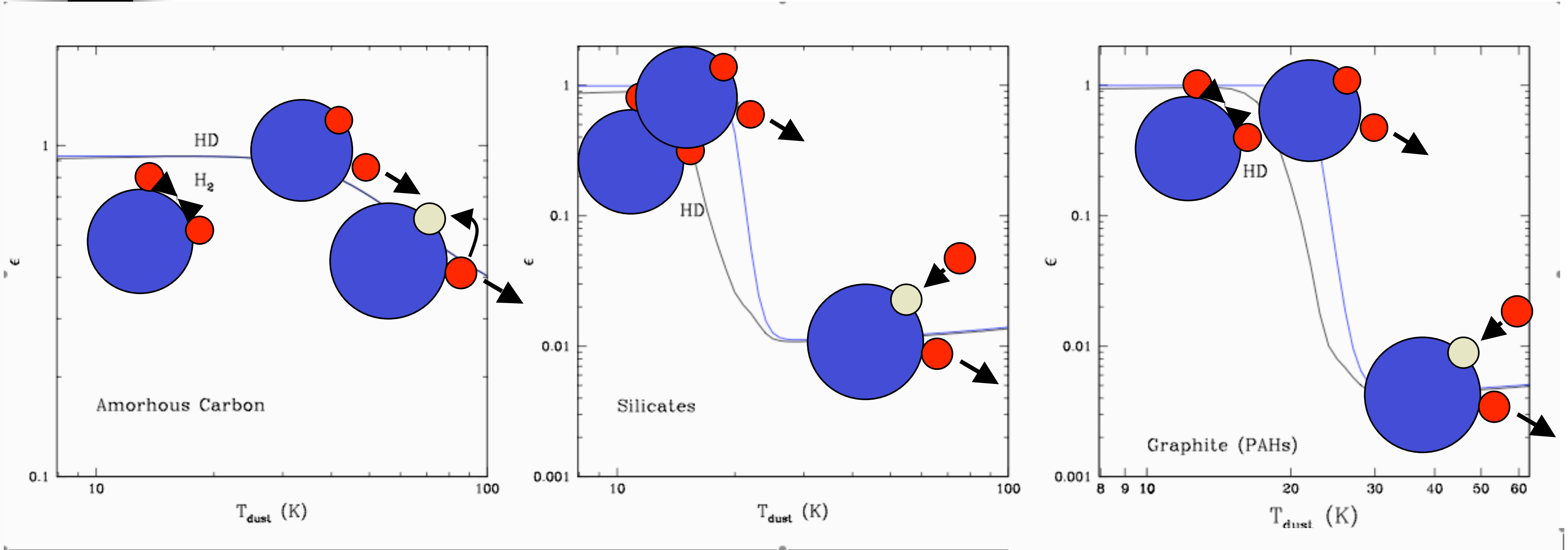
t=-ln(xrand)/t(evt)

List of accretions times (random number depending on the flux of atoms)

Each time an atom arrives on the grain ➔ possible events

Determine the next event that is ordered in the list

Results



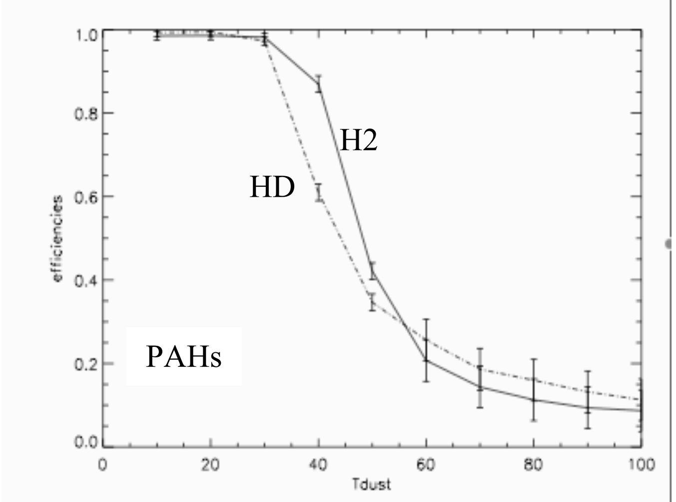
Formation of H_2 and HD

→**physisorbed** atoms @ **low T_{dust}**

→**chemisorbed** atoms @ **high T_{dust}**

Inclusion **para sites**

→ Increase the efficiency >1 mag

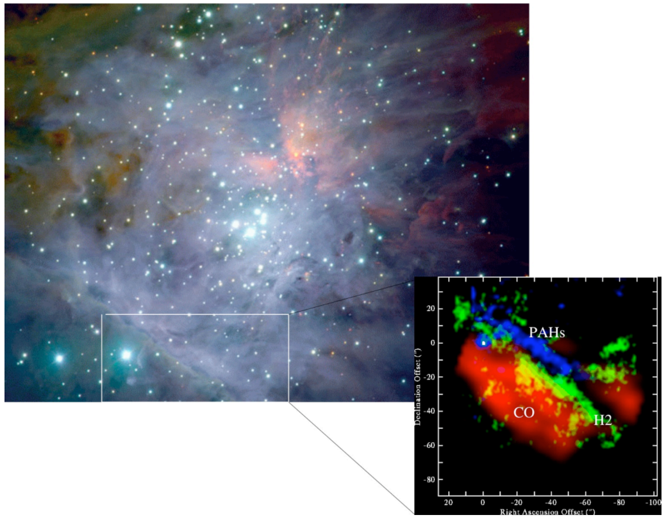


H_2 formation rate in the ISM

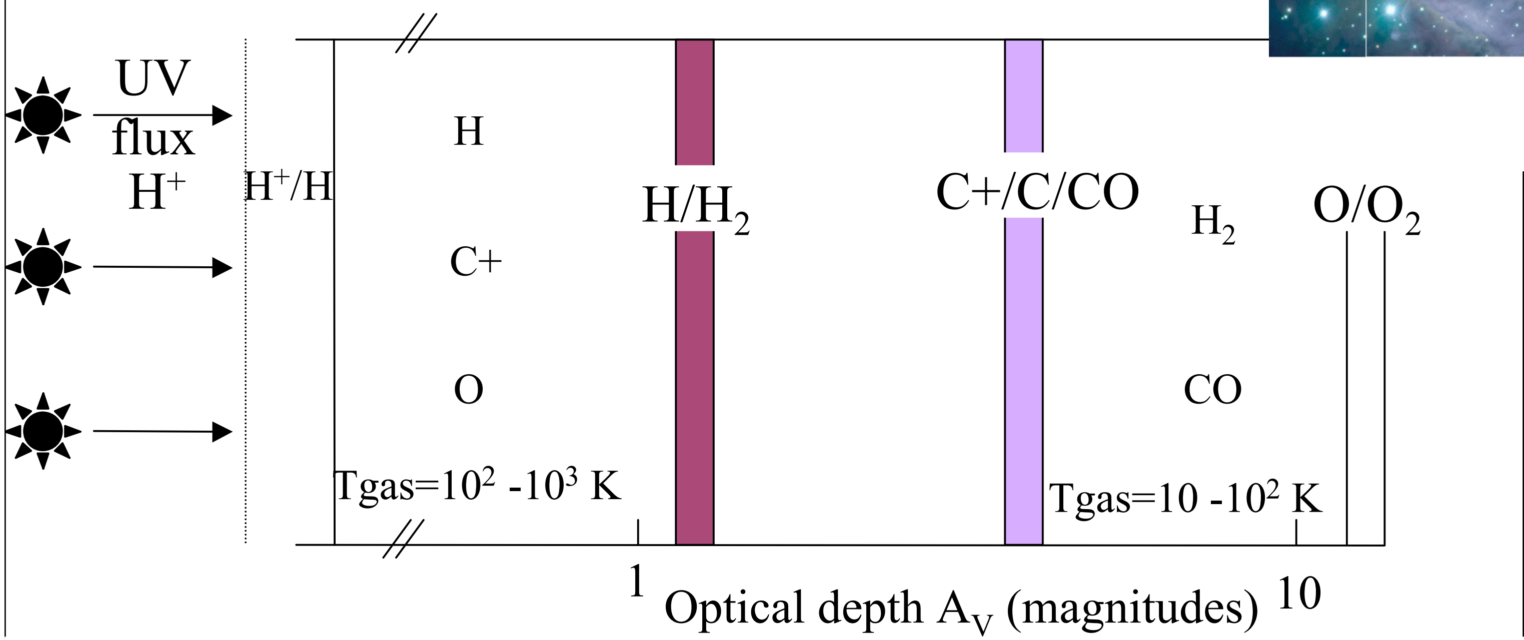
$$R(H_2)=(1/2)\ n_H\ v_H\ \sigma\ n_d\ S_H\ \underline{\boldsymbol{\varepsilon}}$$

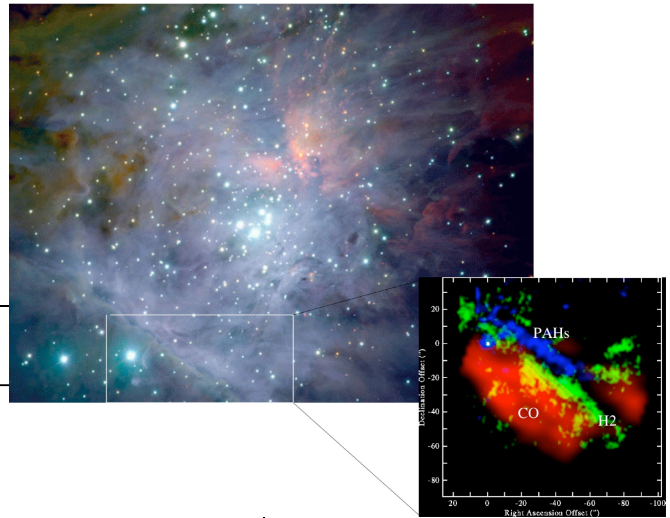
- n_H number density of H atoms
- v_H speed of H atoms in the gas phase
- $\boldsymbol{\sigma}$ area of the grain
- n_d number density of dust grain
- S_H sticking coefficient of the H atoms on the grain
- $\boldsymbol{\varepsilon}$ H_2 recombination efficiency

Photo-dissociation regions



H_2 formation rate: Photo-dissociation Regions



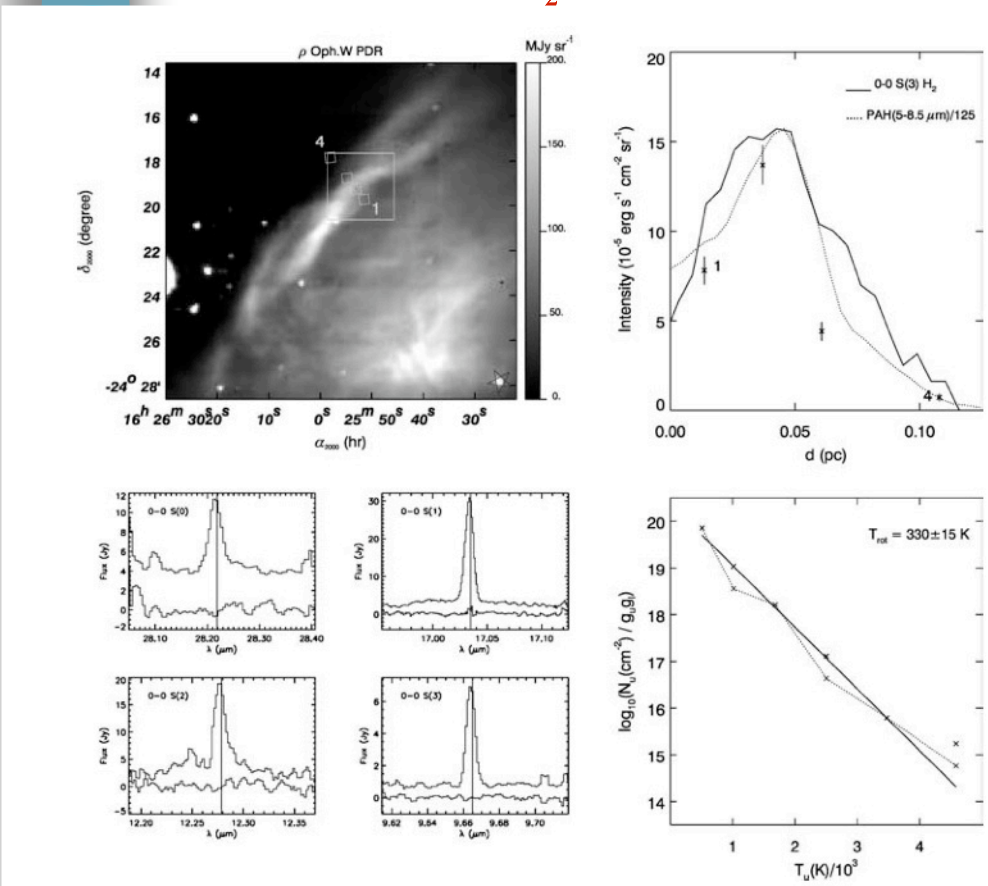


Schematic diagram of a photodissociation region. A PRD extends from the atomic surface region to the point where O_2 is not appreciably photodissociate (~ 10 visual magnitude). In PDRs, hydrogen is mainly into the H_2 form and carbon mostly into CO. From Hollenbach and Tielens 1997.

H_2 formation rate: Photo-dissociation Regions

ISOCAM MAP (in the LW2 filter)

Rotational transitions of H_2 and PAHs emission



Abergel et al. 1996
Habart et al. 2003

□ ISO SWS

Rotational transitions of H_2

○ ISO LWS

ISOCAM- CVF

Spectro- imaging

Rotational transitions of H_2

Gas temperature

Photodissociation of H_2

Formation rate of H_2

Grain temperature

H_2 formation rate: Photo-dissociation Regions

Region	Tsg	Tbg	Tgas	Rate H2
	K	K	K	$cm^3 s^{-1}$
chamaeleon	>2.7	15	60	$4\ 10^{-17}$
Oph W	10	36	330	$1.5\ 10^{-16}$
S 140	10	36	500	$1.5\ 10^{-16}$
IC 63	12	44	620	$1.5\ 10^{-16}$
NGC 2023	25	60	330	$3\ 10^{-17}$
Orion bar	62	90	390	$3\ 10^{-17}$

Habart et al. 2004

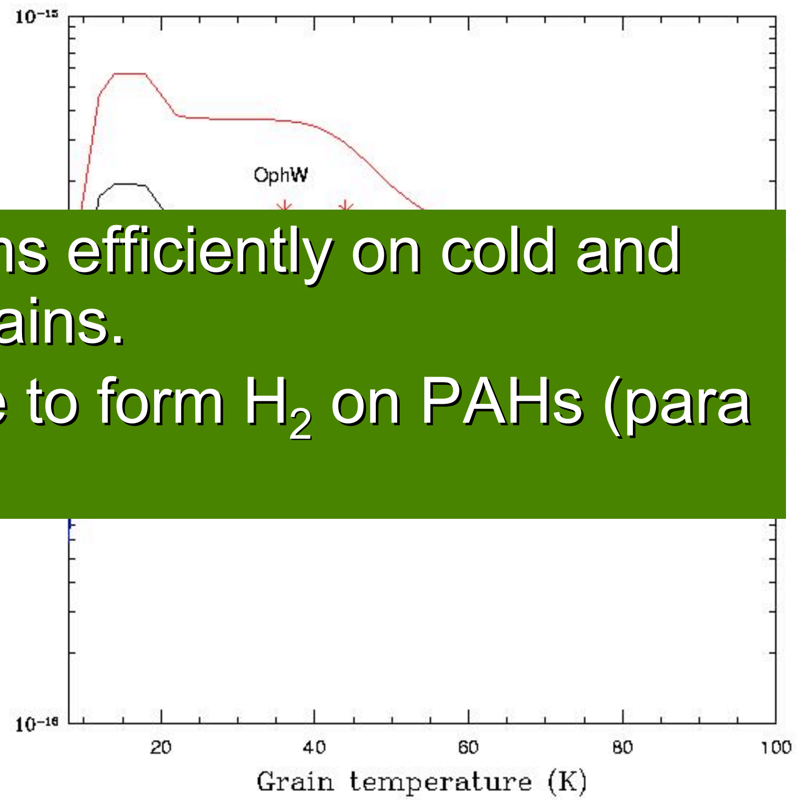
H_2 formation rate: Photo-dissociation Regions

Observations of several PDRs

(*Abergel et al. 1996; Habart et al. 2003)*

T_{dust} = 15 - 90K

T = 60 - 620K



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

→ inclusion of the barrier-less route to form H_2 on PAHs (para sites).

H_2 formation @ high Tdust and Tgas → para sites properties

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

≠ abundances PAHs/very small grains (AC)

(*C iegne et al. 2008, Joblin et al*)

H_2
Summary and Conclusions

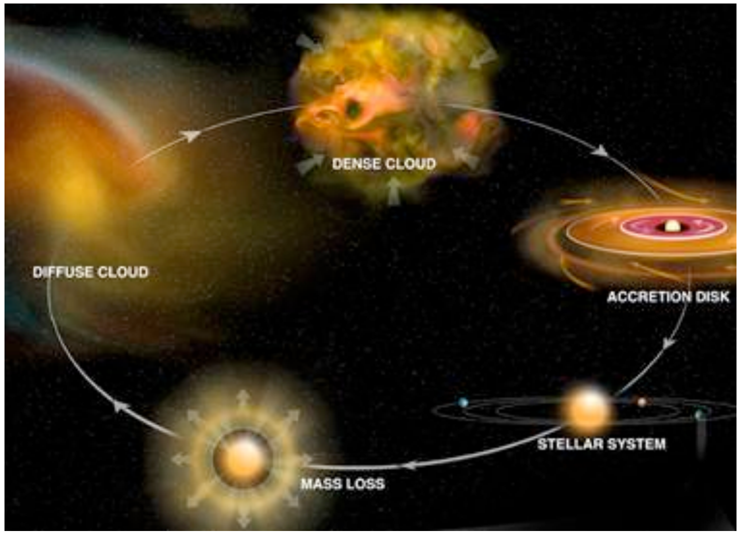
- H_2 forms in **cold** and **warm** environments.
- Formation of H_2 on cold and warm dust grains:
  - **2 interactions** atom/surface: physisorption and chemisorption.
  - Mobility: **tunnel** and **thermal**
- Observations of PDRs show an **efficient** formation of H_2 formation for **wide range of T_{dust}**.
- To reproduce the observations of PDRs → **barrier-less route** to form H_2 on PAHs (para sites properties)

Water formation on interstellar dust

- Water could be an important coolant for star formation (T > 100 K, nH > 106 cm-3; Neufeld 1995).
- Water locked on dust grains in the early ages of our solar system → ocean
- The snow line in planetary disks is determined by the freeze out of water on grains
- Interpretation of observations (HIFI)

Water formation on interstellar dust

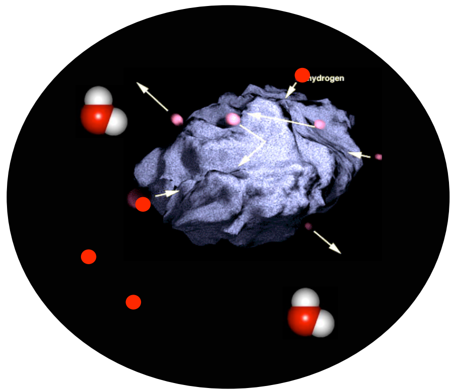
- Star form in clouds made of gas + dust



- Molecules such as CO, O_2, H_2O, cool the gas

(Neufeld et al. 1995)

- Impact of grain surface chemistry on interstellar gas?



Formation of water

Formation of water on dust grains has been studied by several authors for the formation of ices *(Tielens & Hagen 1982; Cuppen & Herbst 2007)*

Ion-molecule reactions: cold gas phase

$H_3^+ + O \rightarrow OH^+ + H_2$

$OH^+ + H_2 \rightarrow H_2O^+ + H_2 \rightarrow H_3O^+$

$H_3O^+ + e \rightarrow H_2O + H$

Neutral-neutral reactions: warm / hot gas phase

$O + H_2 \rightarrow OH + H$

$OH + H_2 \rightarrow H_2O + H$

On interstellar dust grains

$O + H \rightarrow OH$

$OH + H \rightarrow H_2O$

$O_2 + H \rightarrow HO_2$

$HO_2 + H \rightarrow H_2O_2$

$H_2O_2 + H \rightarrow H_2O + H$

(Miyauchi et al. 2008, Iopollo et al. 2008)

$O_3 + H \rightarrow OH + O_2$

$OH + H \rightarrow H_2O$

(Mokrane et al. 2009)

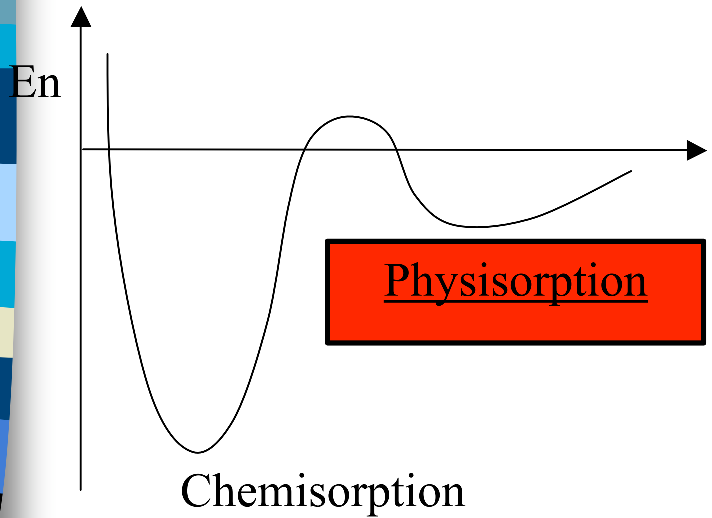
Water on bare grains: Monte carlo simulations

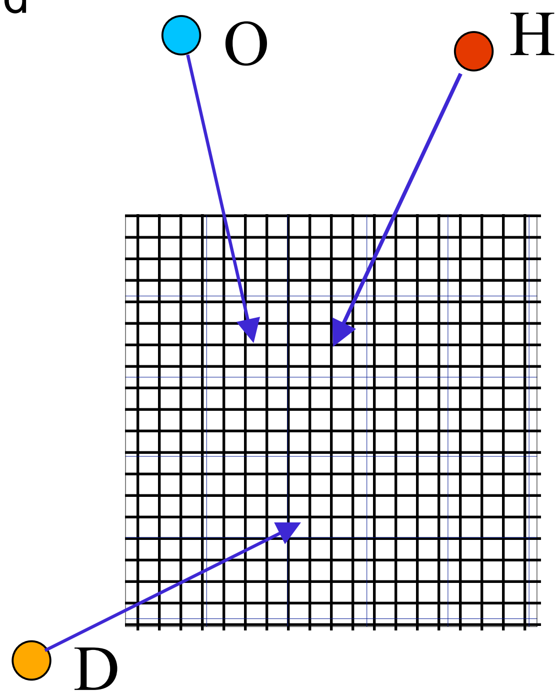
Carbon grains

Grain surface = grid

Atoms arrive randomly on the grid execute random walk

Each point of the grid is a site: physisorbed and chemisorbed





Each time an atom arrives on the grain: possible events

Evaporation

Phys ➔ Phys

Phys ➔ Chem

UV

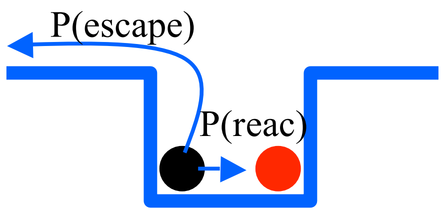
CR

Water on bare grains: Monte carlo simulations

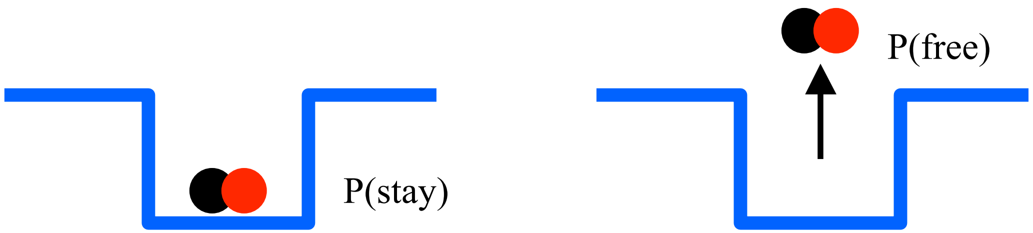
- Chemical network:

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

- Two species in a same site: compare probability to react and probability to escape.



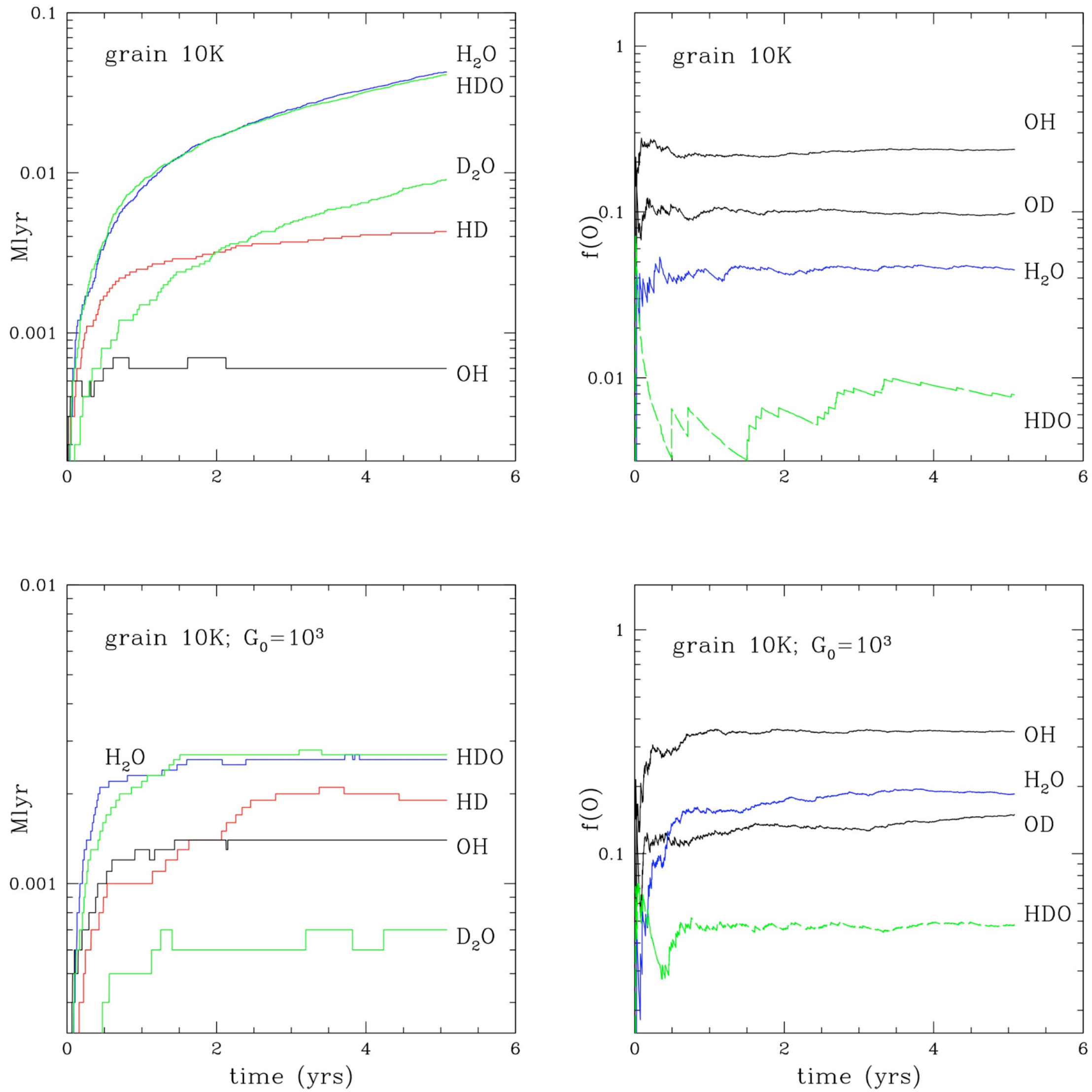
- If reaction occurs probability that the product is released in the gas (Enthalpy and binding energy).



- Include photo-dissociation due to UV photons and CR.

Results

Grain surface   Gas phase



Test case:

Grain 10K

nH=10^3

D/H =0.1

O/H=0.1

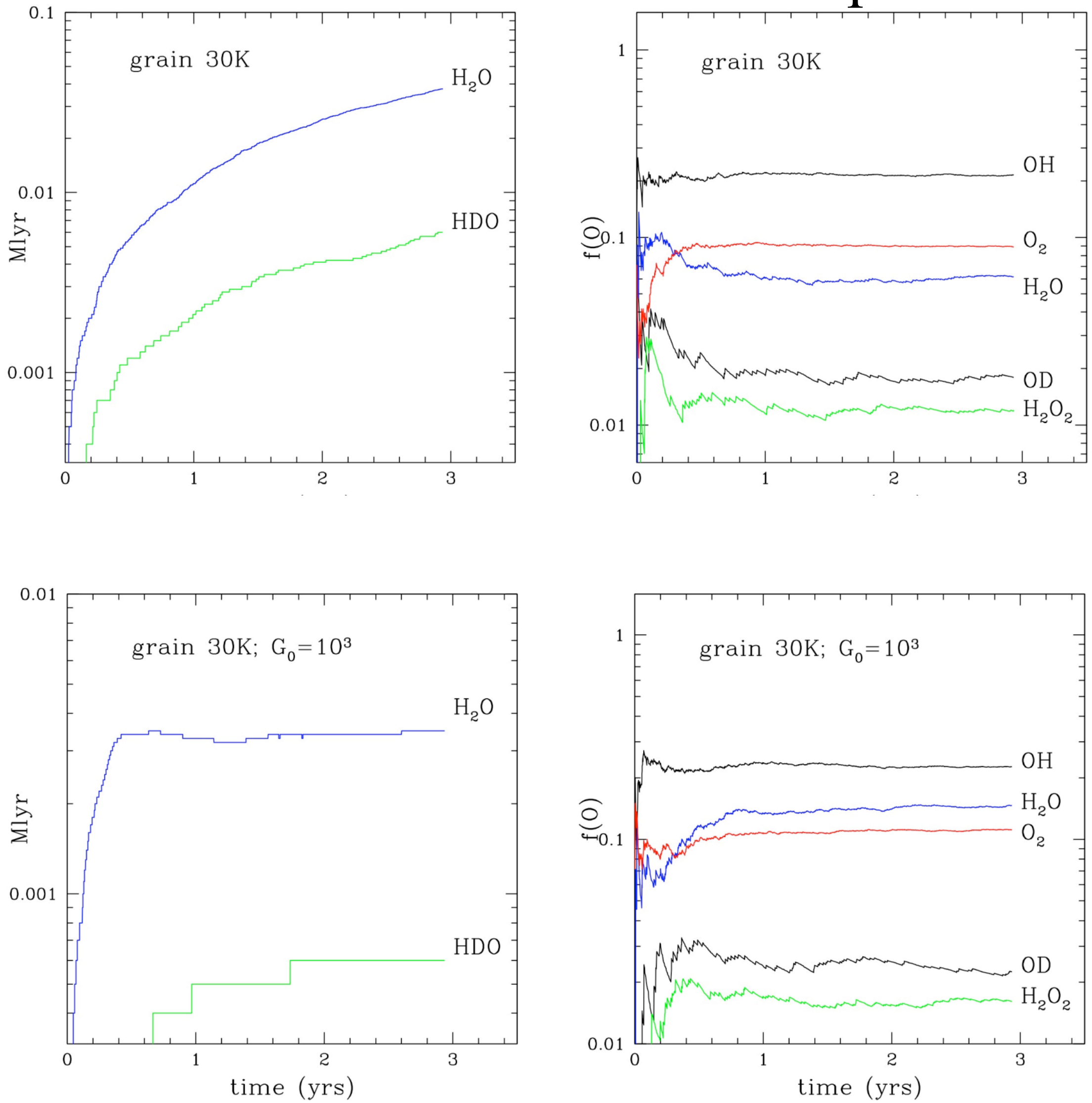
$$O + H \xrightarrow{P0} OH + H \xrightarrow{P1} H_2O$$

$$O + H \xleftarrow[h\nu]{} OH + H \xleftarrow[h\nu]{} H_2O$$

Grain 10K
Hydrogenated species
UV boosts water desorption

Results

Grain surface   Gas phase



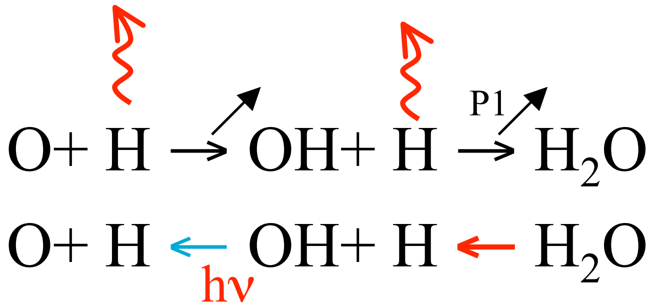
Test case:

Grain 30K

nH=10^3

D/H =0.1

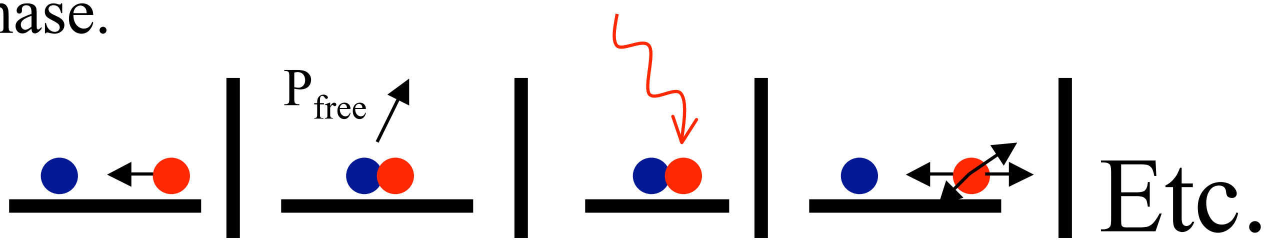
O/H=0.1



Grain 30K
Species rich in oxygen
UV boosts H_2O desorption

Results

Grains **10 K** favours **hydrogenation**
Warmer grains (**30 K**) favours **oxygenation**
UV photons **dissociate** species that **recombine**.
"dissociation-formation-dissociation" boost gas phase.



Species released in gas ➔ photo-dissociated.
Boost VS photo-dissociation?

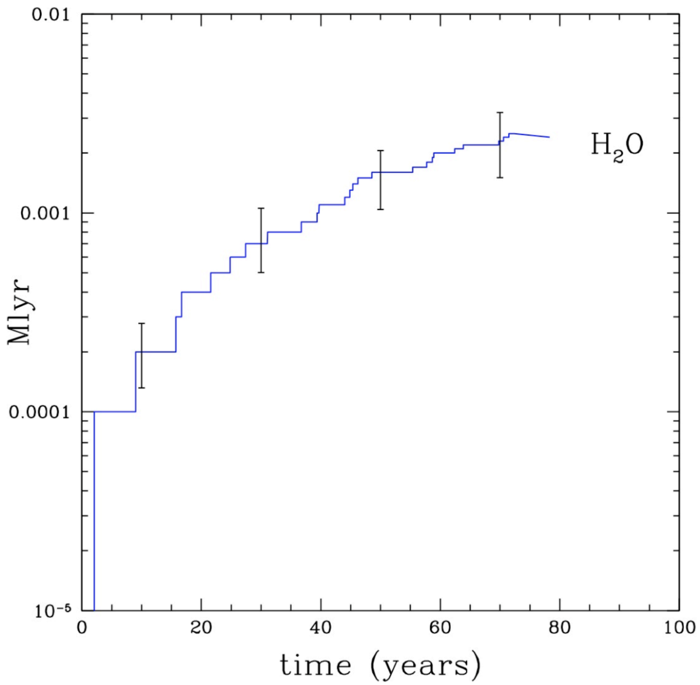
Diffuse clouds

Diffuse clouds: H atomic

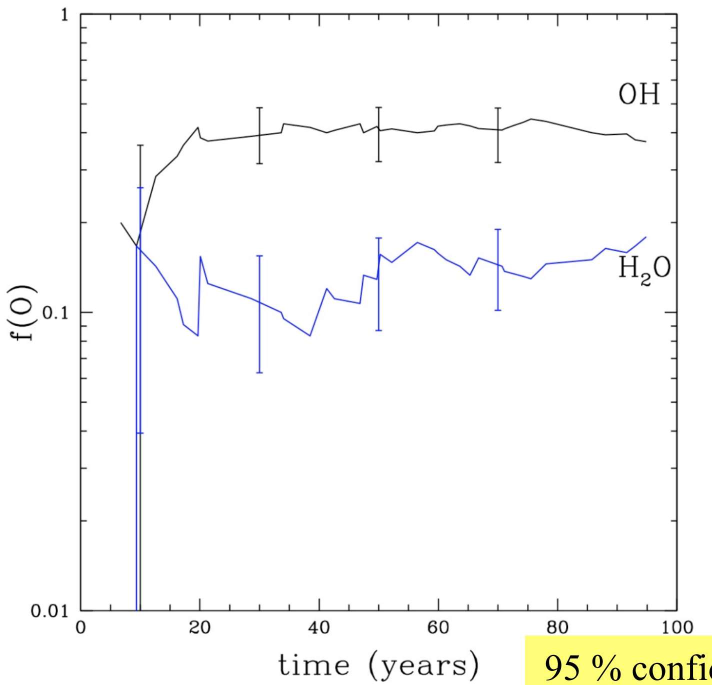
H + O → OH + H → H_2O

T_{dust}=18K, T_{gas}=100K, nH=100 cm^{-3}, O/H =3 10^{-4}, D/H=2 10^{-5}

Grain surface



Gas phase



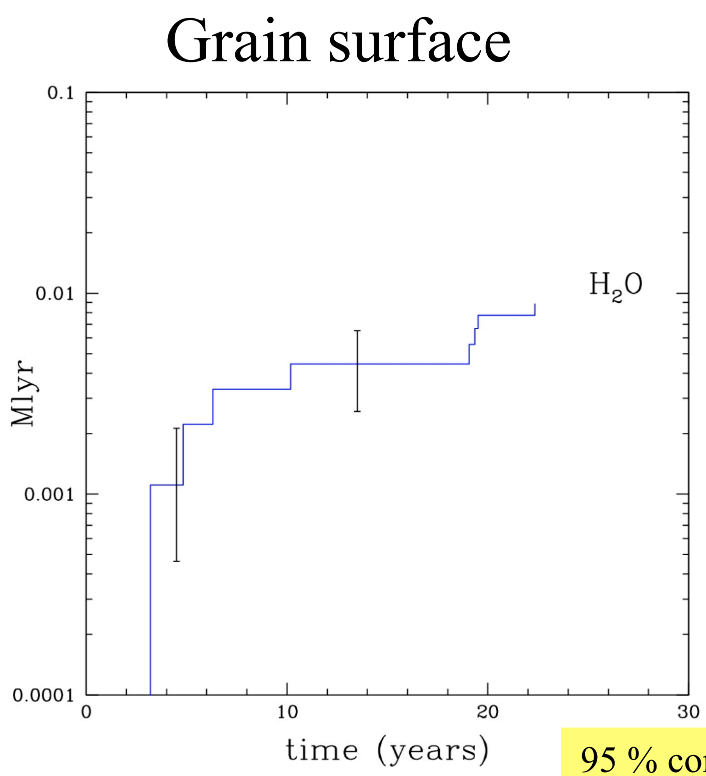
95 % confidence level

Transluscents clouds

Transluscents clouds: H molecular

$\mathbf{H_2 + O \rightarrow OH + H}$ $\mathbf{OH + H_2 \rightarrow H_2O + H}$

T_{dust}=14K, T_{gas}=50K, nH=500 cm^{-3}, O/H =3 10^{-4}, D/H=2 10^{-5}



95 % confidence level

No desorption gas phase

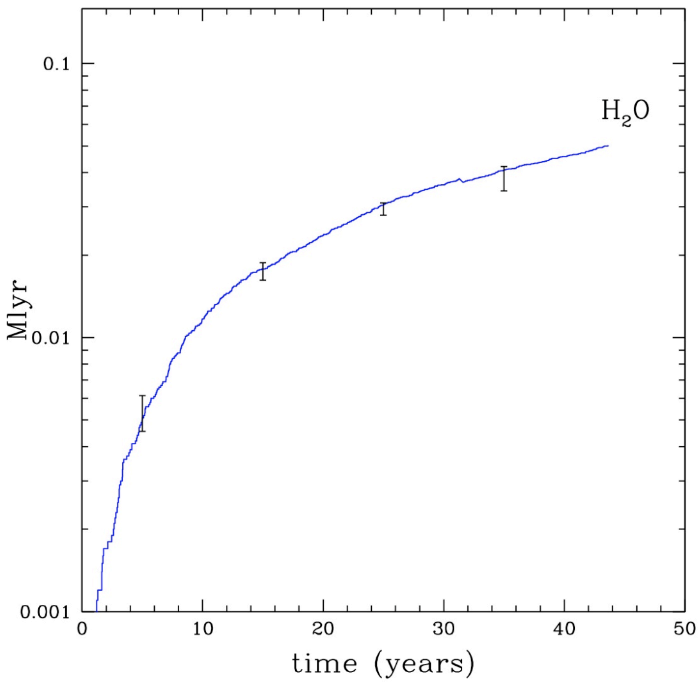
Dense clouds

Dense clouds: H molecular

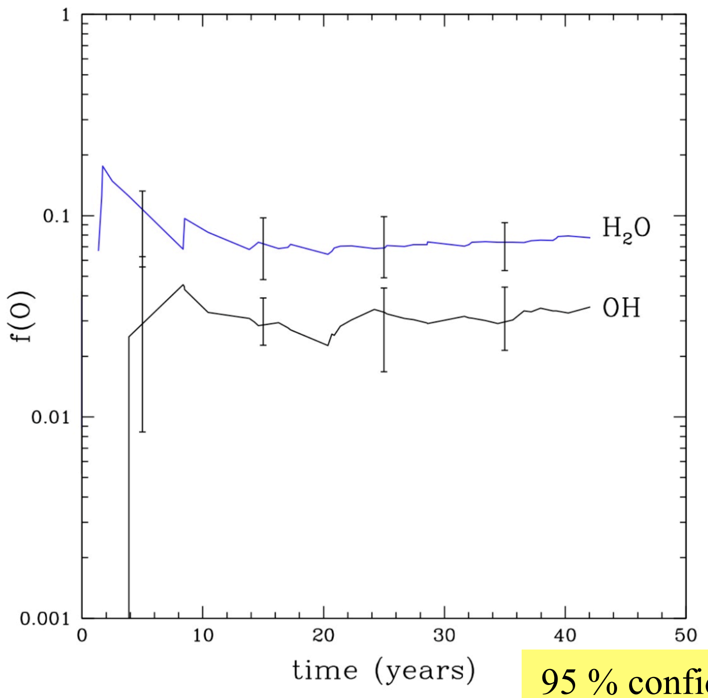
H2 + O → OH + H → H2O

T_{dust}=12K, T_{gas}=20K, G_0=1, Av=5
nH=5000 cm^{-3}, O/H =3 10^{-4}, D/H=2 10^{-5}

Grain surface



Gas phase

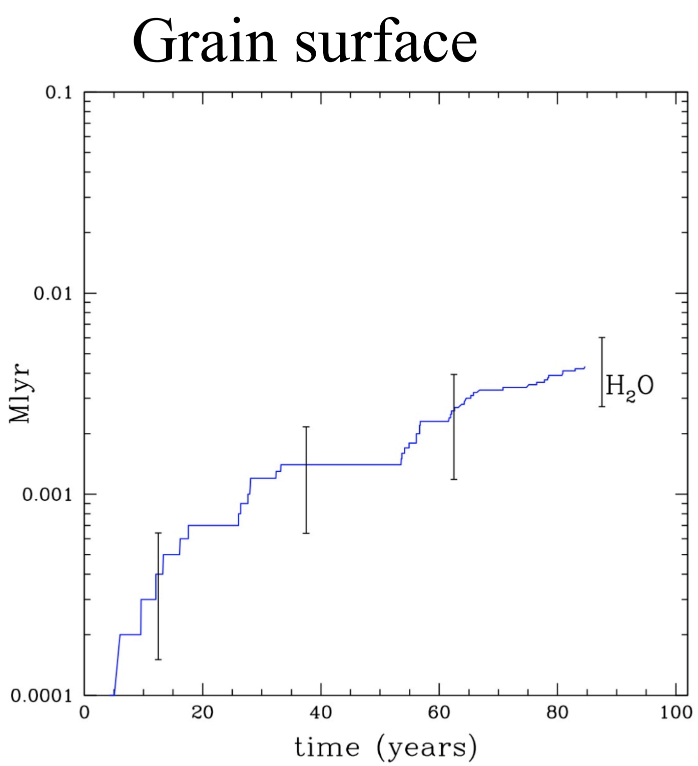


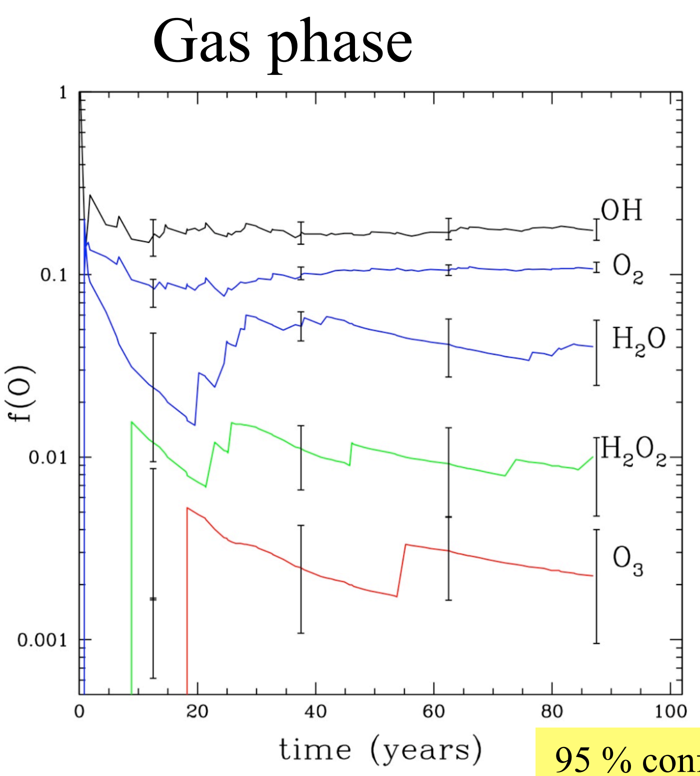
95 % confidence level

Photo-dissociation regions

PDR: H molecular
H_2O formation involves O_2 and O_3

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}





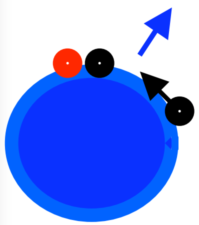
95 % confidence level

Formation of water

Diffuse clouds

Atomic OH + H

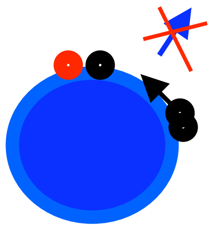
Ice coverage 0.3%



Transluscents clouds

Molecular OH + H_2

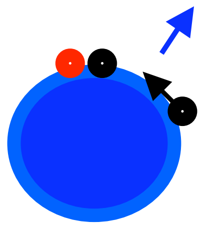
Ice coverage 1%



Dense clouds

Molecular O + $H_2 \rightarrow$ OH + H

Ice coverage > 100%



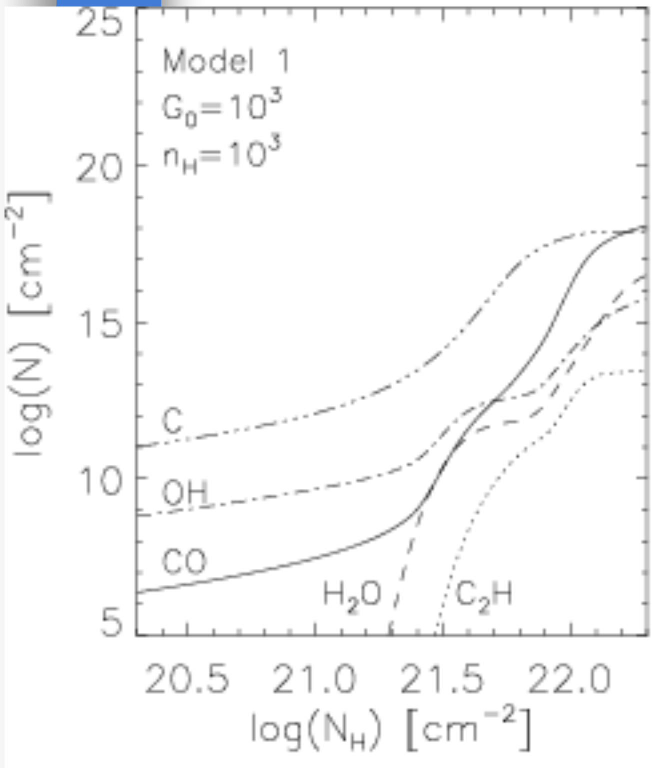
Warm grains O_2 and O_3

Chemistry on **bare grains** impacts **gas phase chemistry**

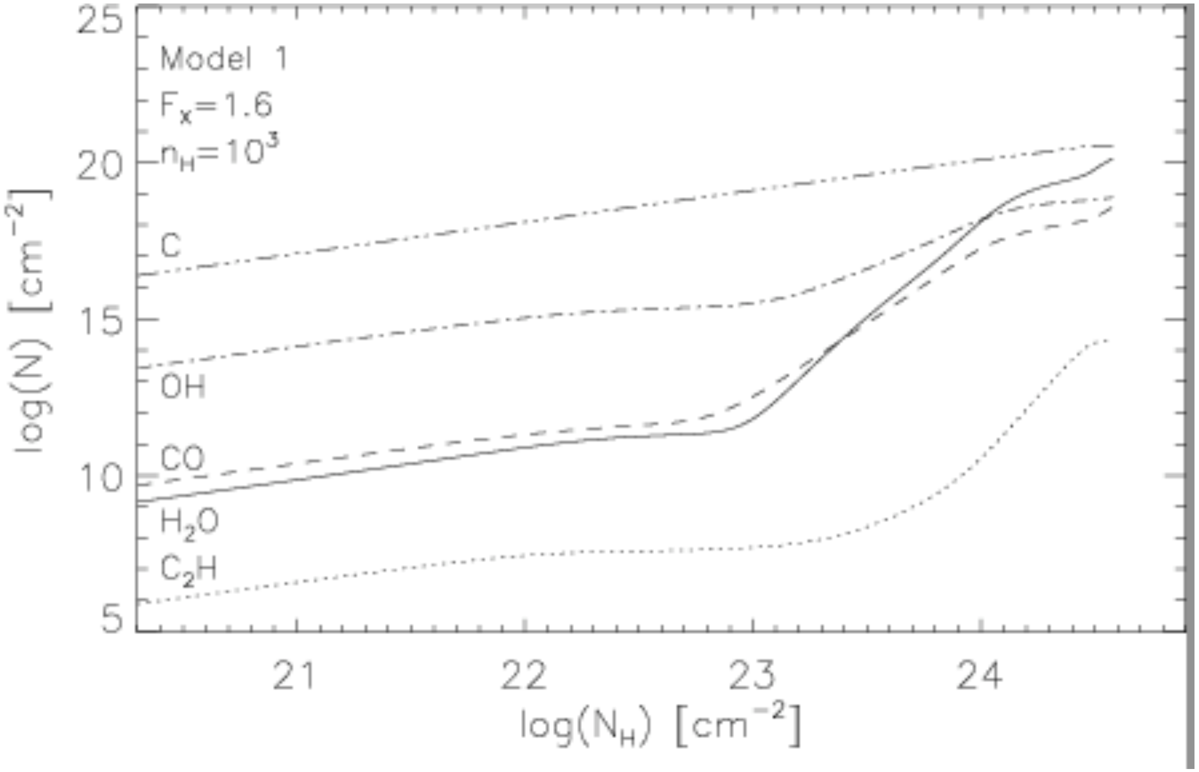
Once **icy mantles** formed, this process no longer exists

UV vs Xray star forming regions

PDR



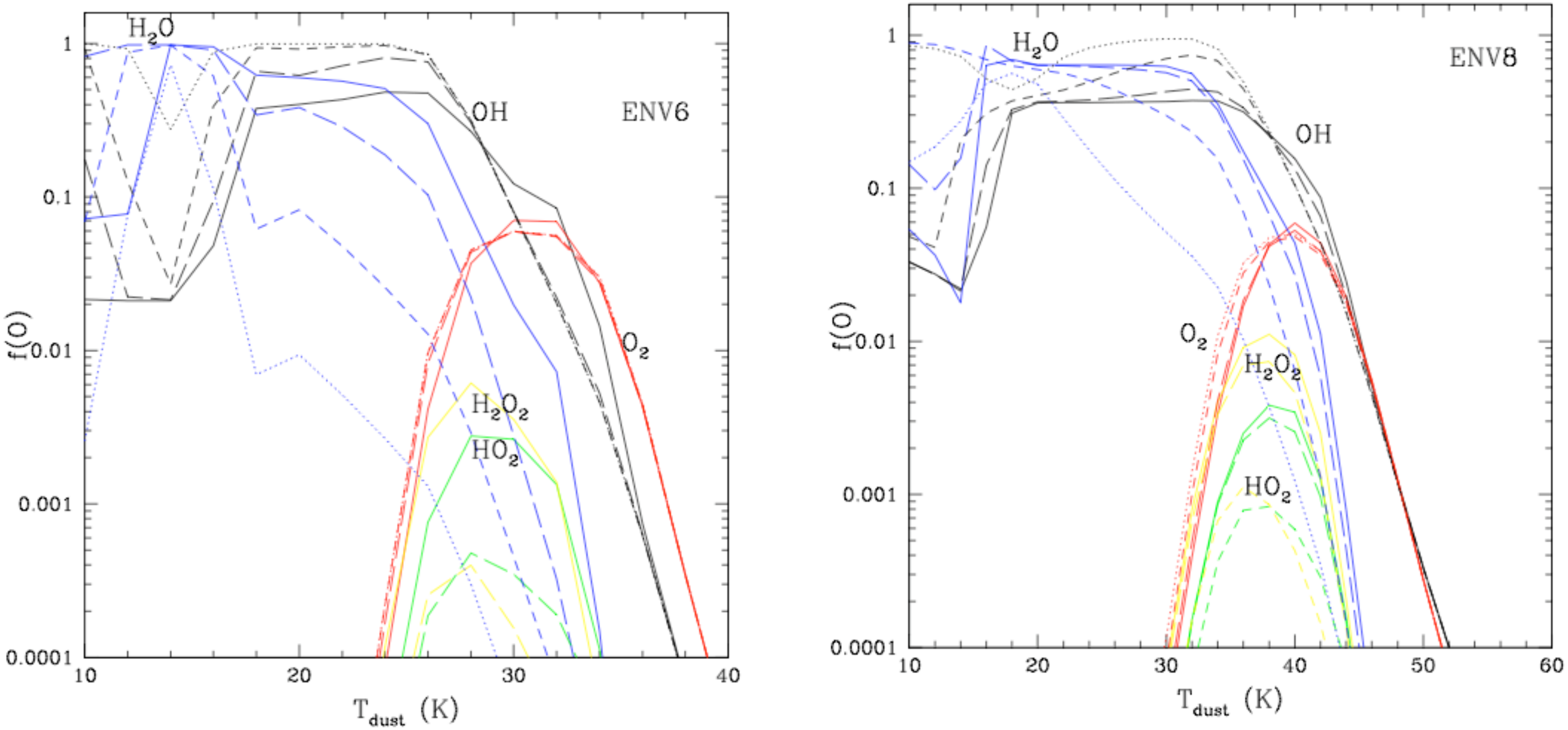
XDR



Grain surface chemistry in XDR

nH=10^3 cm^{-3}
G0=1,10,100,1000

nH=$10^{5.5}$ cm^{-3}
G0=10^3, 10^4, 10^5, 10^6

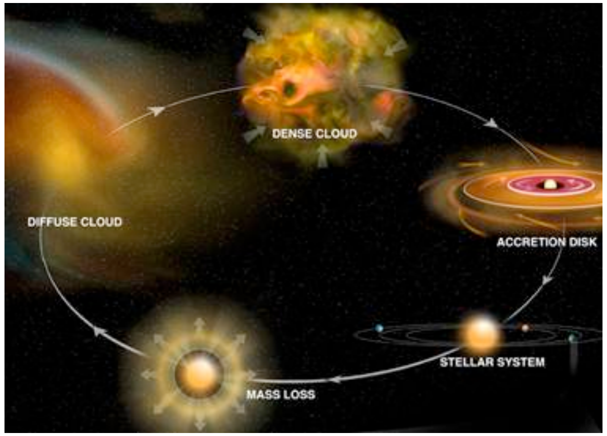


Summary and Conclusions

Very first stages of star formation: atomic / molecular / PDR (warm grains).

water forms on dust through different routes

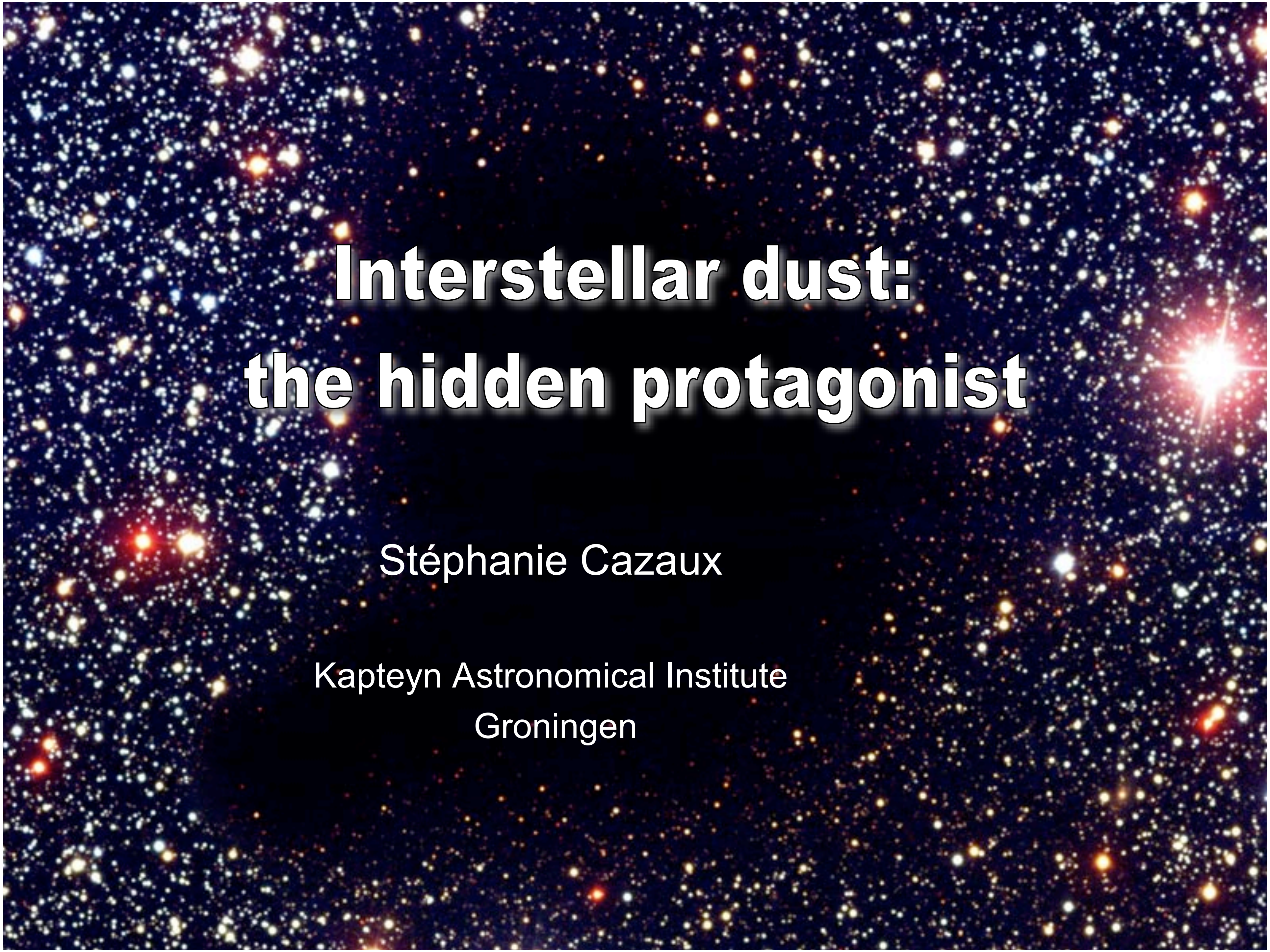
Reactions involve different routes with ≠ exothermicity: ≠ impact on gas



UV → photo-dissociate species that reform → enhance the fraction released in the gas upon formation.

Chemistry gas + dust during the collapse of a cloud

- Interstellar gas
- thermal balance
- star formation efficiency

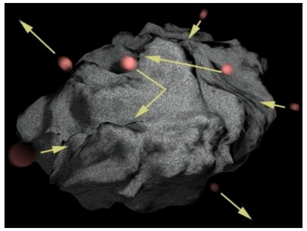


Interstellar dust: the hidden protagonist

Stéphanie Cazaux

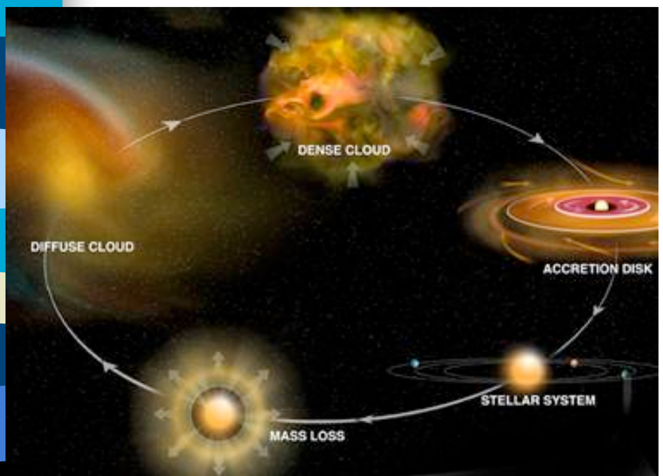
Kapteyn Astronomical Institute
Groningen

The real role of dust

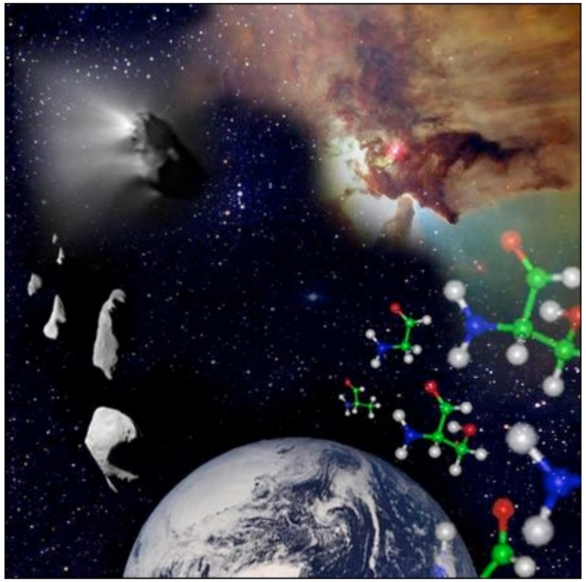


Interplay dust/gas

Star form in clouds (gas + dust)
cules cool the gas
Dust ➔ impact gas ➔ **star formation**



On dust ➔ **complex molecules**
➔ building blocks of **life**



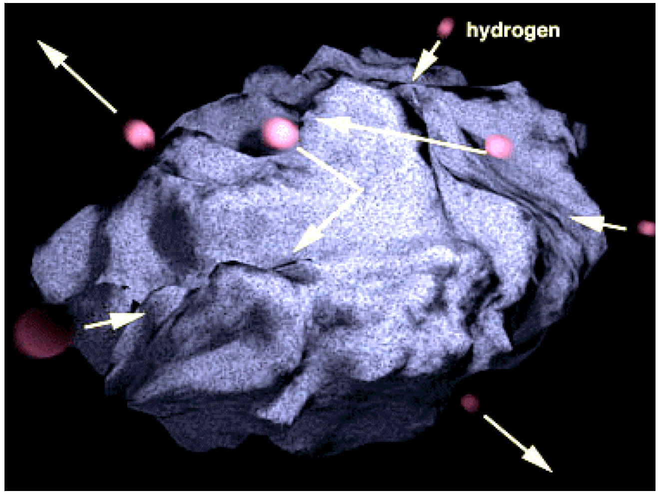
The real role of dust

Projects:

•Grain surface chemistry and molecular complexity (PHD)

•Primordial star formation (Post-doc)

•Diagnostics of star forming regions (Applicant)



Grain surface chemistry:

H_2 & HD

Cazaux & Tielens 2002, 2004
Cazaux et al. 2002, 2005
Cazaux & Spaans 2004, 2009

H_2O, O_2, ices

Cazaux et al. 2010, submitted, in prep

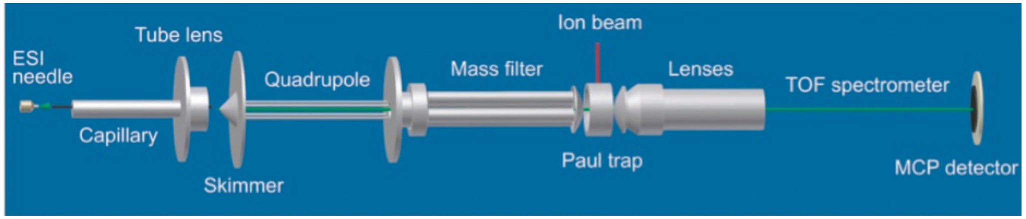
Complex molecules

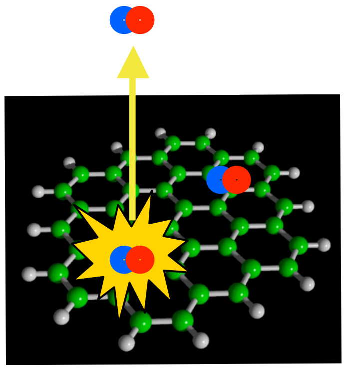
Cazaux et al. 2003

Grain surface chemistry and molecular complexity

Experiments

Available @ KVI (Kernfysisch Versneller Instituut) Groningen.





Exothermic

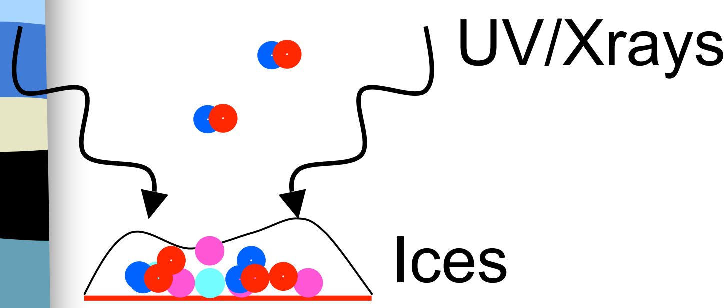
➡ Grain surface chemistry impacts gas

Project 1

Grain surface chemistry and molecular complexity

Model

Laboratory results ➔ surface chemistry code (Cazaux et al. 2010)



Goals:

➔ Tool for astrophysical models: include dust

➔ Complexity in ices VS comets and star forming regions

➔ Issue for astrochemistry/ planetology/ astrobiology

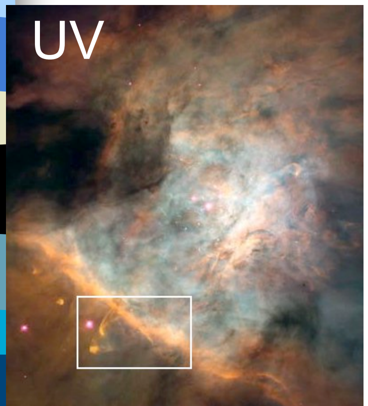
Project 2

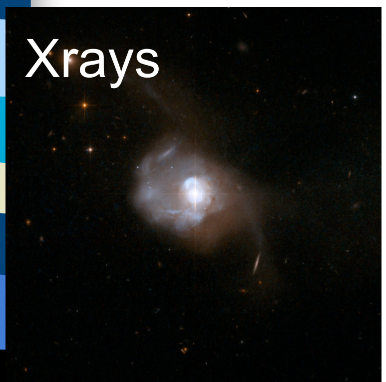
Diagnostics of star forming regions

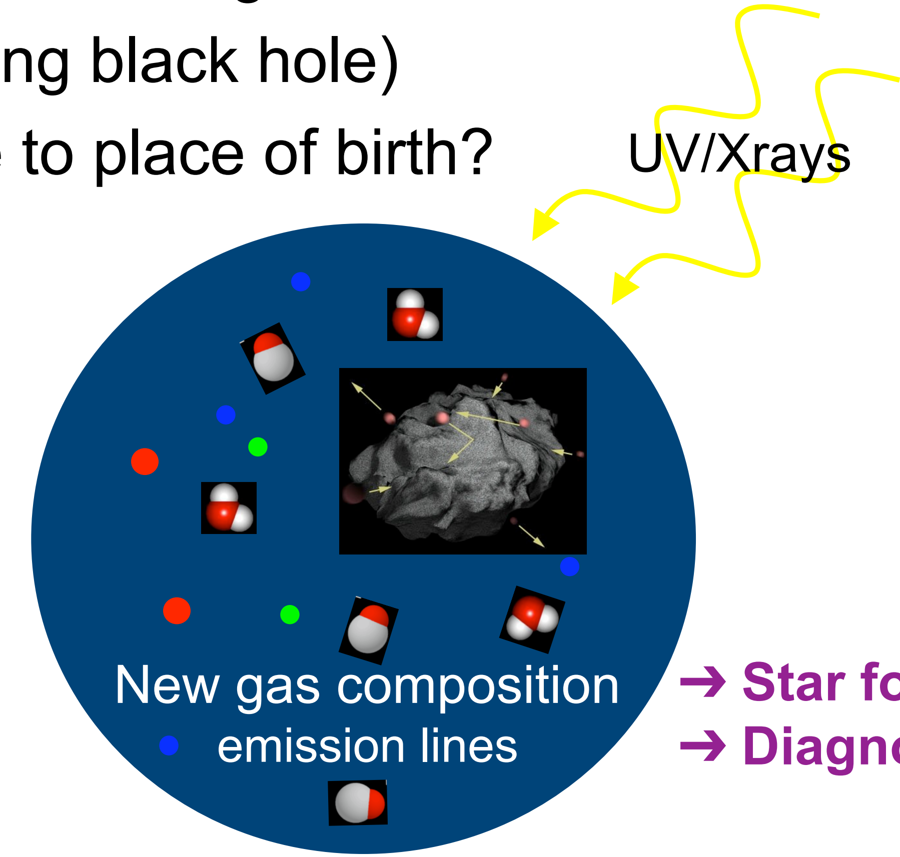
Molecular content of star forming environments

UV (star)/Xrays (accreting black hole)

Star formation sensitive to place of birth?







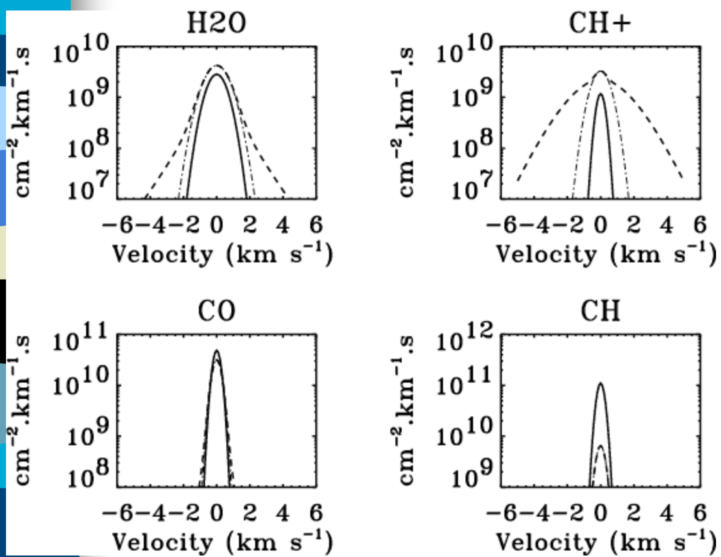
→ **Star formation**

→ **Diagnostics**

PDR/XDR (UV/Xrays dominated regions)
+ radiative transfer code. Kapteyn Institute.

Project 2

Diagnostics of star forming regions



Radio telescopes interferometers

ALMA 2011
(Atacama Large Millimeter Array)

Goals:

➔ Impact of dust on gas in star forming regions

➔ Star formation efficiency

➔ Diagnostics UV/Xrays regions

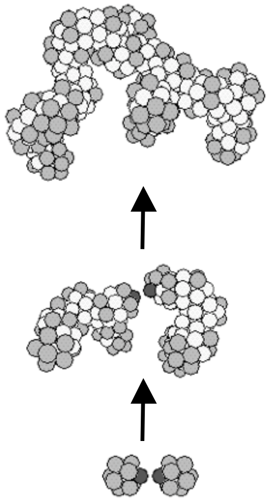
Project 3

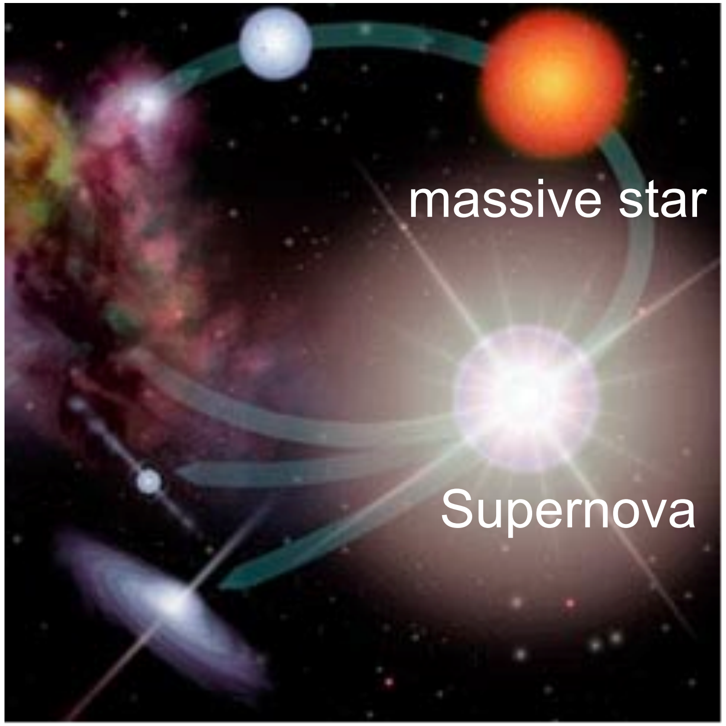
Primordial star formation

Early Universe: simple species / no dust.

Supernovae produce heavy elements ➔ in dust.

Dust enrichment + chemistry changes star formation

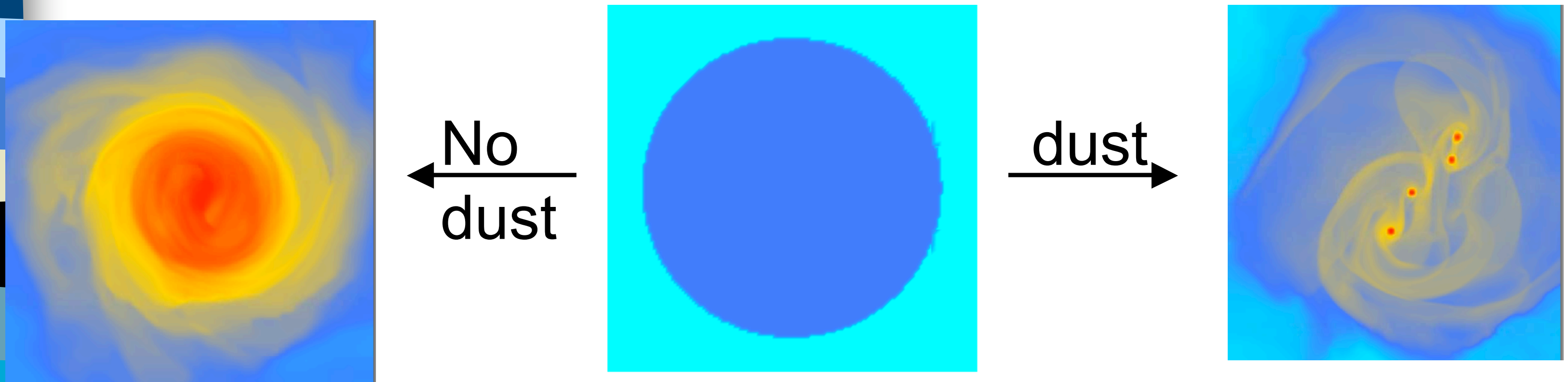




Primordial star formation

Molecular cloud evolution: Hydrodynamic code

Kapteyn Institute



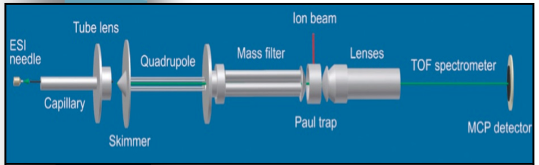
Goals: dust affects

➔Cloud fragmentation

➔Star formation and final masses

Dust as protagonist

Experiment

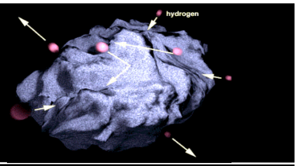


T. Schlathoelter, KVI

P1:15 months /P2:12 months

Model

Dust/gas + ices



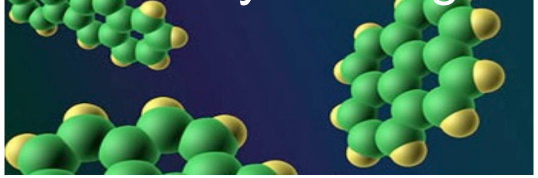
P. Caselli, Leeds

V. Cobut, Paris

P1:18 months /P2:12months

Model

Chemistry PAHs/gas



P3:6 months

Observations

P1:15 months /P2:24months

PDR/XDR + dust + emission lines

M. Spaans, Kapteyn

P2:months

Hydrodynamic code + dust

M. Spaans, Kapteyn

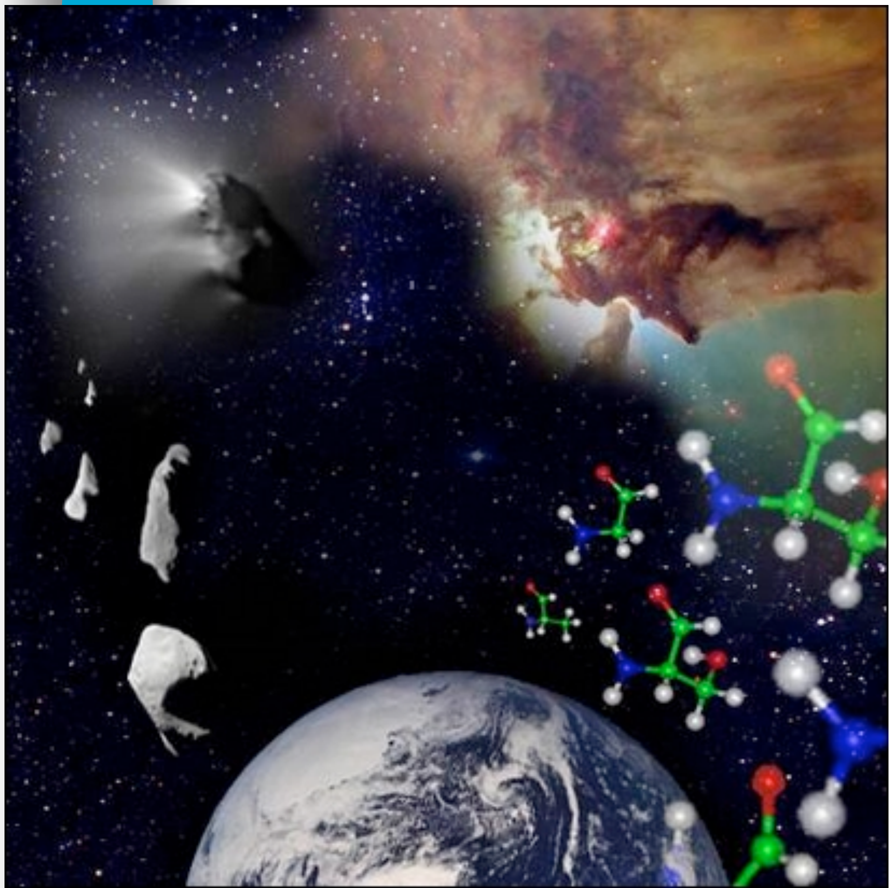
S. Salvadori, Kapteyn

P3: 24 months

P1: PHD P2: Applicant P3: Postdoc

Dust as protagonist

Chemical complexity



Star formation