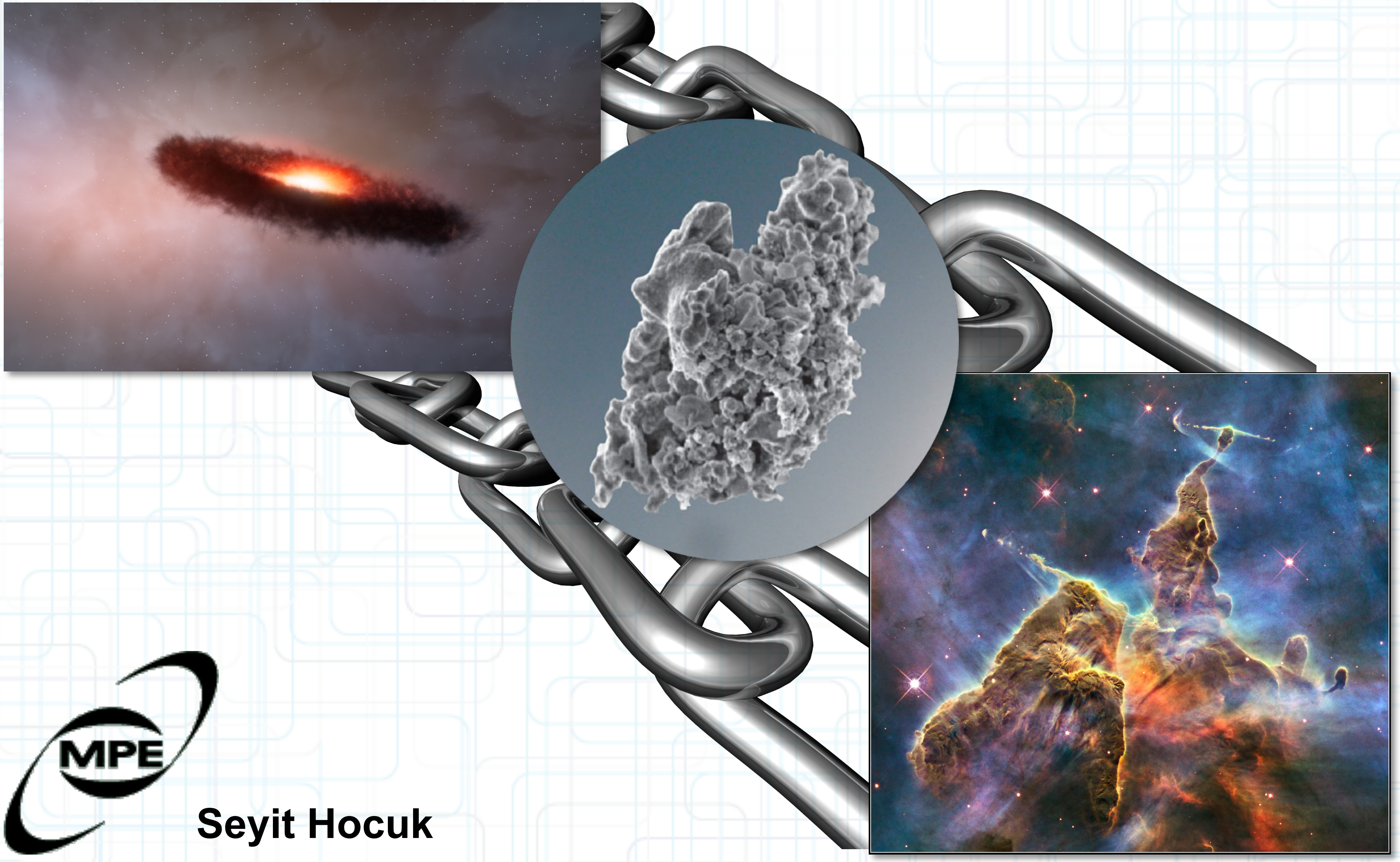
The role of small and large scale physics

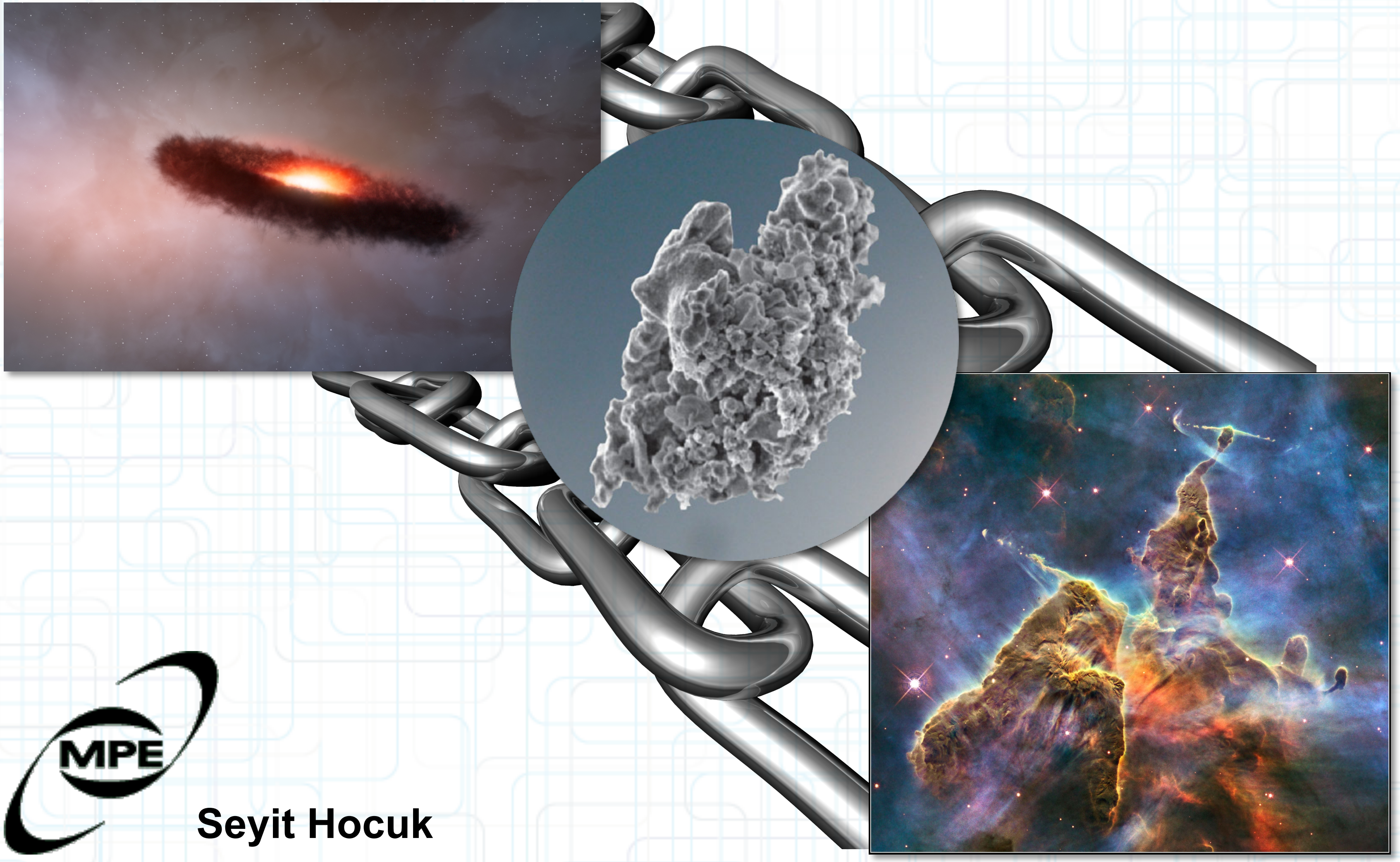
in numerical studies of star formation



Seyit Hocuk

The role of small ~~and large~~ scale physics

in numerical studies of star formation



Seyit Hocuk

In collaboration with

S. Cazaux

P. Caselli

M. Spaans

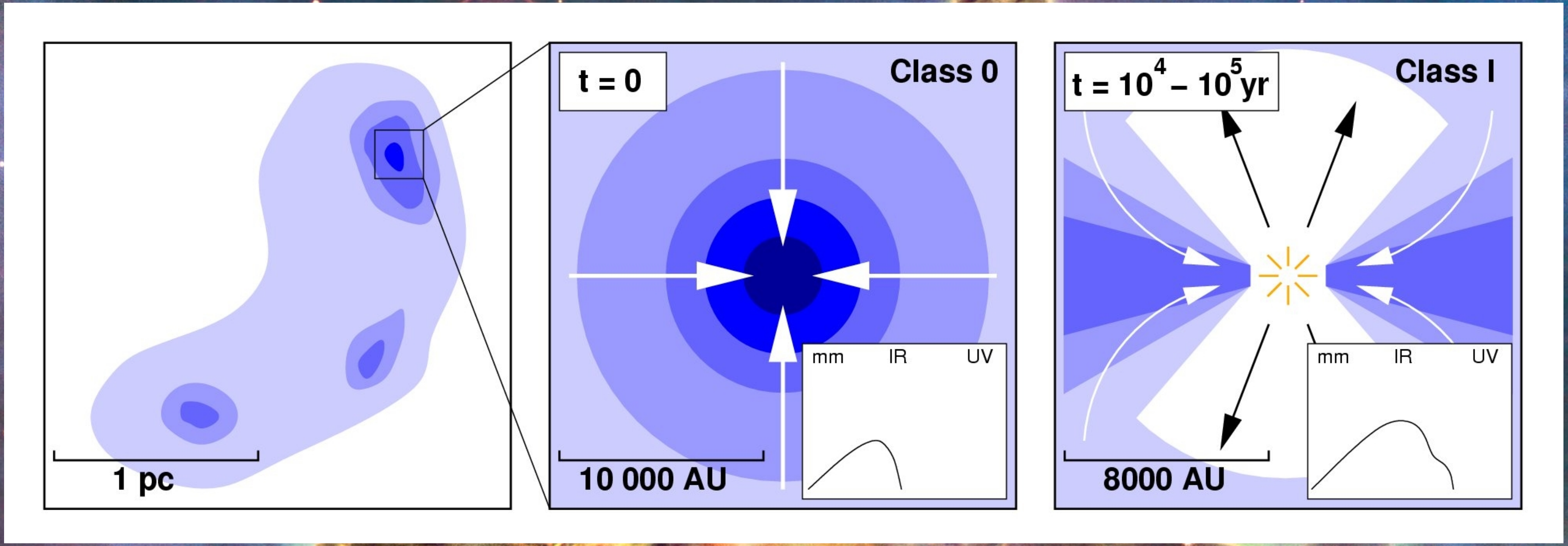
In collaboration with

S. Cazaux: The dust expert, experiments

P. Caselli: Expert on observations of star-forming regions

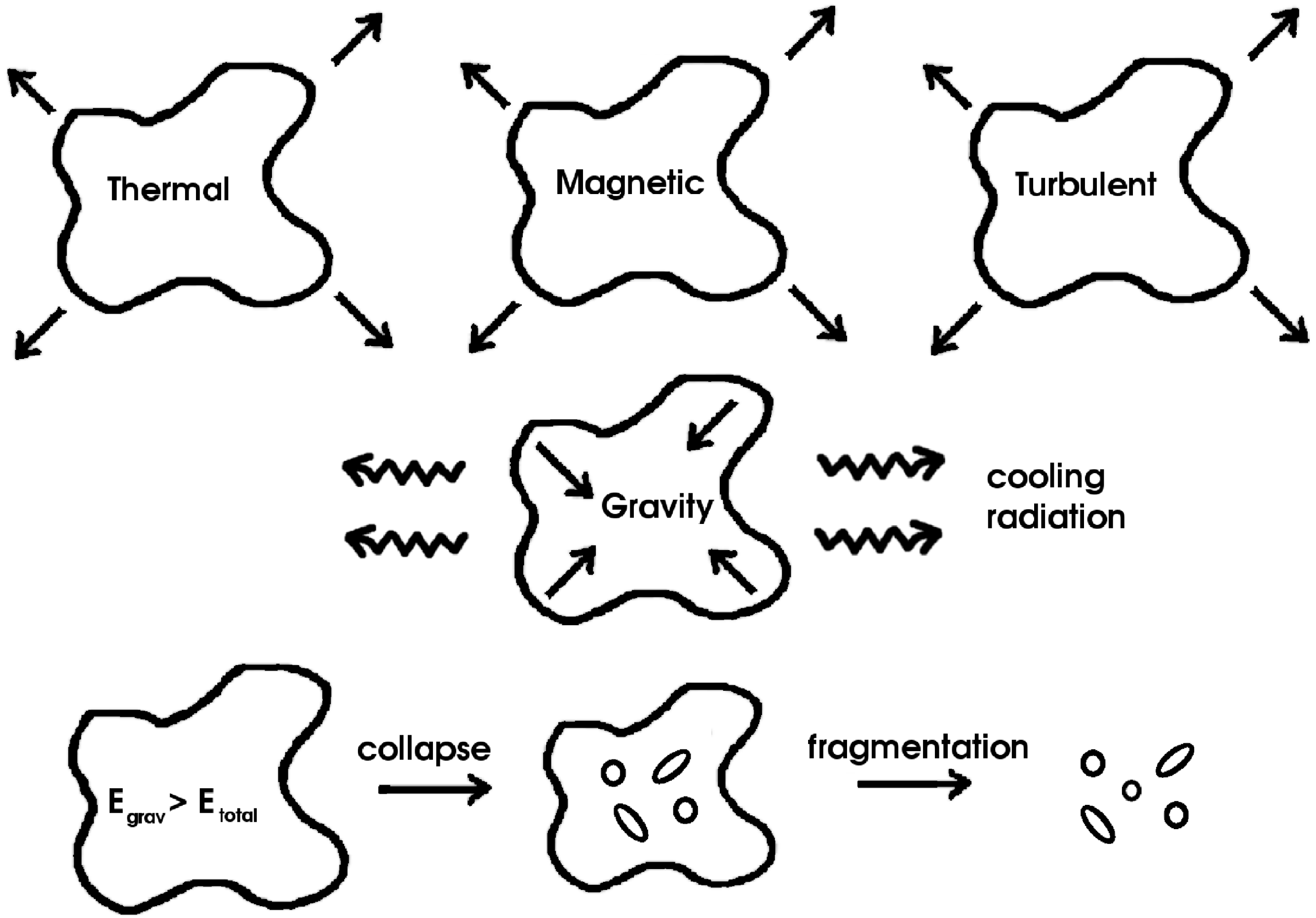
M. Spaans: Expert on star-formation theories and the EOS

Star formation



Jonkheid 2006

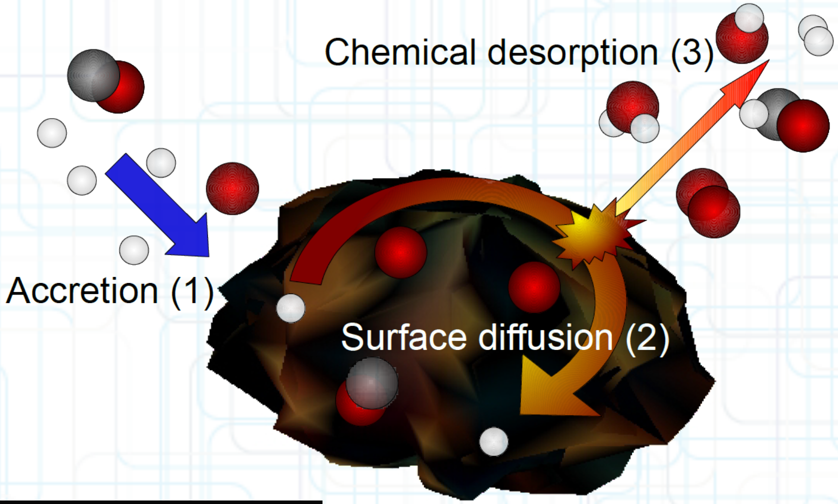
Large scale and feedback processes



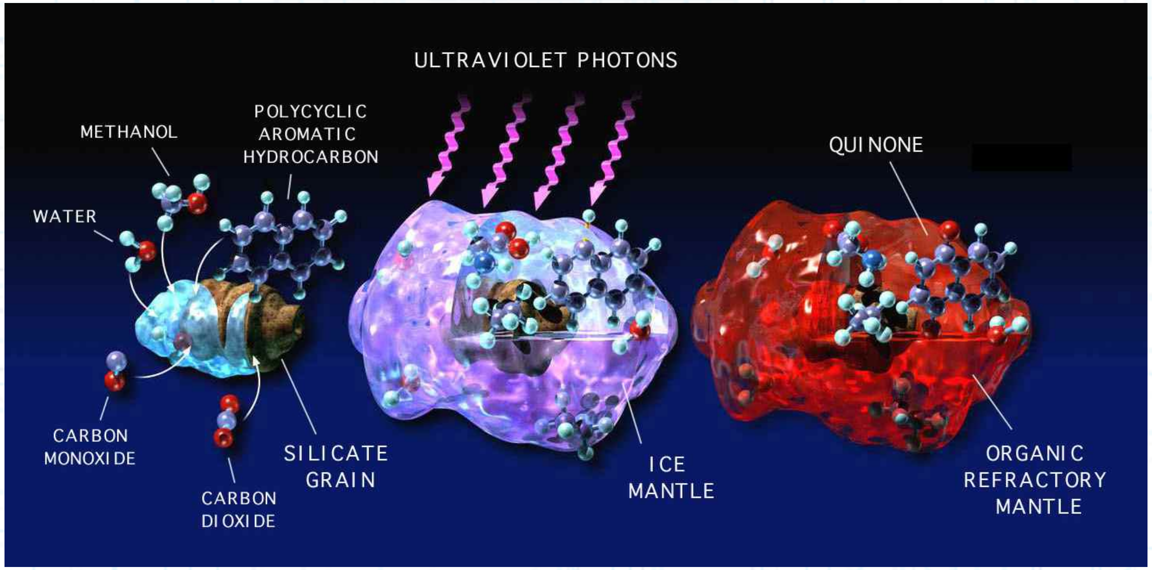
Hocuk 2011

Chemistry, on dust grains

Carbon based or
Silicon based

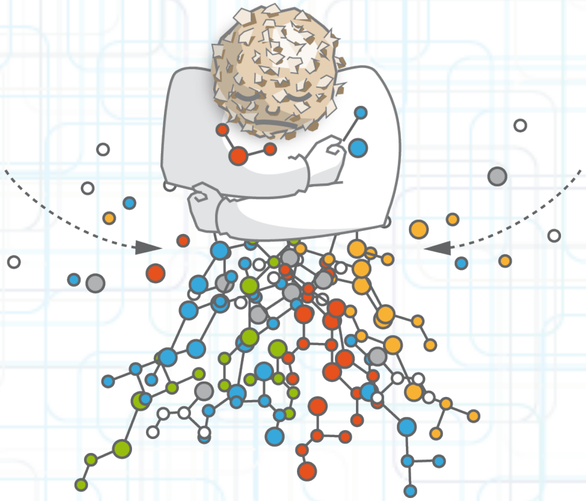


1 micron



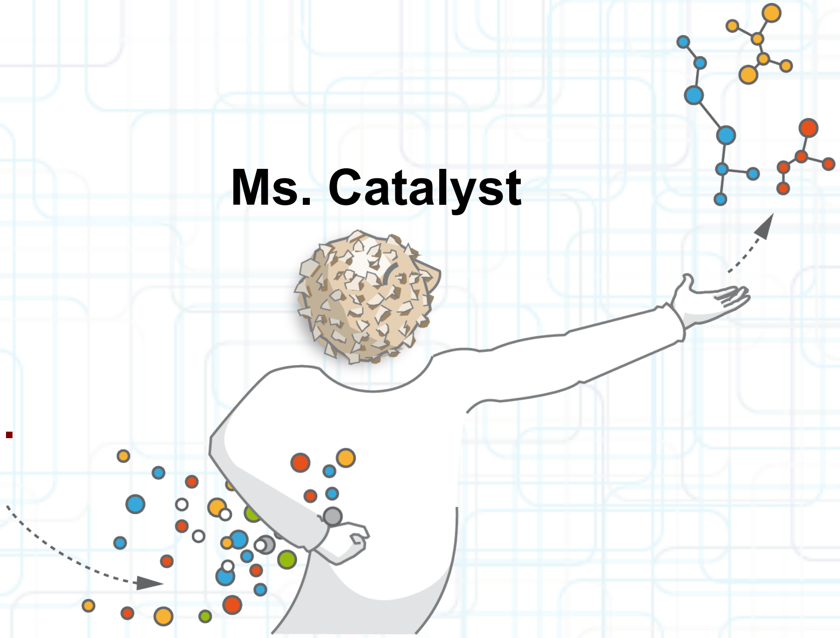
Cosmic Dust dual nature

Mr. Freeze



vs.

Ms. Catalyst



Dust can lock up atoms and molecules when it’s cold, but it can also allow efficient molecule formation.

Why is dust chemistry important?

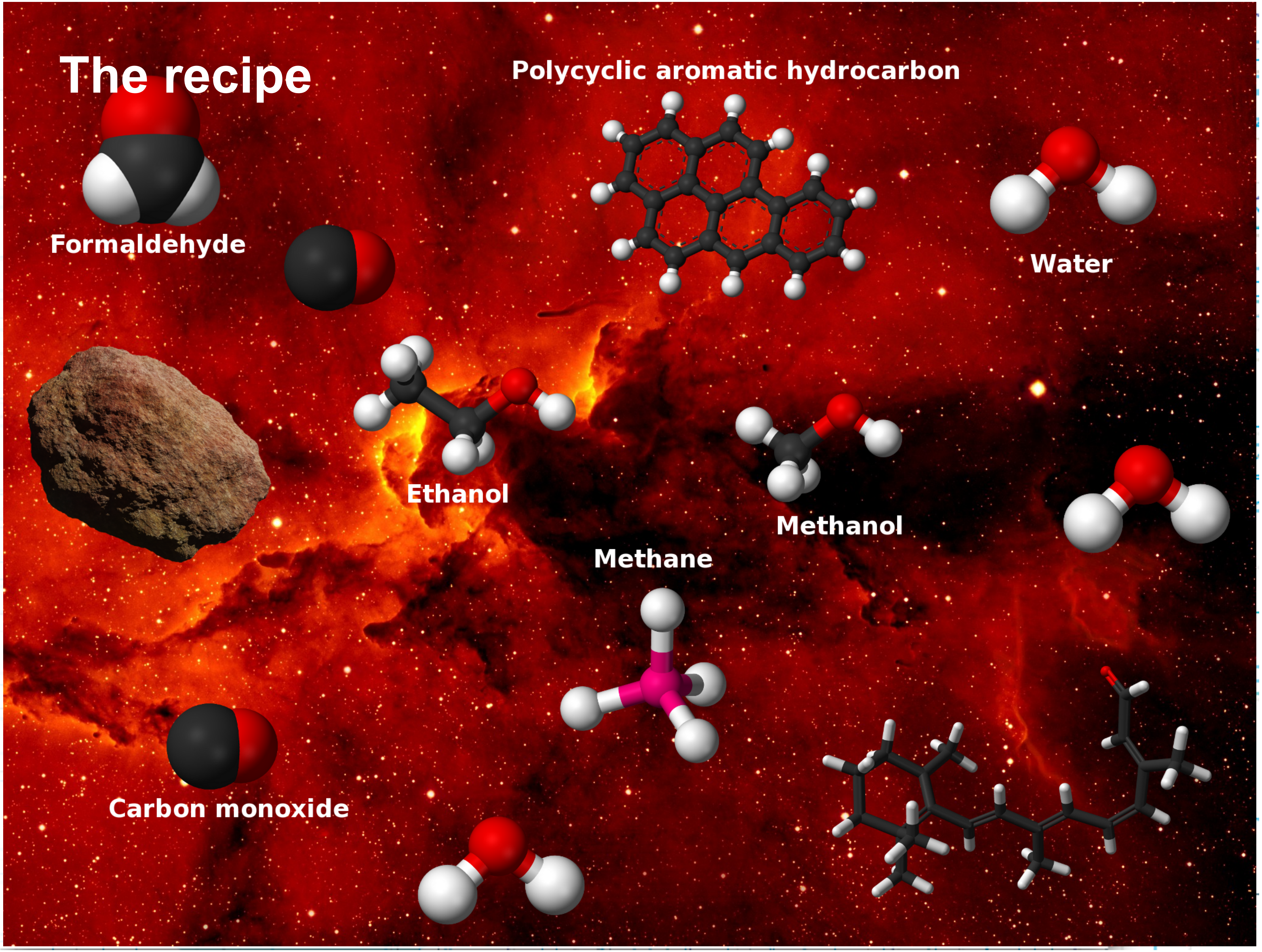
a) It affects the molecule formation in star-forming clouds

b) Molecules control the radiative cooling properties of gas

c) The equation of state will be affected

d) This happens in the very early phases of evolving clouds

The recipe

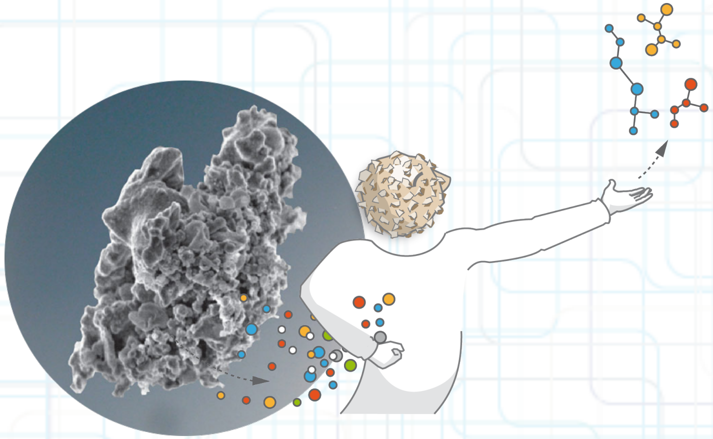

Polycyclic aromatic hydrocarbon
Formaldehyde
Water
Ethanol
Methanol
Methane
Carbon monoxide

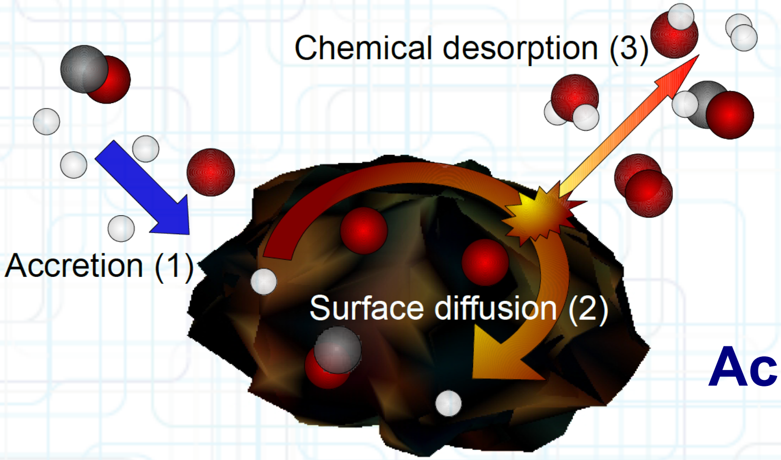
The FLASH code

- AMR hydrodynamical code
- Gas + grain surface chemistry (rate equations)
- Thermal balance (non-equilibrium)
- UV + CR background
- Including processes such as: Freeze-out, Photodesorption, Chemical desorption, Two-phase model
- Upto 7000 reactions in the gas phase over 100 on dust

Dust chemistry

Rate equations



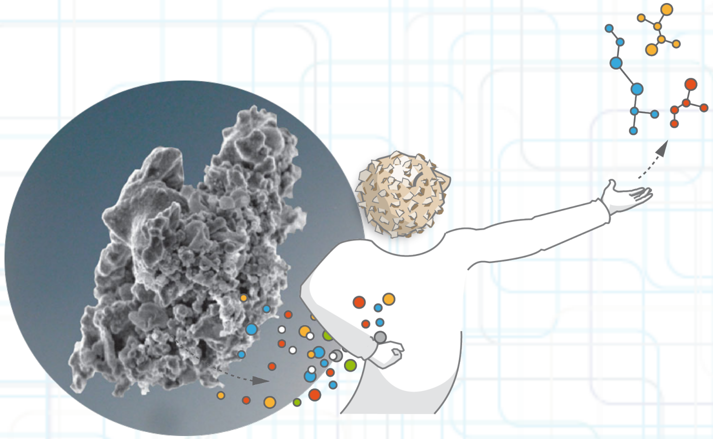


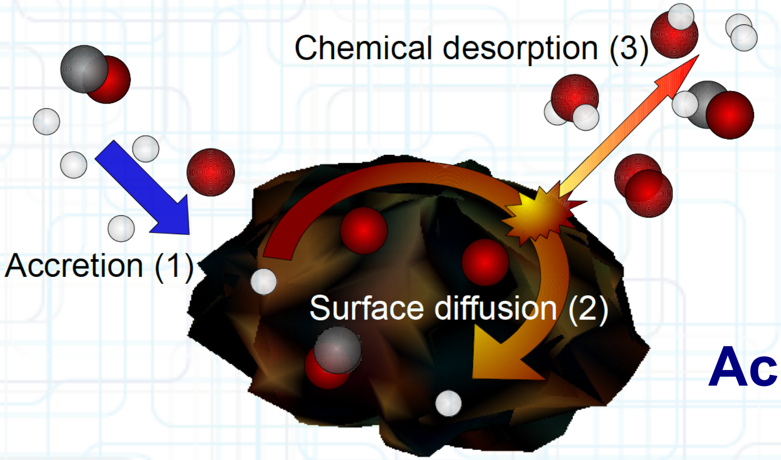
Accretion/Adsorption

$$k_{accr} = \alpha \sqrt{\frac{T_g}{100}} \beta \quad \mathrm{cm}^3 \mathrm{s}^{-1},$$

$$R_{accr} = n_{x_i} n_{<H>} S(T_g) \times k_{accr} \quad \mathrm{cm}^{-3} \mathrm{s}^{-1},$$

Dust chemistry
Rate equations





Accretion/Adsorption

thermal velocity

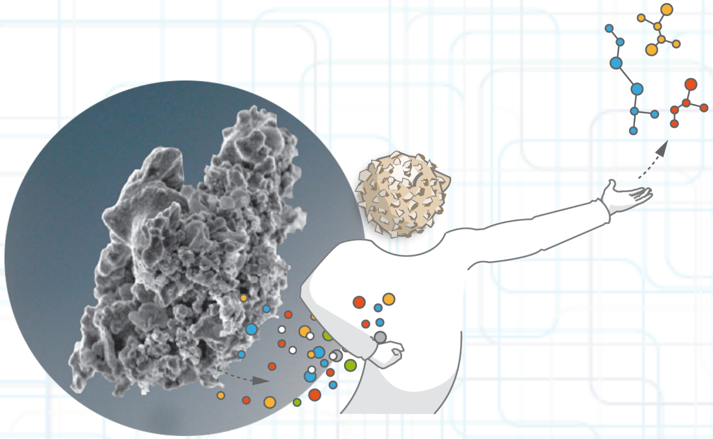
total cross-section

$$k_{accr} = \alpha \sqrt{\frac{T_g}{100}} \beta \quad \mathrm{cm}^3 \mathrm{s}^{-1},$$

$$R_{accr} = n_{x_i} n_{<H>} S(T_g) \times k_{accr} \quad \mathrm{cm}^{-3} \mathrm{s}^{-1},$$

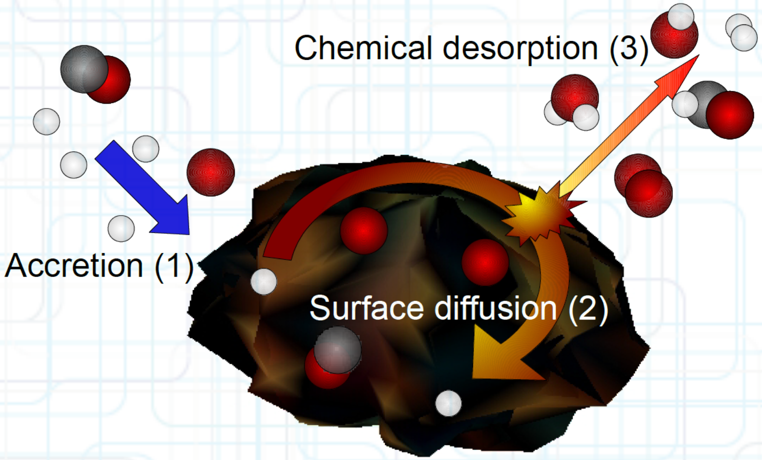
Species number density

Sticking coefficient



Dust chemistry

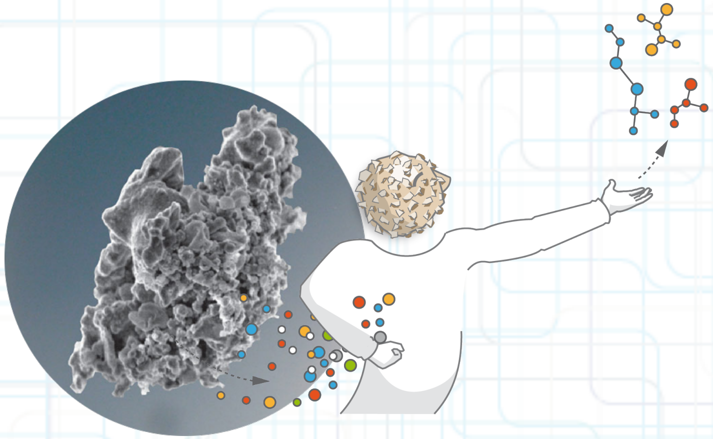
Rate equations



Evaporation

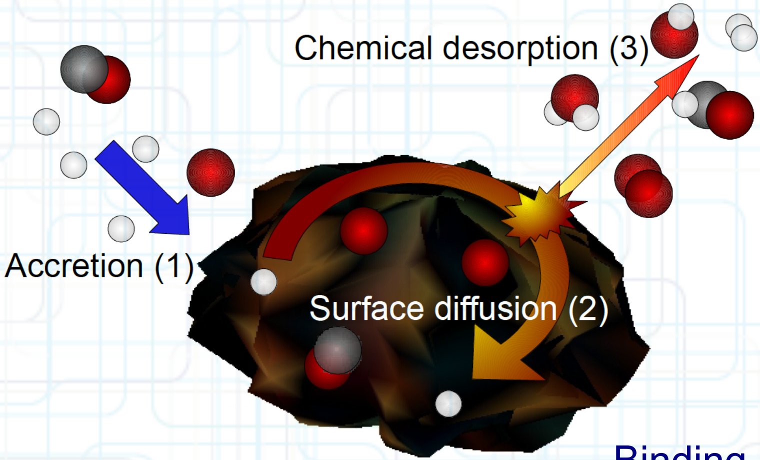
$$k_{evap} = \alpha \left(\mathcal{F}_{bare} \exp\left(-\frac{E_{bare,i}}{T_d}\right) + \mathcal{F}_{ice} \exp\left(-\frac{E_{ice,i}}{T_d}\right)\right) \quad s^{-1},$$

$$R_{evap} = n_{x_i} \times k_{evap} \quad cm^{-3}s^{-1},$$



Dust chemistry

Rate equations



Evaporation

Binding energy bare

Binding energy ice

oscillation frequency

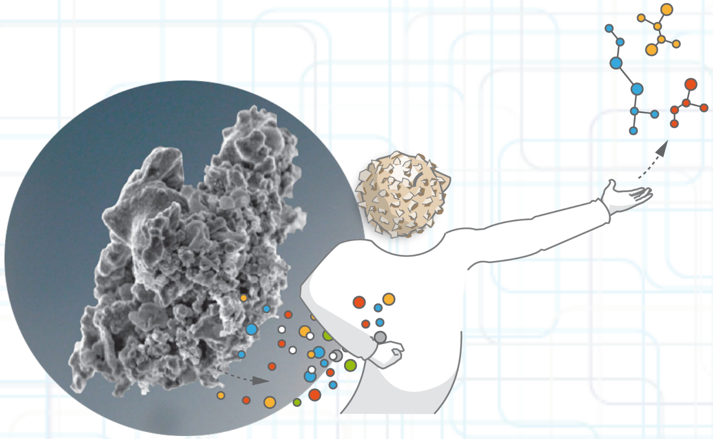
$$k_{evap} = \alpha\left(\mathcal{F}_{bare}\exp\left(-\frac{E_{bare,i}}{T_d}\right) + \mathcal{F}_{ice}\exp\left(-\frac{E_{ice,i}}{T_d}\right)\right) \quad \mathrm{s}^{-1},$$

$$R_{evap} = n_{x_i} \times k_{evap} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1},$$

dust temperature

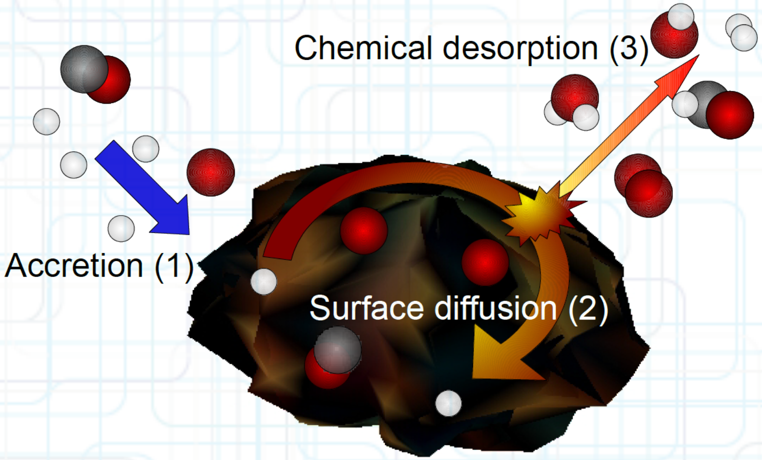
bare grain fraction

icy dust fraction



Dust chemistry

Rate equations



Reaction

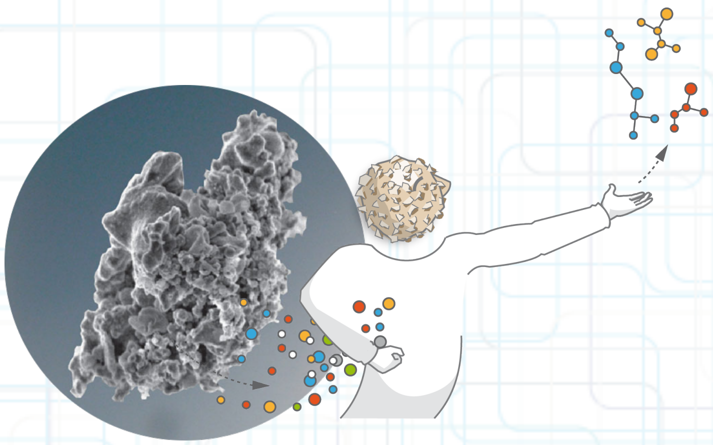
$$k_{2body} = \alpha \mathcal{F}_{bare} \left(\exp\left(-\frac{2E_{bare,i}}{3T_d}\right) + \exp\left(-\frac{2E_{bare,j}}{3T_d}\right)\right)\beta$$

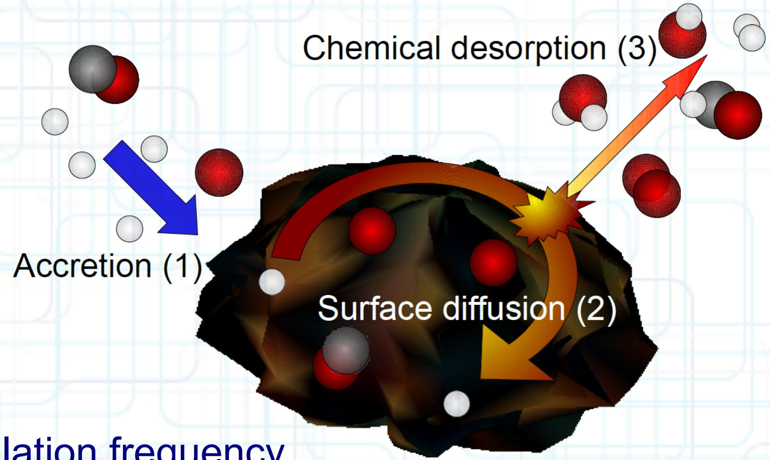
$$+ \alpha \mathcal{F}_{ice} \left(\exp\left(-\frac{2E_{ice,i}}{3T_d}\right) + \exp\left(-\frac{2E_{ice,j}}{3T_d}\right)\right)\gamma \quad \mathrm{s}^{-1},$$

$$R_{2body} = \frac{n_{x_i} n_{x_j}}{n_d n_{sites}} P_{reac} \times k_{2body} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1},$$

Dust chemistry

Rate equations





Reaction

oscillation frequency

chemical desorption

$$k_{2body} = \alpha\mathcal{F}_{bare}\left(\exp\left(-\frac{2E_{bare,i}}{3T_d}\right)+\exp\left(-\frac{2E_{bare,j}}{3T_d}\right)\right)\beta + \alpha\mathcal{F}_{ice}\left(\exp\left(-\frac{2E_{ice,i}}{3T_d}\right)+\exp\left(-\frac{2E_{ice,j}}{3T_d}\right)\right)\gamma \quad \mathrm{s}^{-1},$$

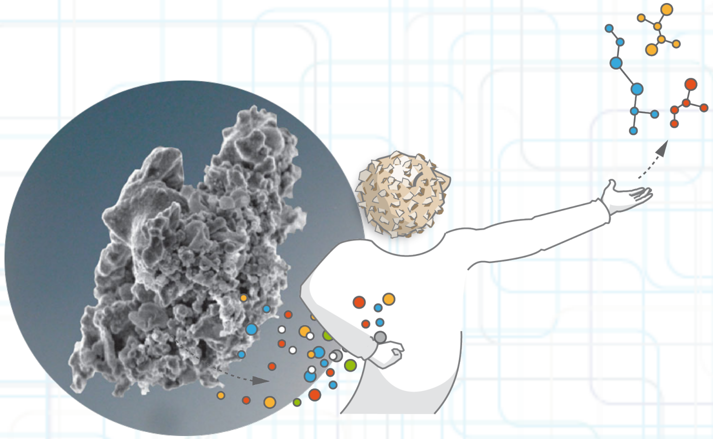
monolayer conversion

reaction probability

$$R_{2body} = \frac{n_{x_i}n_{x_j}}{n_d n_{sites}} P_{reac}\times k_{2body} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1},$$

Dust chemistry

Rate equations



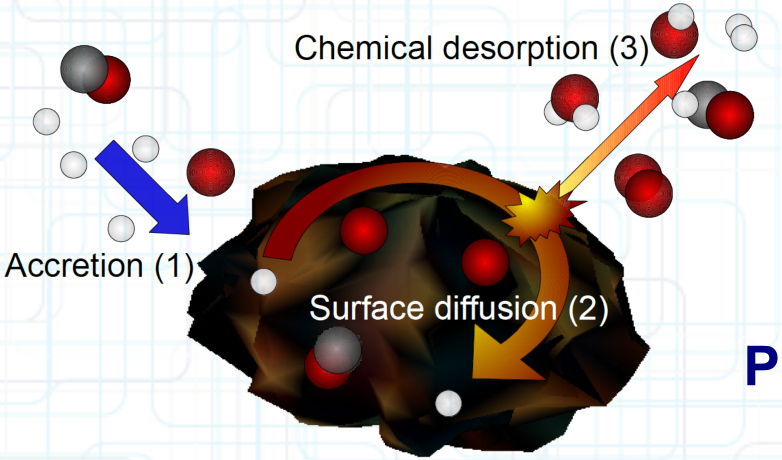
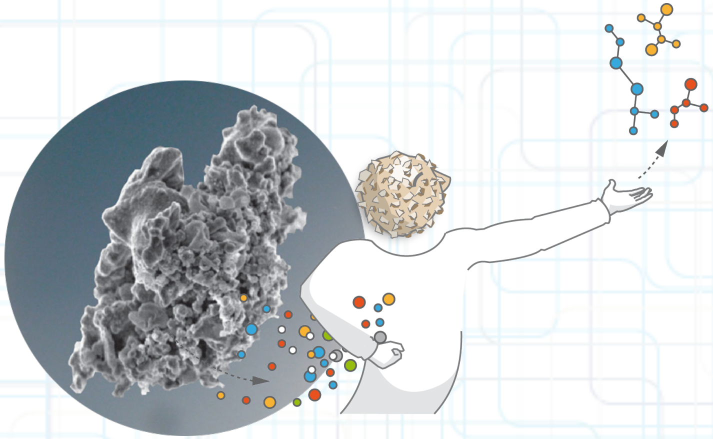


Photo-dissociation

$$
\begin{aligned}
k_{phot} &= \alpha e^{-\gamma A_v} \quad \mathrm{s}^{-1}, \\
R_{phot} &= \chi\, n_{x_i} \times k_{phot} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1}.
\end{aligned}
$$

Dust chemistry

Rate equations



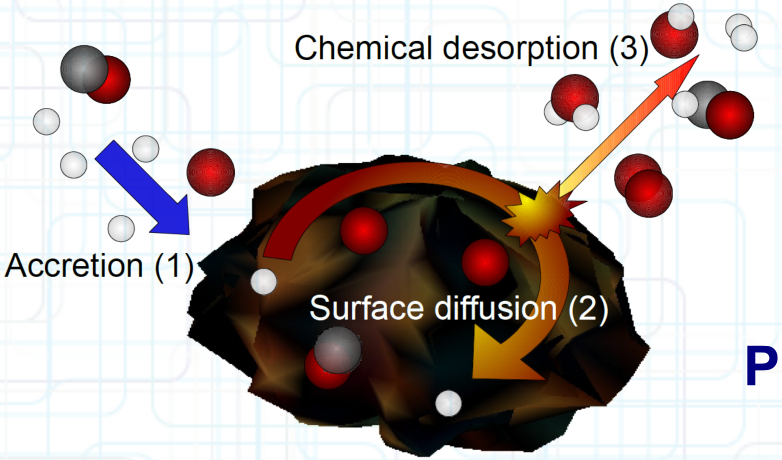


Photo-dissociation

extinction factor

visual extinction

$$k_{phot} = \alpha e^{-\gamma A_v} \quad \mathrm{s}^{-1},$$

unattenuated rate

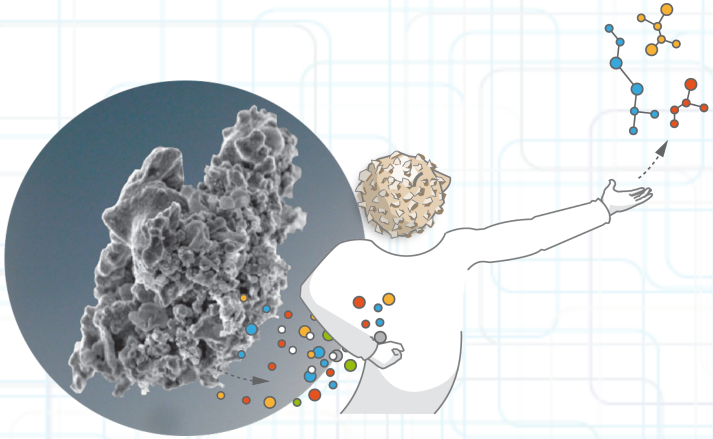
$$R_{phot} = \chi\, n_{x_i} \times k_{phot} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1}.$$

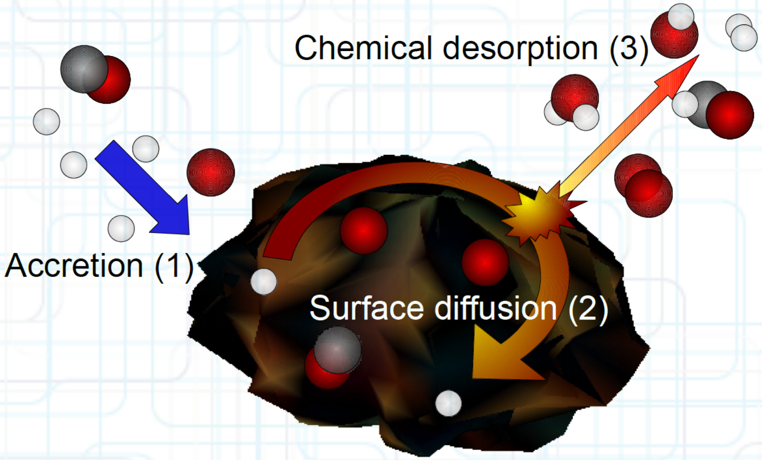
UV field strength

self-shielding is included for CO and H_2

Dust chemistry

Rate equations





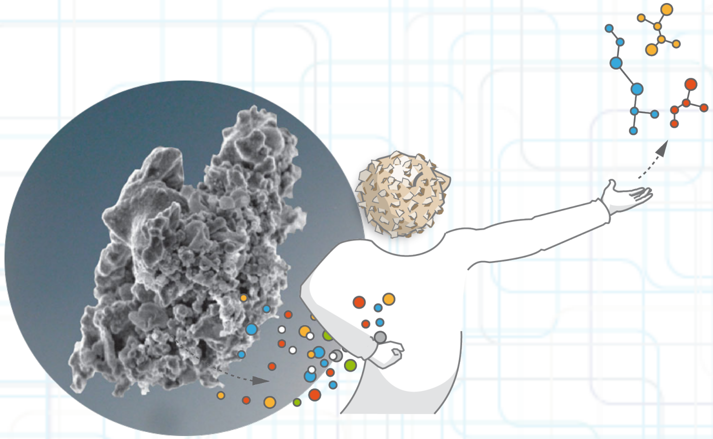
CR processes

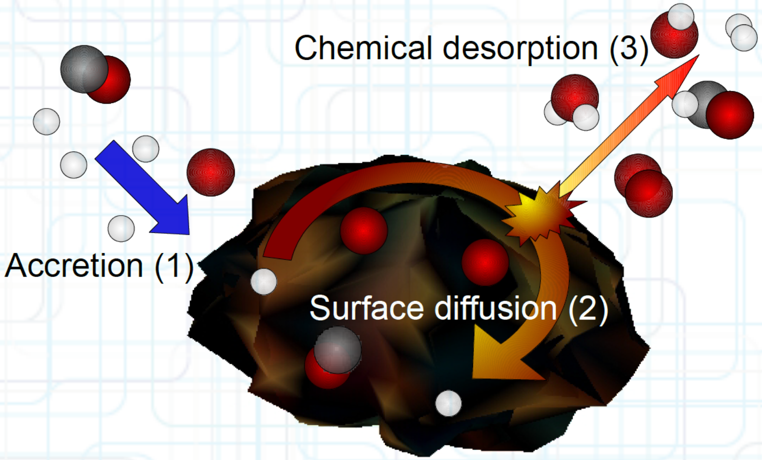
$$k_{CR} = \alpha\zeta_{H_2} \quad \mathrm{s}^{-1},$$

$$R_{CR} = n_{x_i} \times k_{CR} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1},$$

Dust chemistry

Rate equations





CR processes

fractional rate per reaction

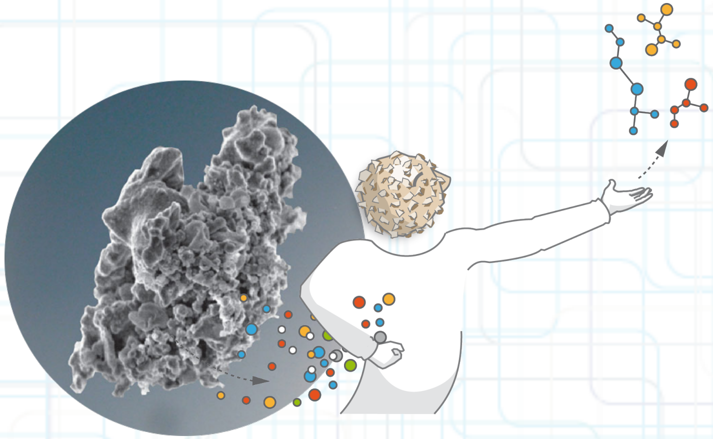
Cosmic ray ionisation rate

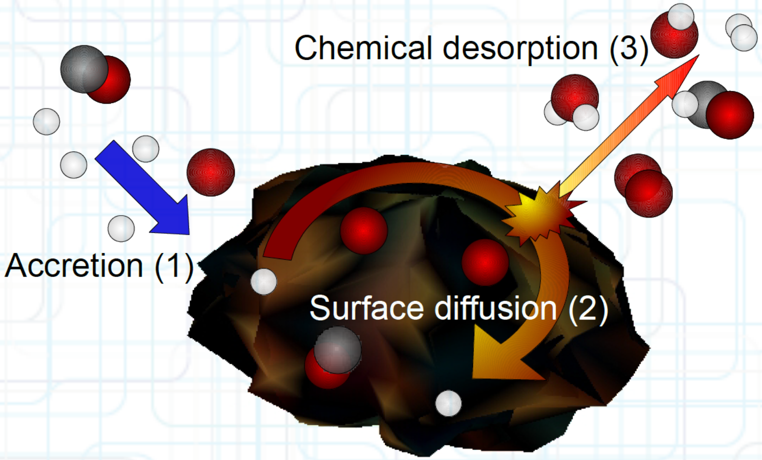
$$k_{CR} = \alpha\zeta_{H_2} \quad \mathrm{s}^{-1},$$

$$R_{CR} = n_{x_i} \times k_{CR} \quad \mathrm{cm}^{-3}\mathrm{s}^{-1},$$

Dust chemistry

Rate equations



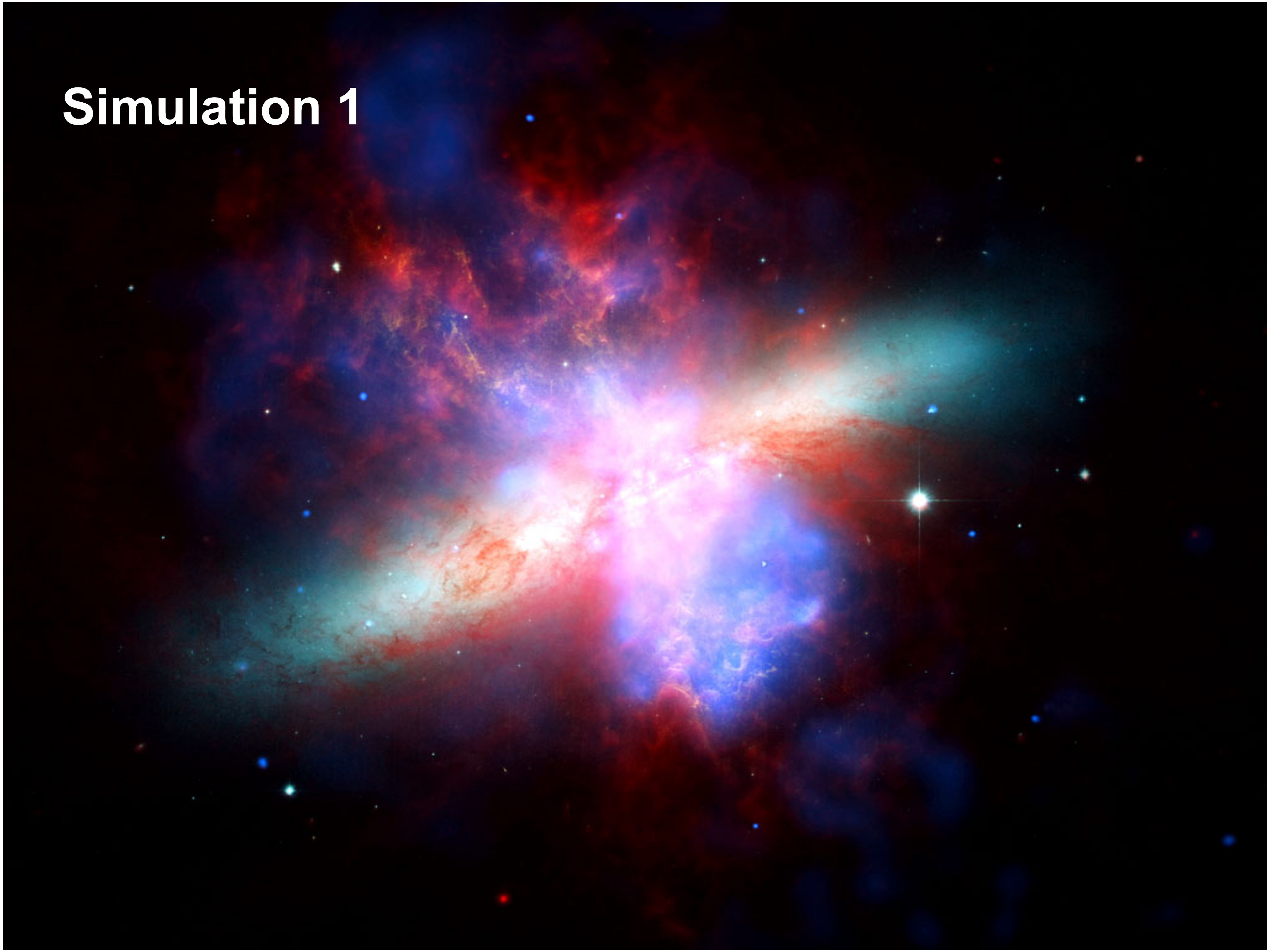


Photodesorption

Secondary UV from CR

Chemical adsorption

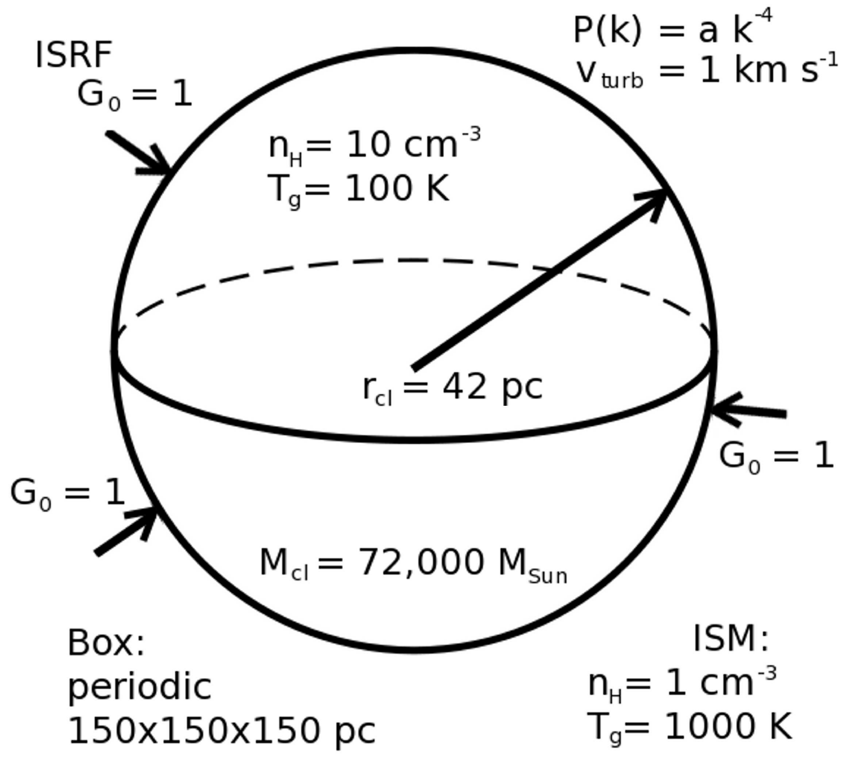
Simulation 1



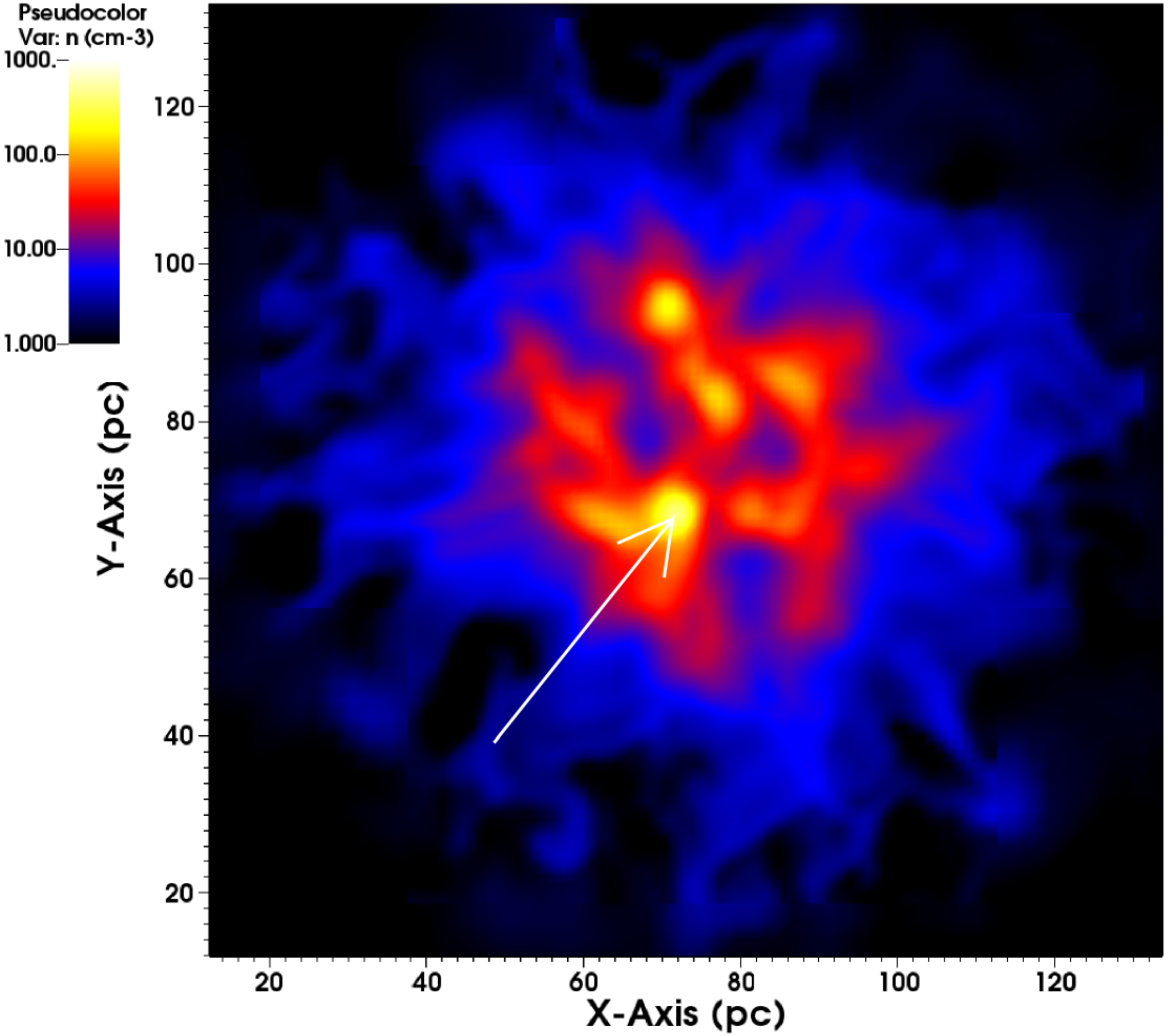
Diffuse cloud simulation

Ingredients:

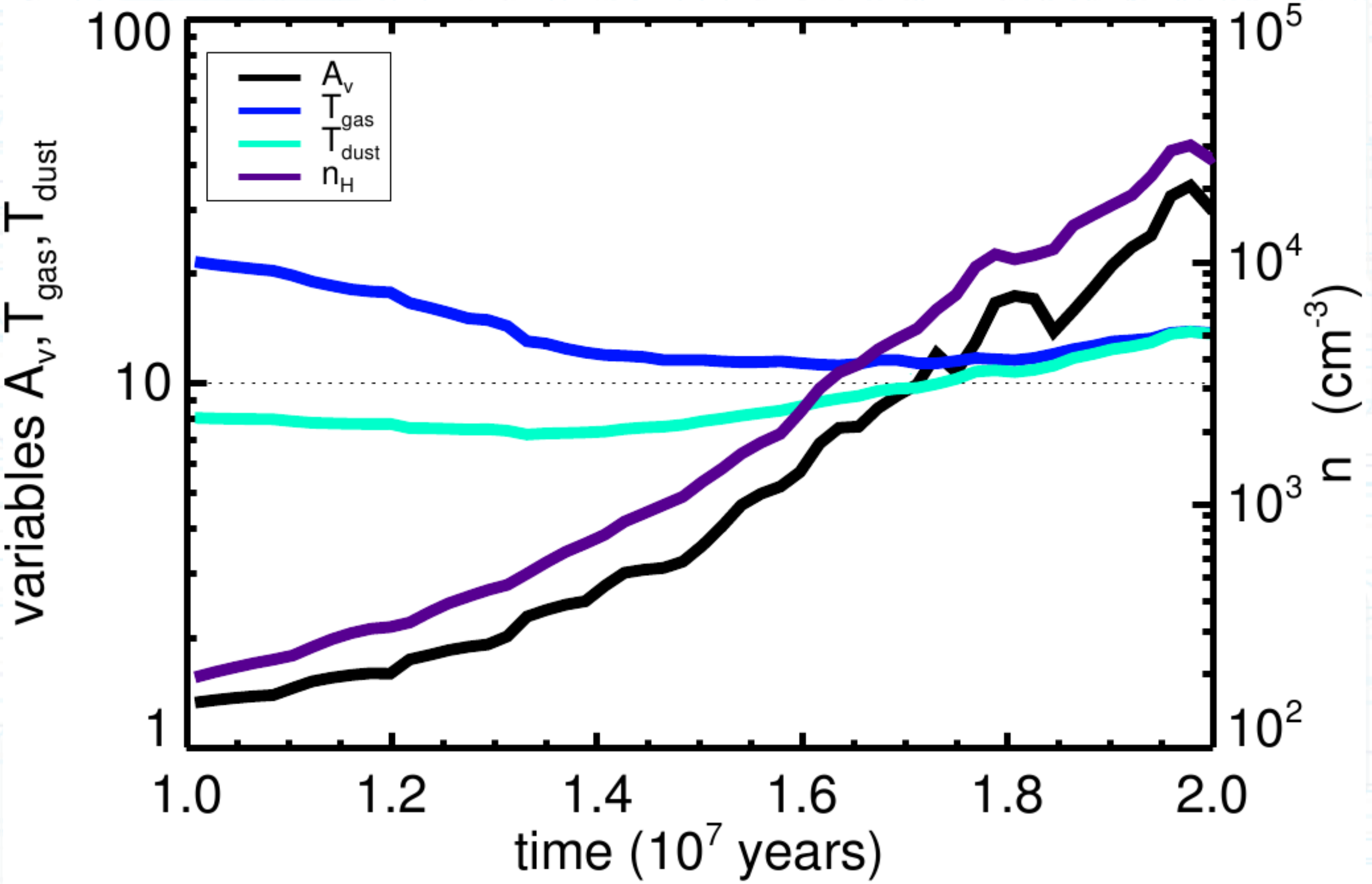
Gravity
Turbulence
Chemistry (gas+dust)
42 species
UV radiation
Heating & Cooling



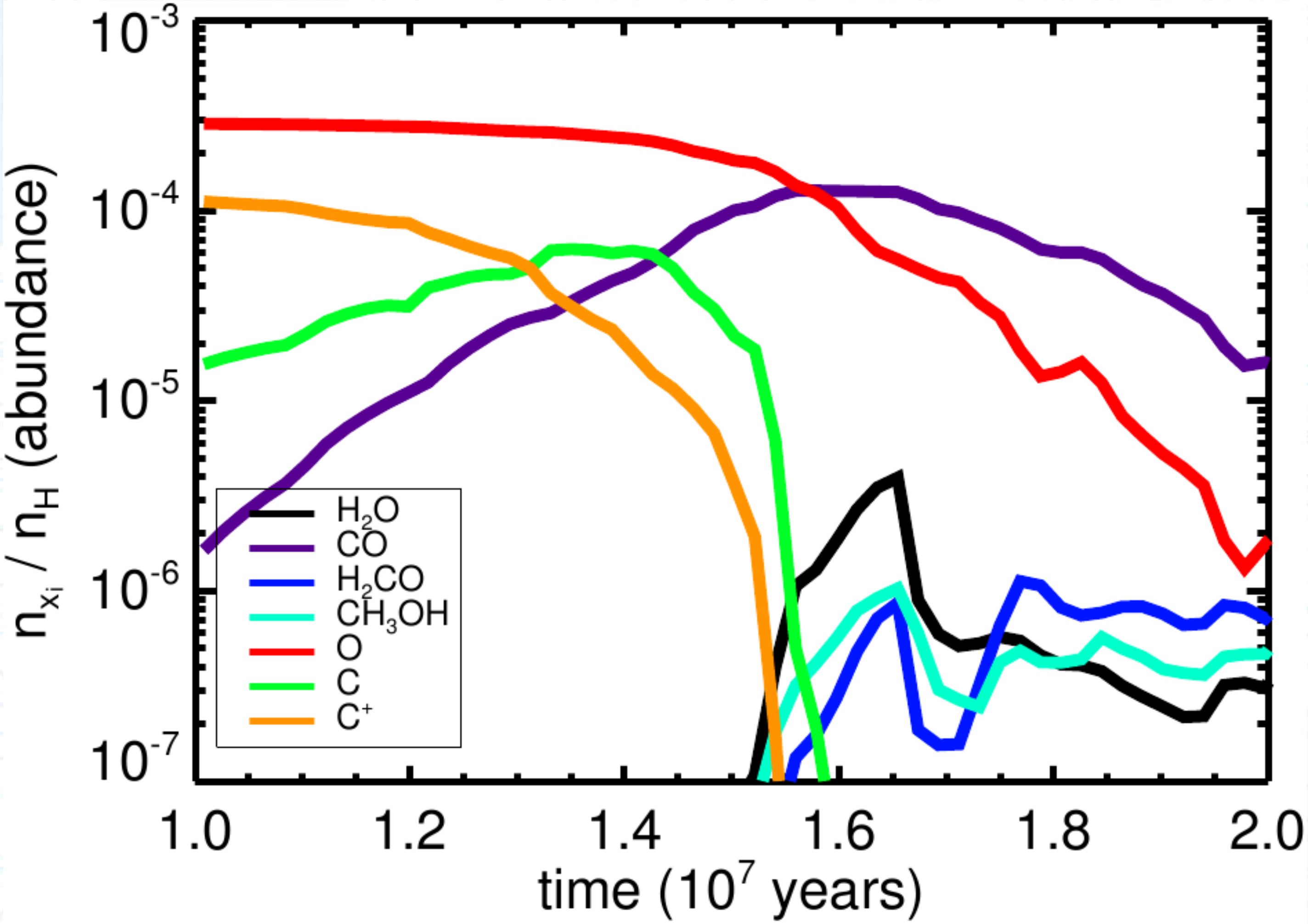
After 13 Myr evolution



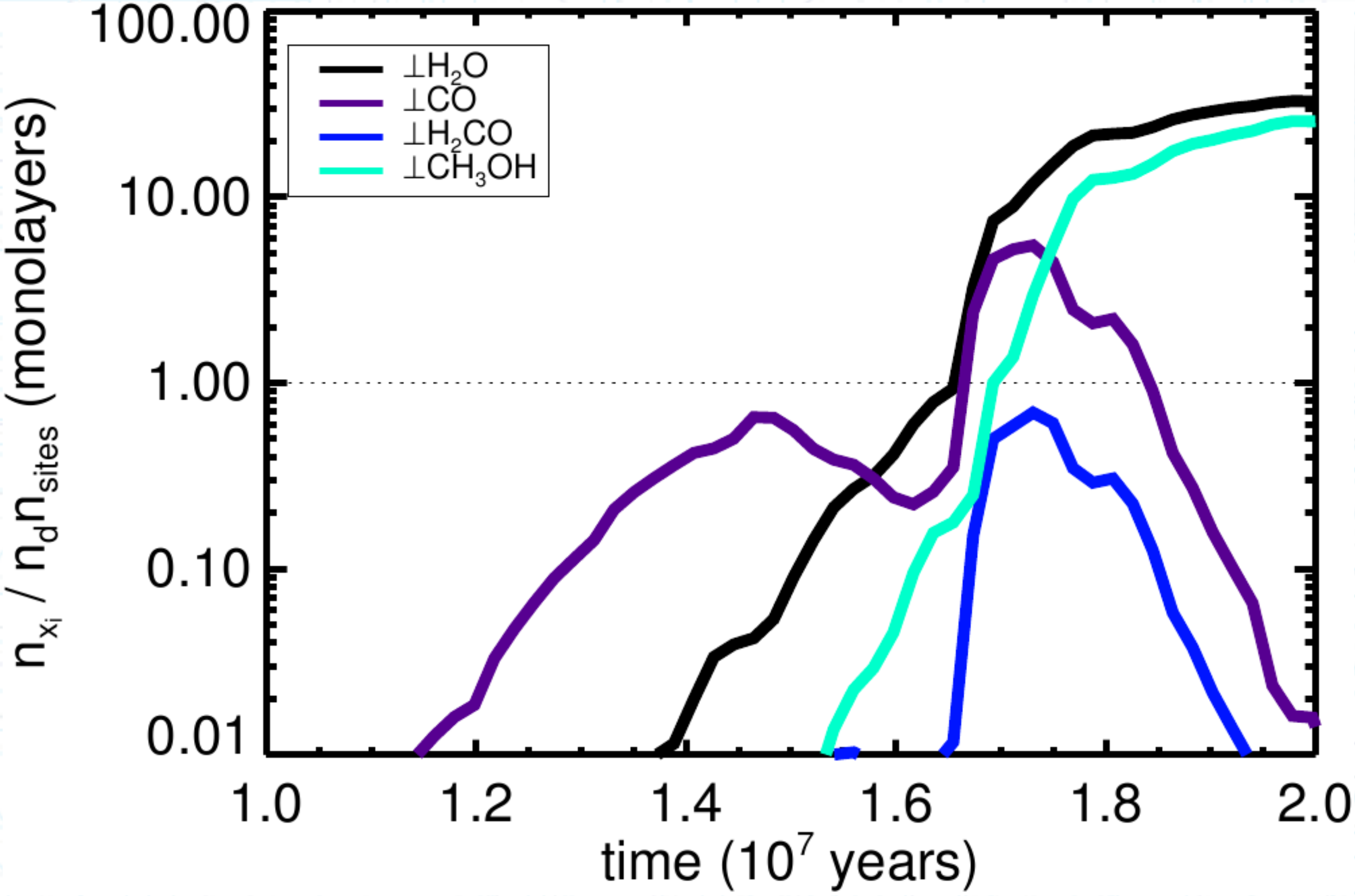
Cloud evolution



Gas-phase species

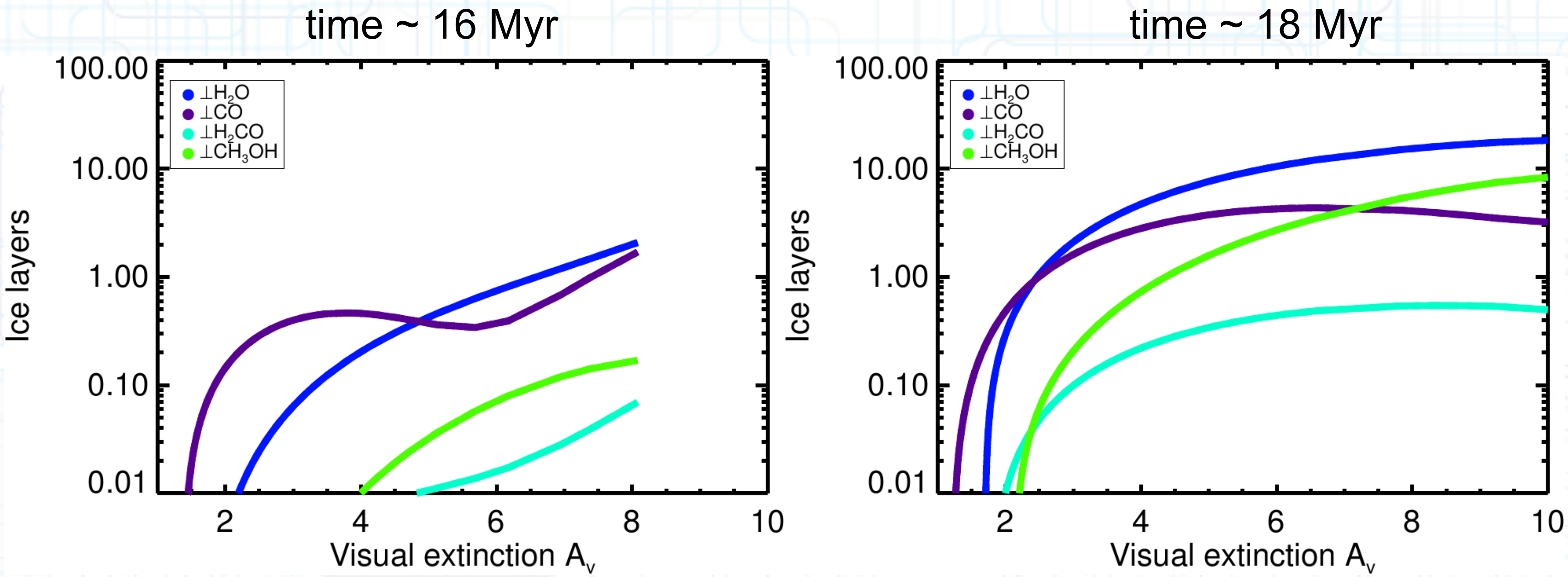


Ice species

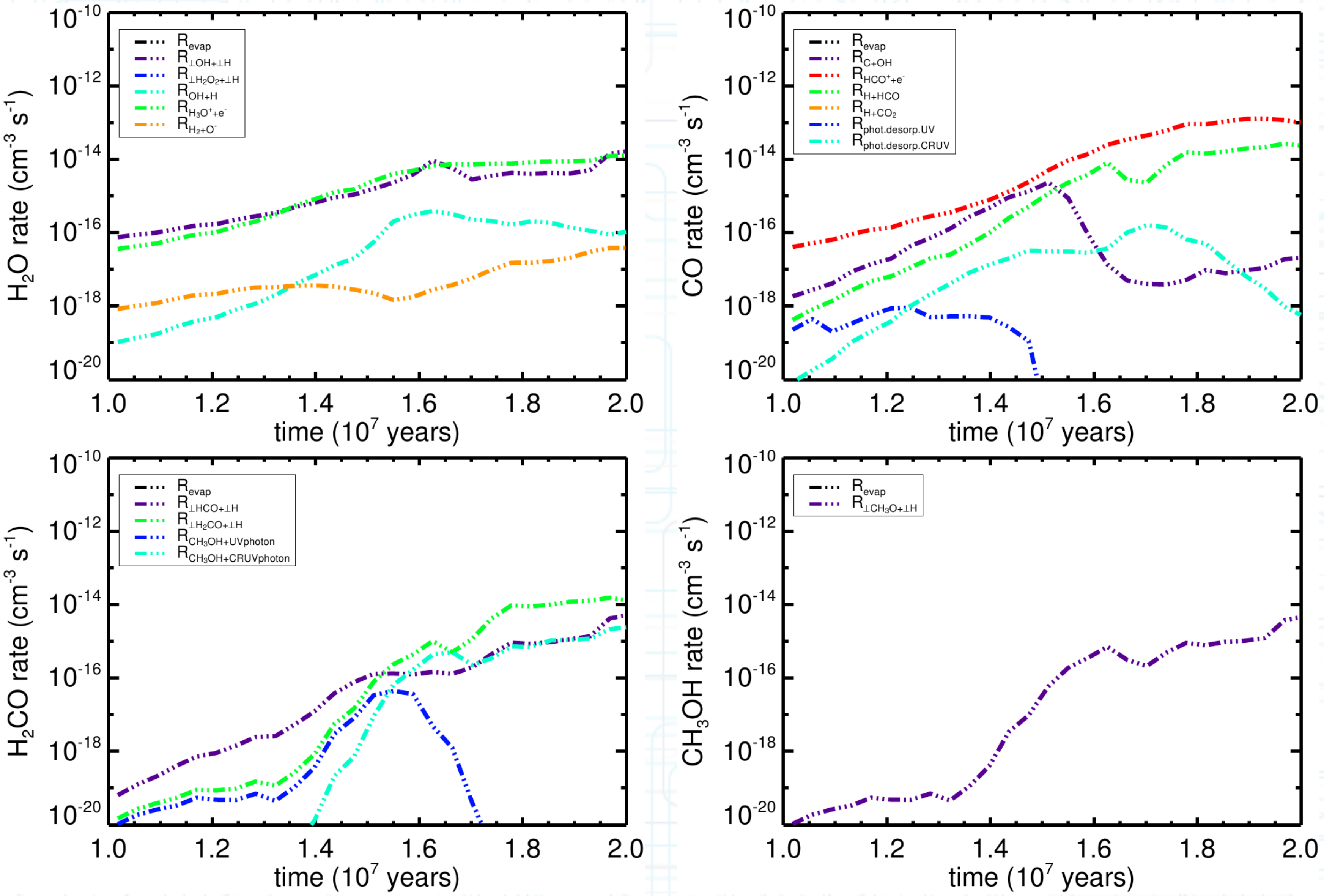


⊥H_2O
⊥CO
⊥H_2CO
⊥CH_3OH
100.00
10.00
1.00
0.10
0.01
$n_{x_i} / n_d n_{sites}$ (monolayers)
1.0
1.2
1.4
1.6
1.8
2.0
time (10^7 years)

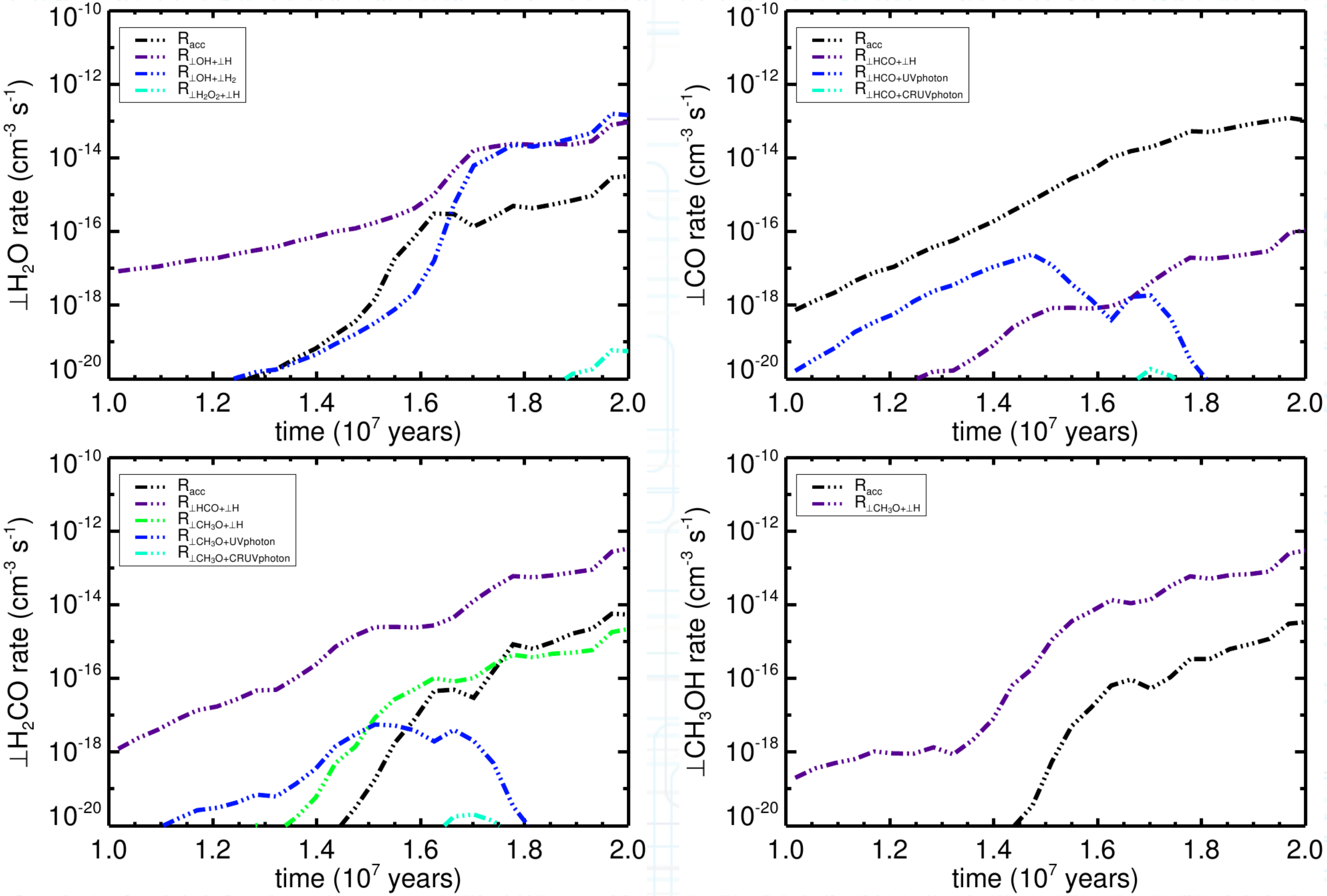
Ice coverage vs. extinction



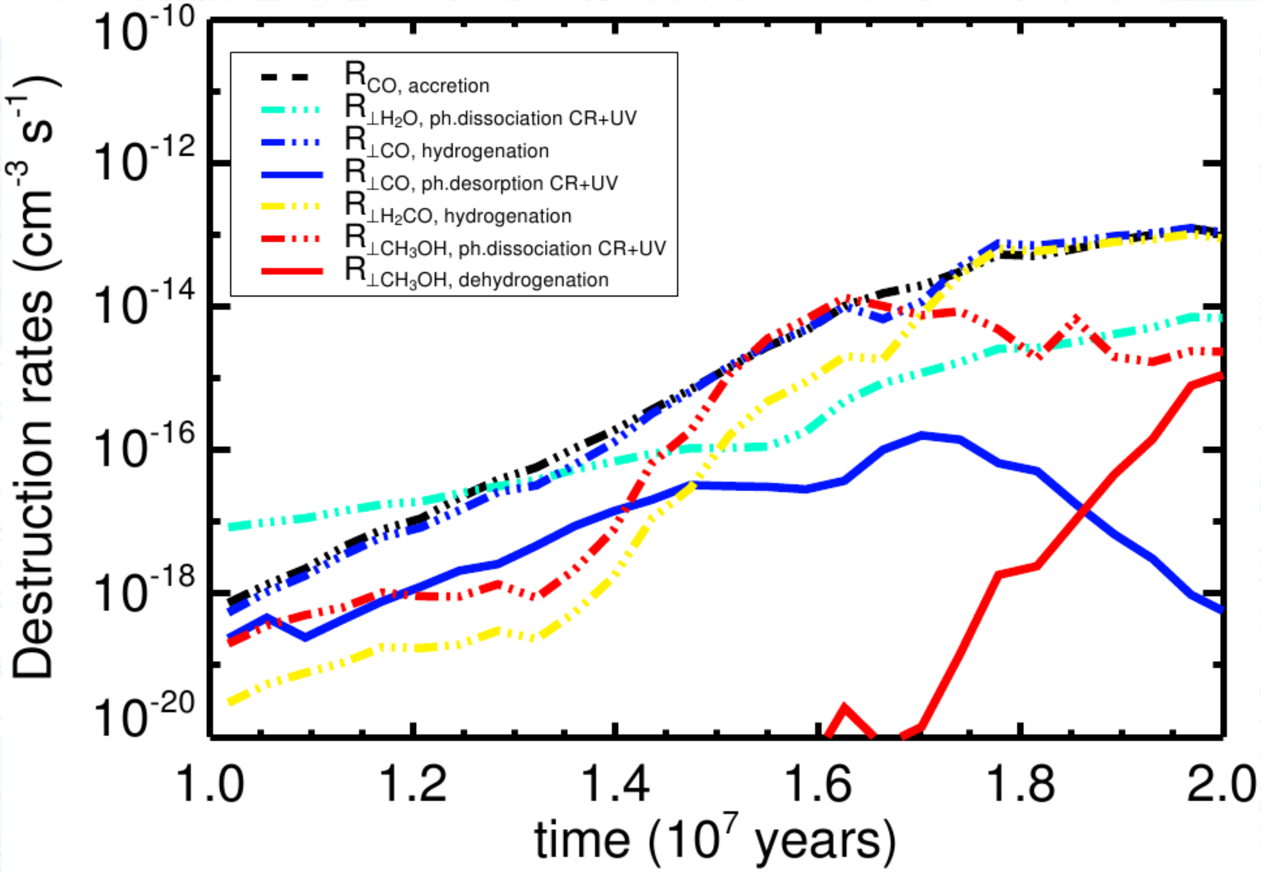
Gas-phase species formation rates



Ice species formation rates



Destruction rates



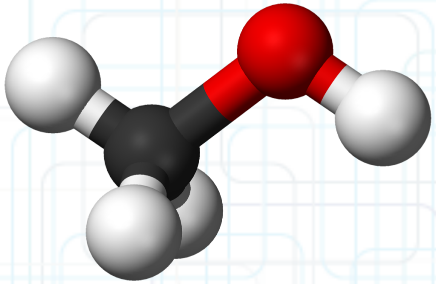
What do we take from this

In the first ice layer(s) CO is well mixed with H_2O ice

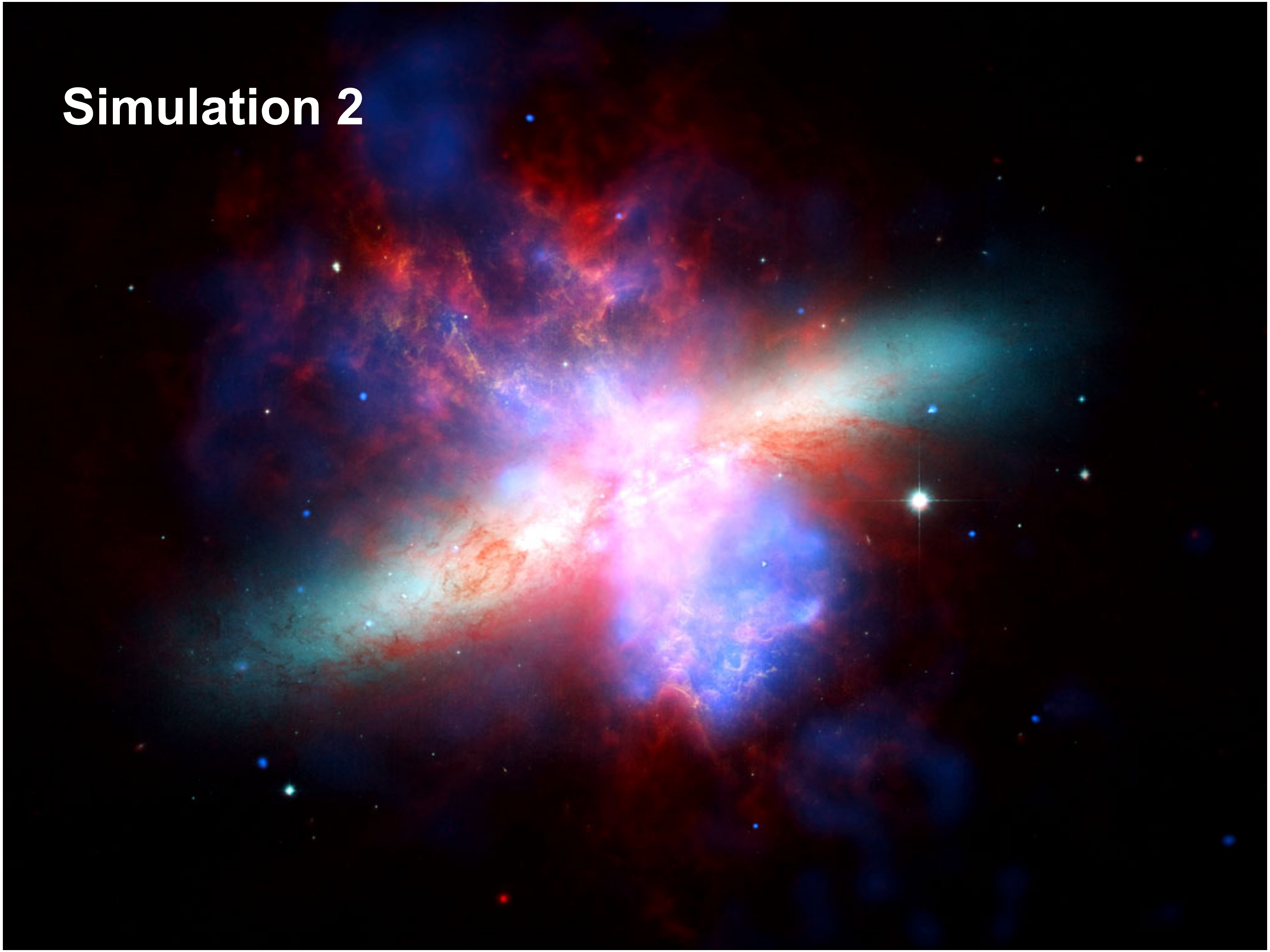
Freeze-out of species greatly increases after the first ice layer has formed

The abundance of formaldehyde in molecular clumps can be explained by chemical desorption

Grain surface chemistry does strongly alter the abundances in translucent clouds, which will affect cloud evolution



Simulation 2

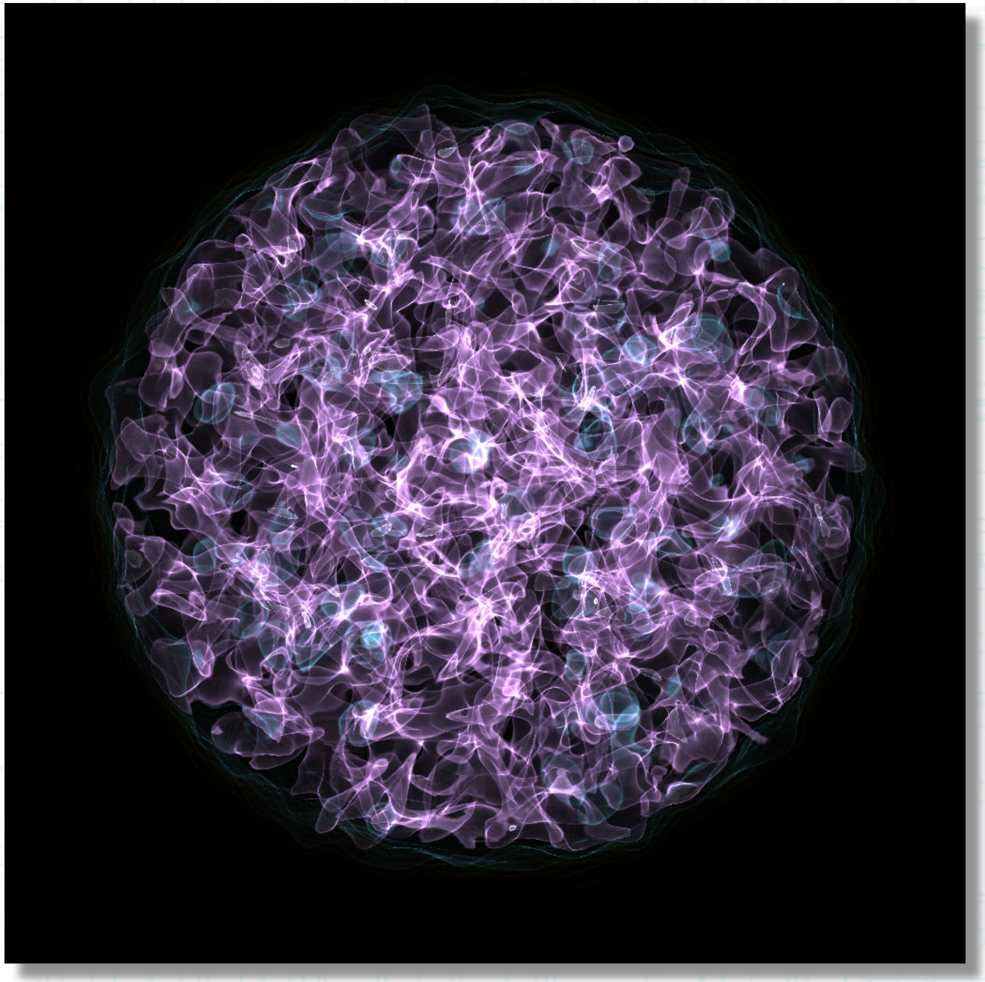


Starting from translucent stage

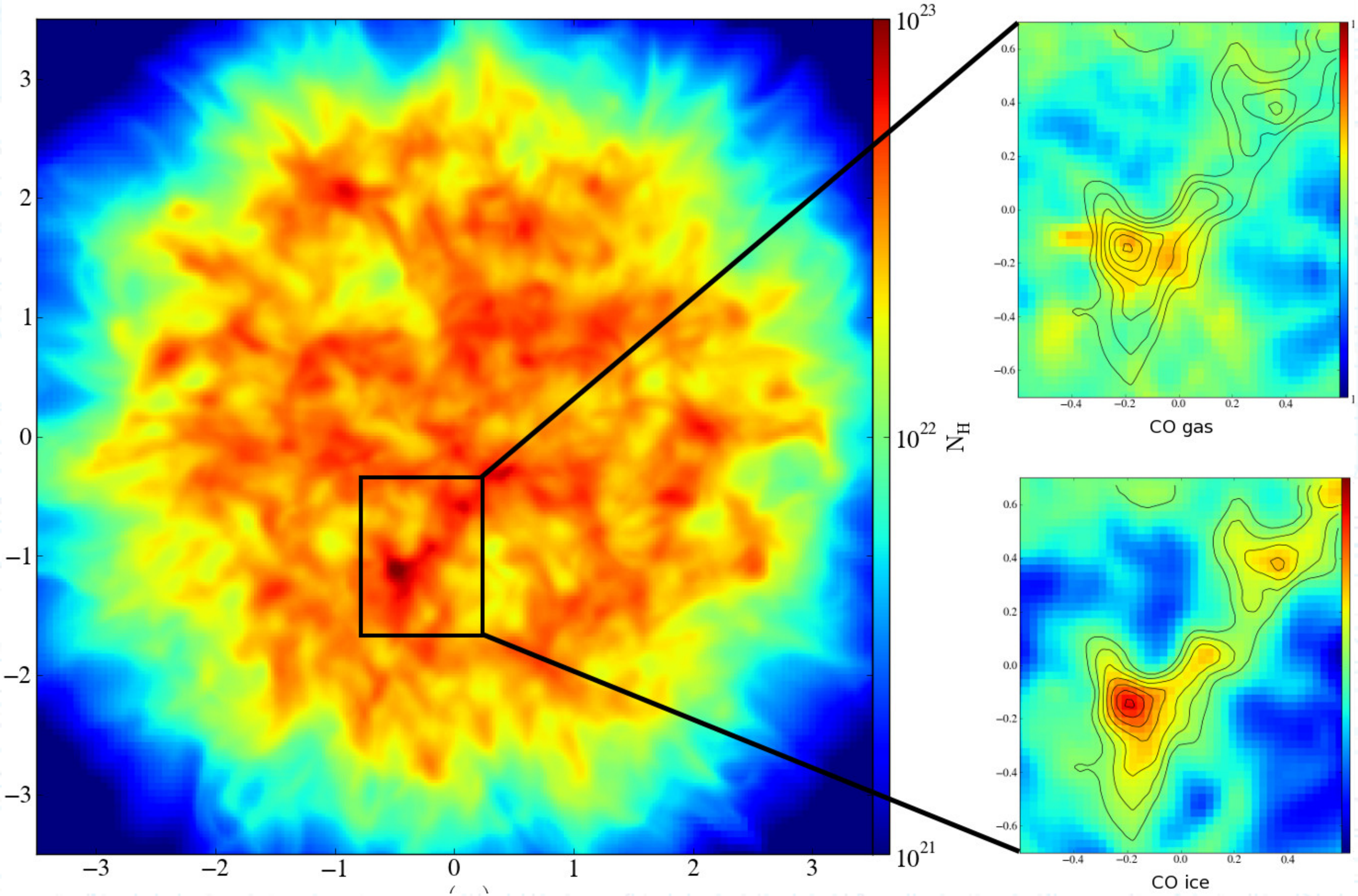
Ingredients:

Gravity
Turbulence
Chemistry (gas+dust)
32 species
UV radiation
Heating & Cooling

Cloud:
r = 4.2 pc
T_g = 10 K
density =1000 cm^{-3}
Two different models

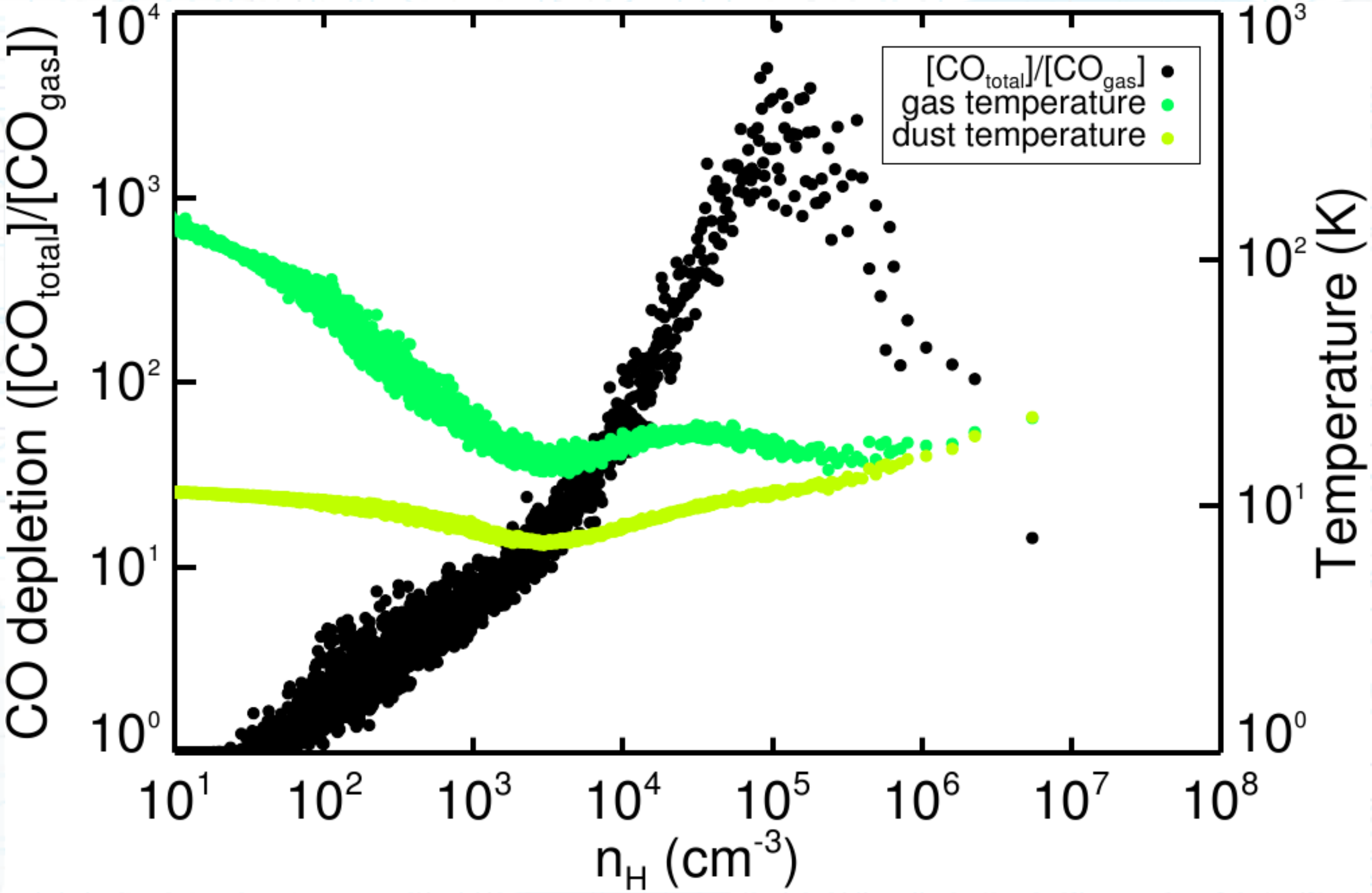


CO freeze-out



Cloud Evolution

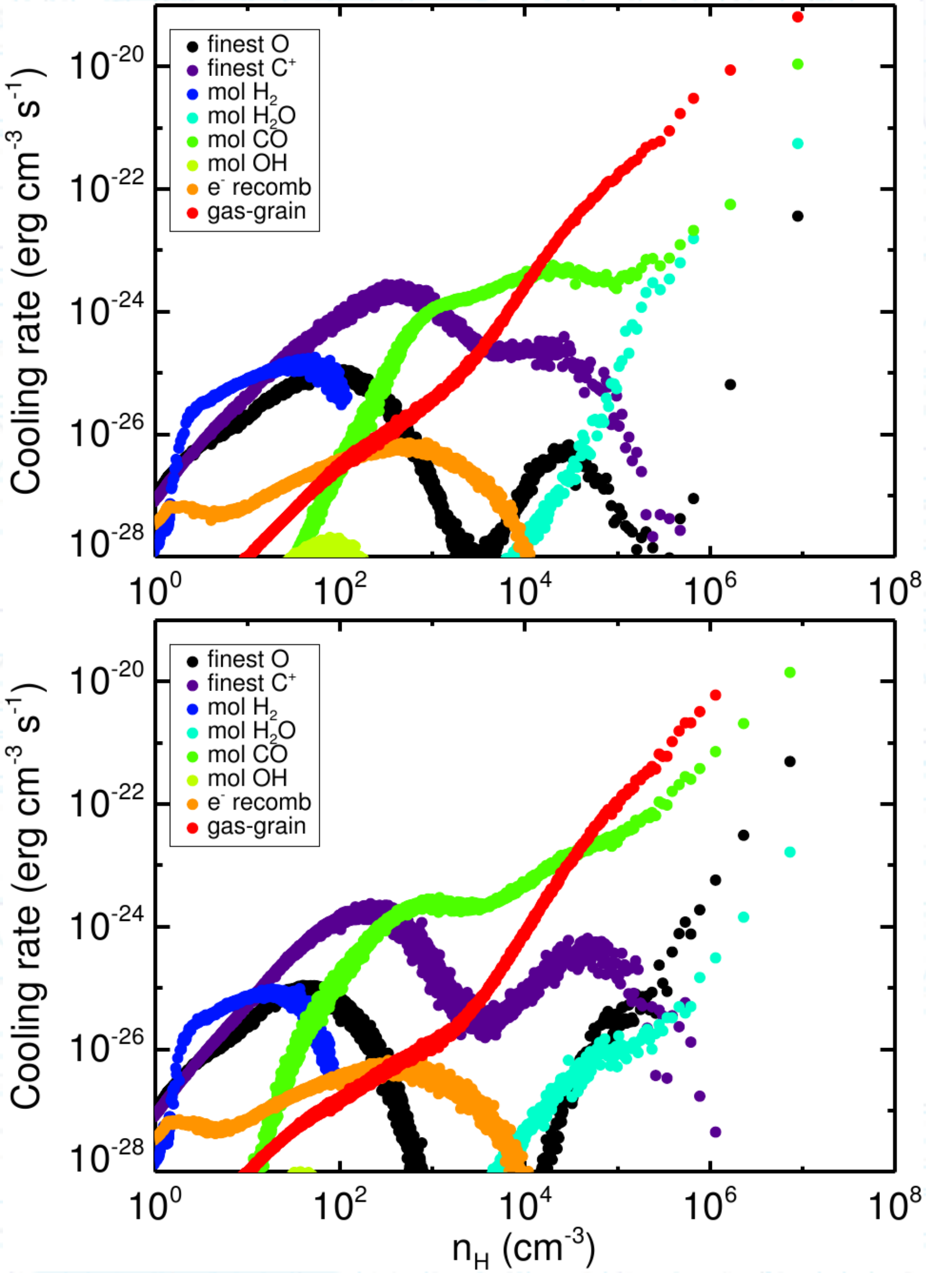
CO depletion



Cloud Evolution
cooling rates

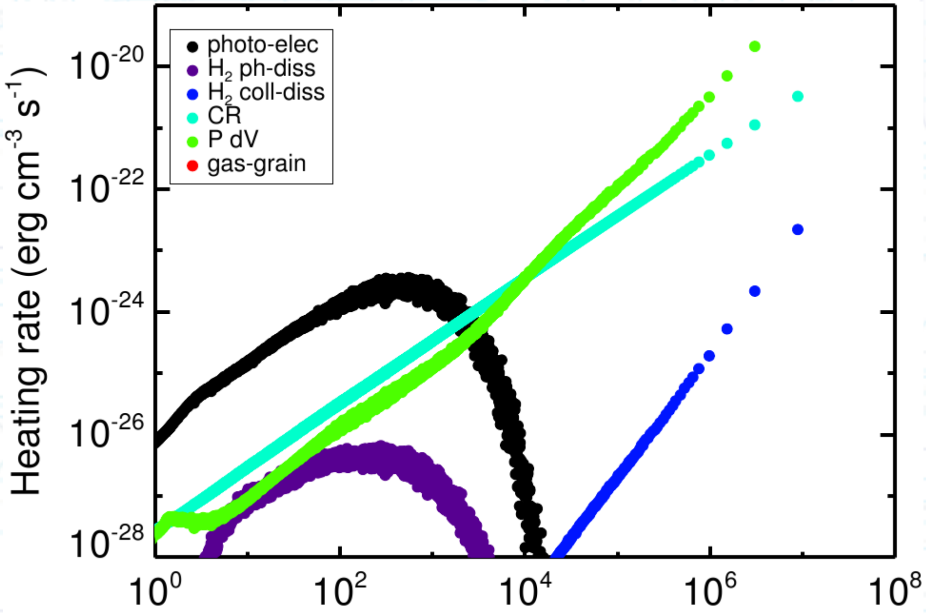
With grain
surface chemistry

Without grain
surface chemistry

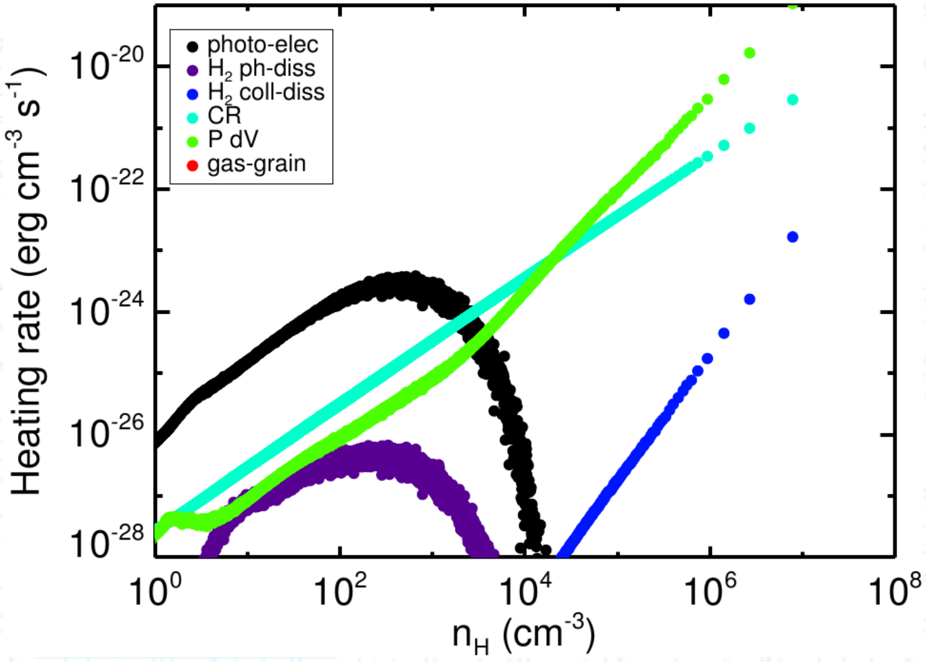


Cloud Evolution
heating rates

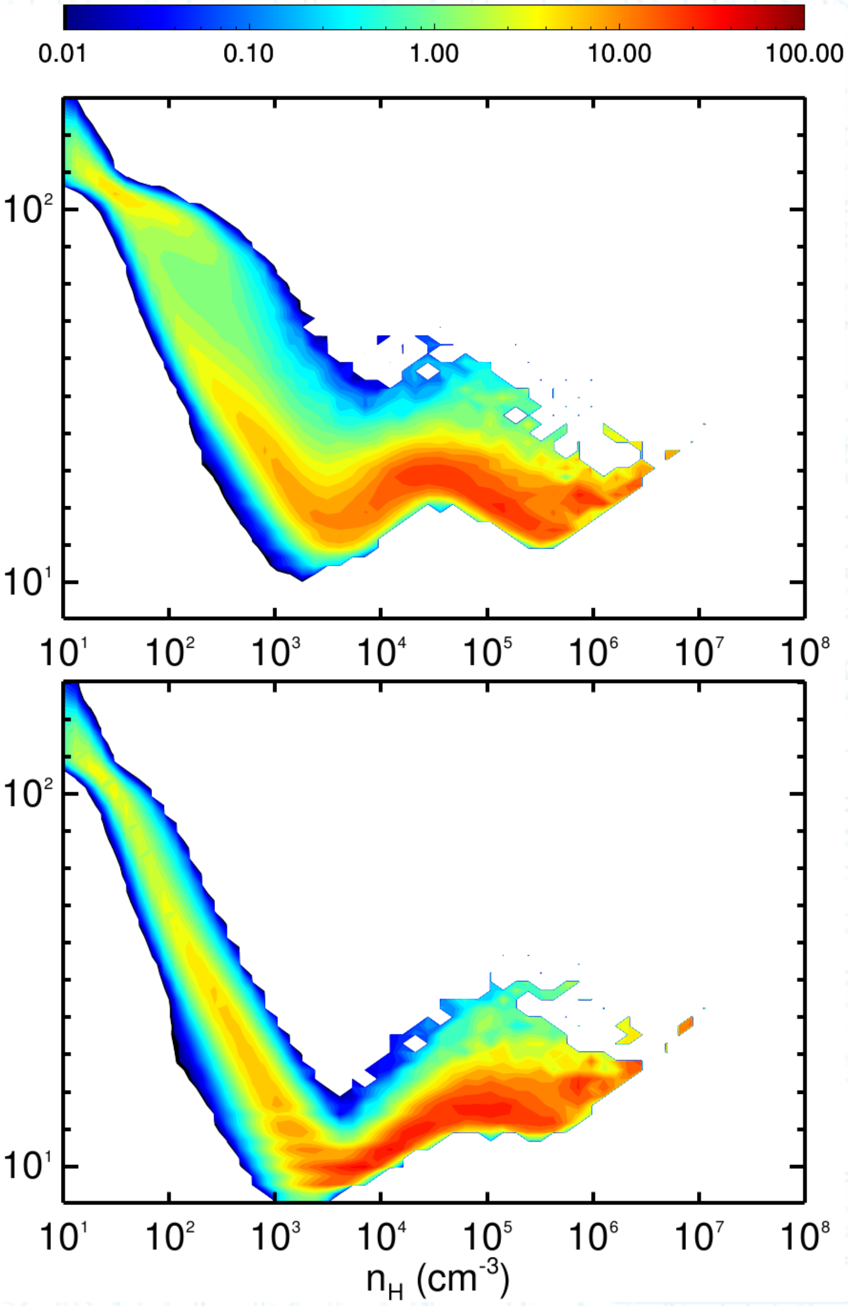
With grain
surface chemistry



Without grain
surface chemistry



Cloud Evolution
phase diagram



With grain surface chemistry

Without grain surface chemistry

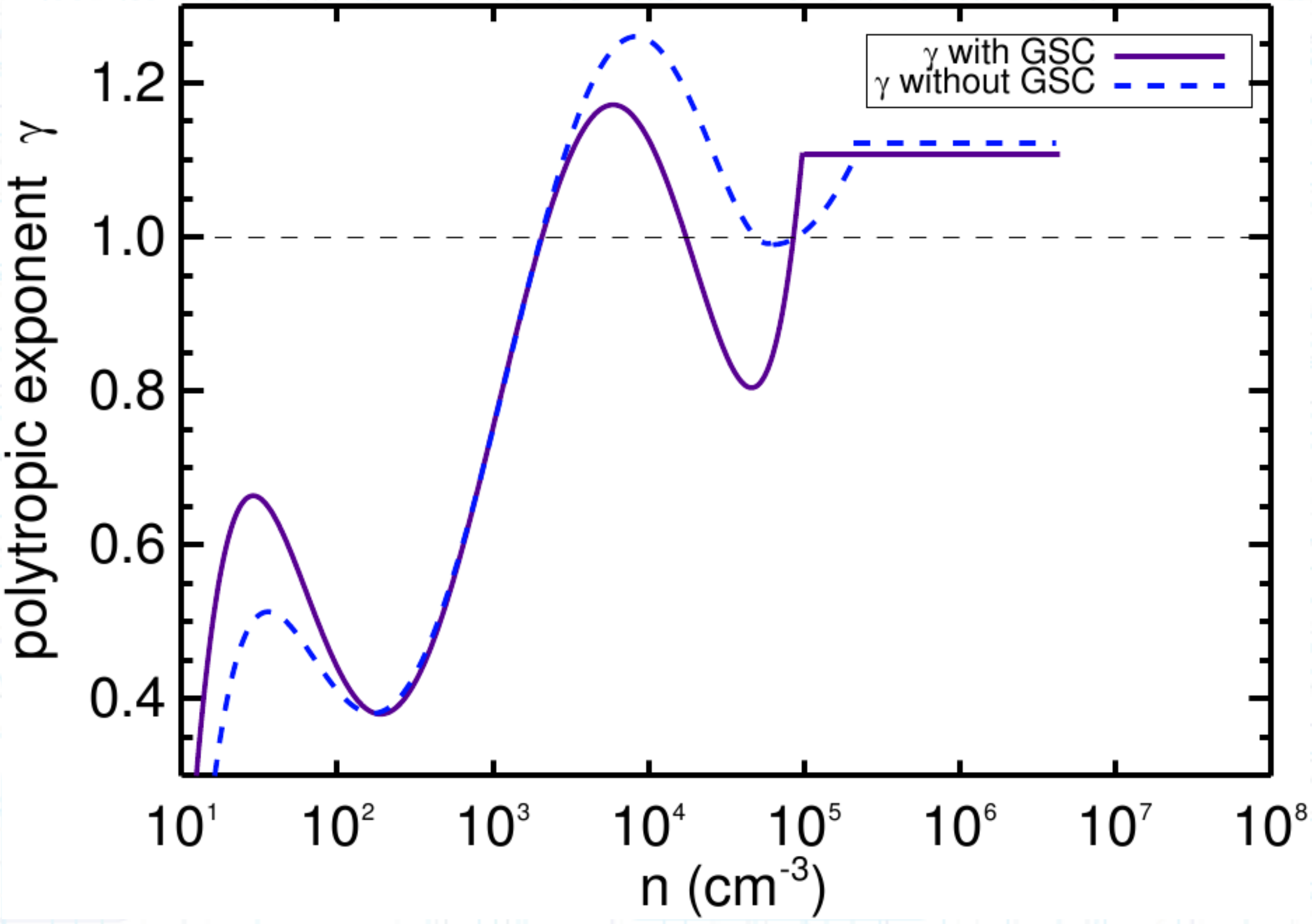
Cloud Evolution
equation of state

The EOS is defined as

$\mathbf{P = \rho^{\gamma}}$

ideal gas $\mathbf{P = \rho T}$

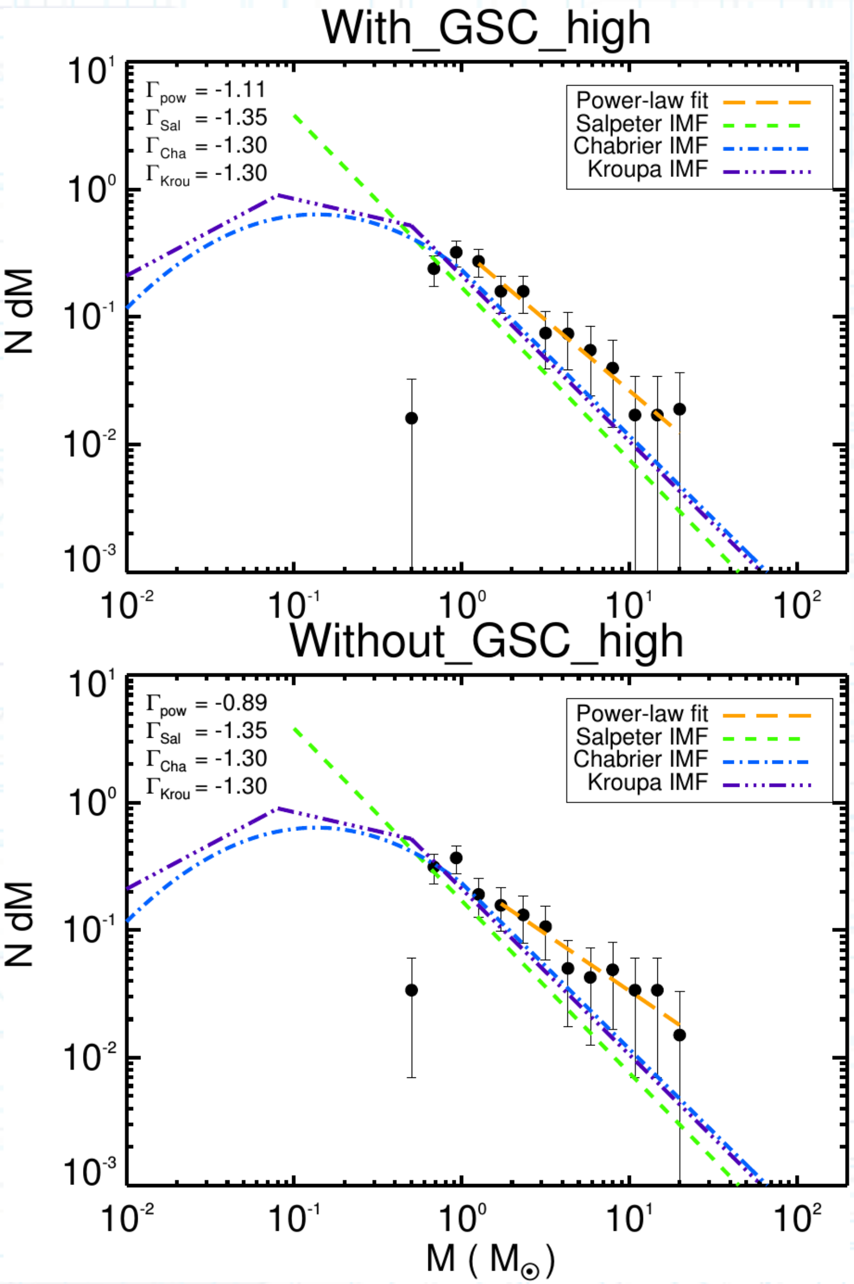
$\boldsymbol{\gamma = 1 + d\log T / d\log \rho}$



Star formation
initial results

With grain
surface chemistry

Without grain
surface chemistry



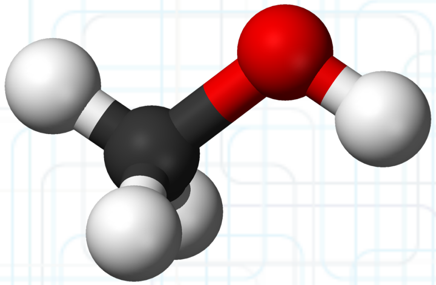
What do we take from this

Freeze-out is able to deplete the main coolant around 10^4 cm^{-3}

Grain surface chemistry influences gas temperatures

The changes in the EOS will affect cloud fragmentation

There is indication that the stars when forming remember the cloud evolution history, such that their masses are affected



Extra

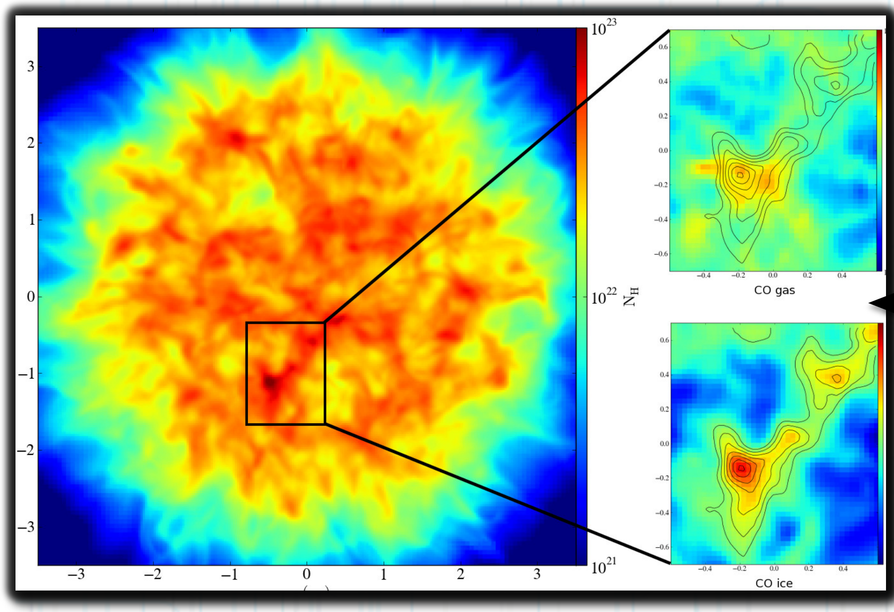
Connecting scales

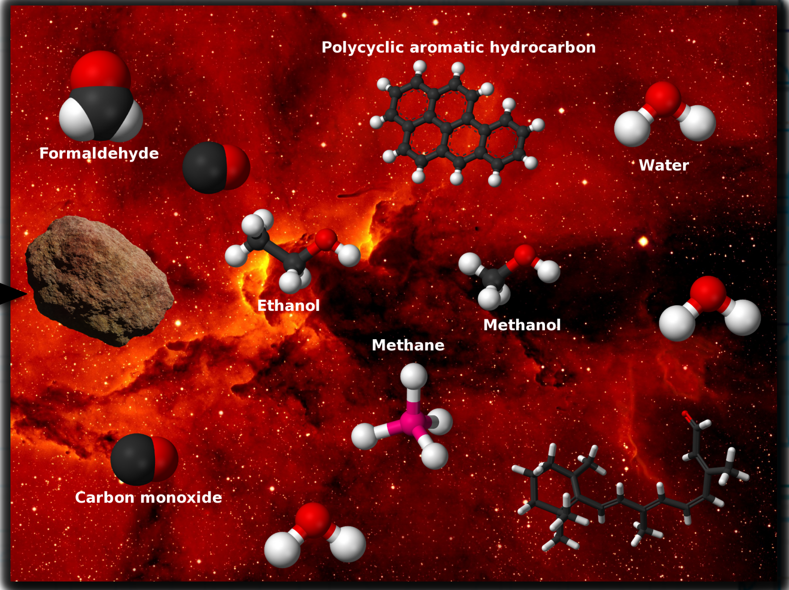
Large scales

Gravity, turbulence

Small scales

Chemistry





To fully understand stars, we need to go back to the beginning

Large scales

Gravity (Hocuk+ 2010)

Tubulence (Hocuk+ 2011)

Magnetic fields (Hocuk+ 2012)

Small scales

Chemistry

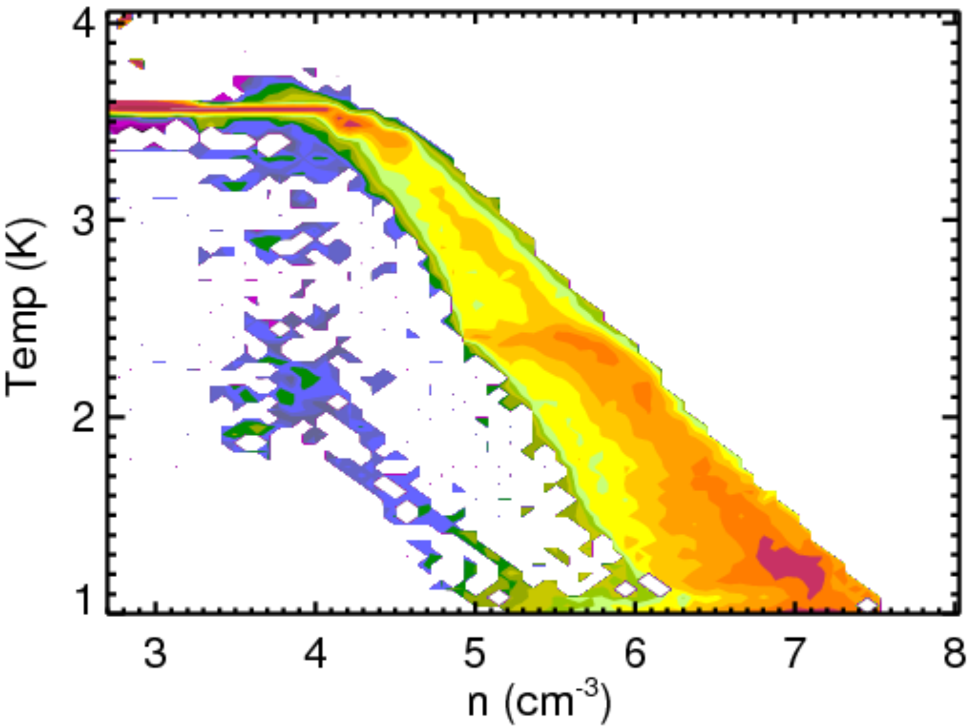
gas phase

solid phase (surface)
(Hocuk+ 2014)

Equation of State (EOS)

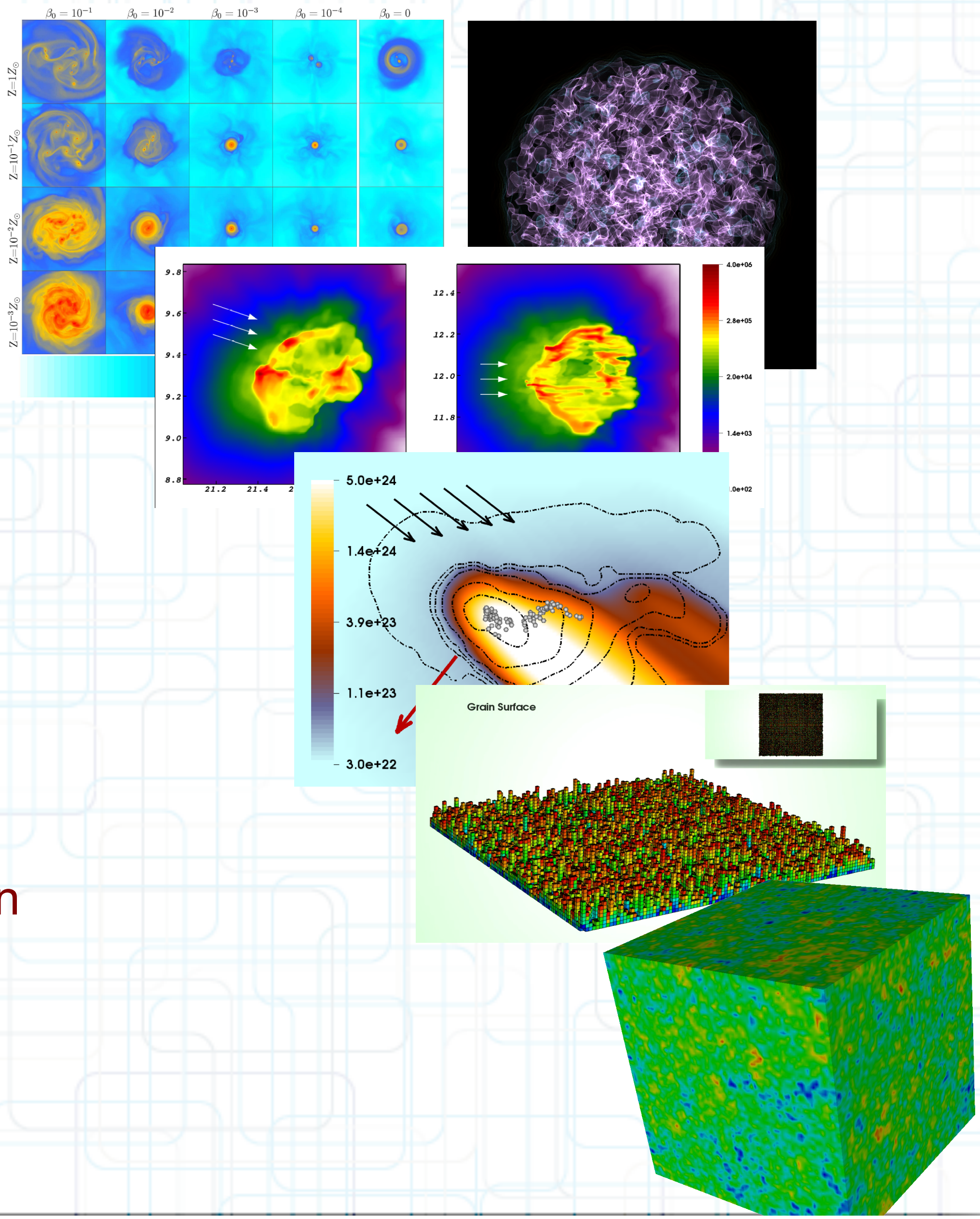
$$P \propto \rho^{\gamma} ,$$

$$\text{where } \gamma = d\log(T)/d\log(\rho) + 1$$



… and me

S. Hocuk: Experienced with hydrodynamical simulations and theories of star formation



We are all made from Stardust