

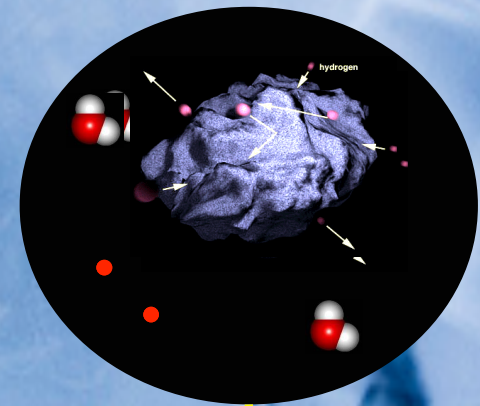
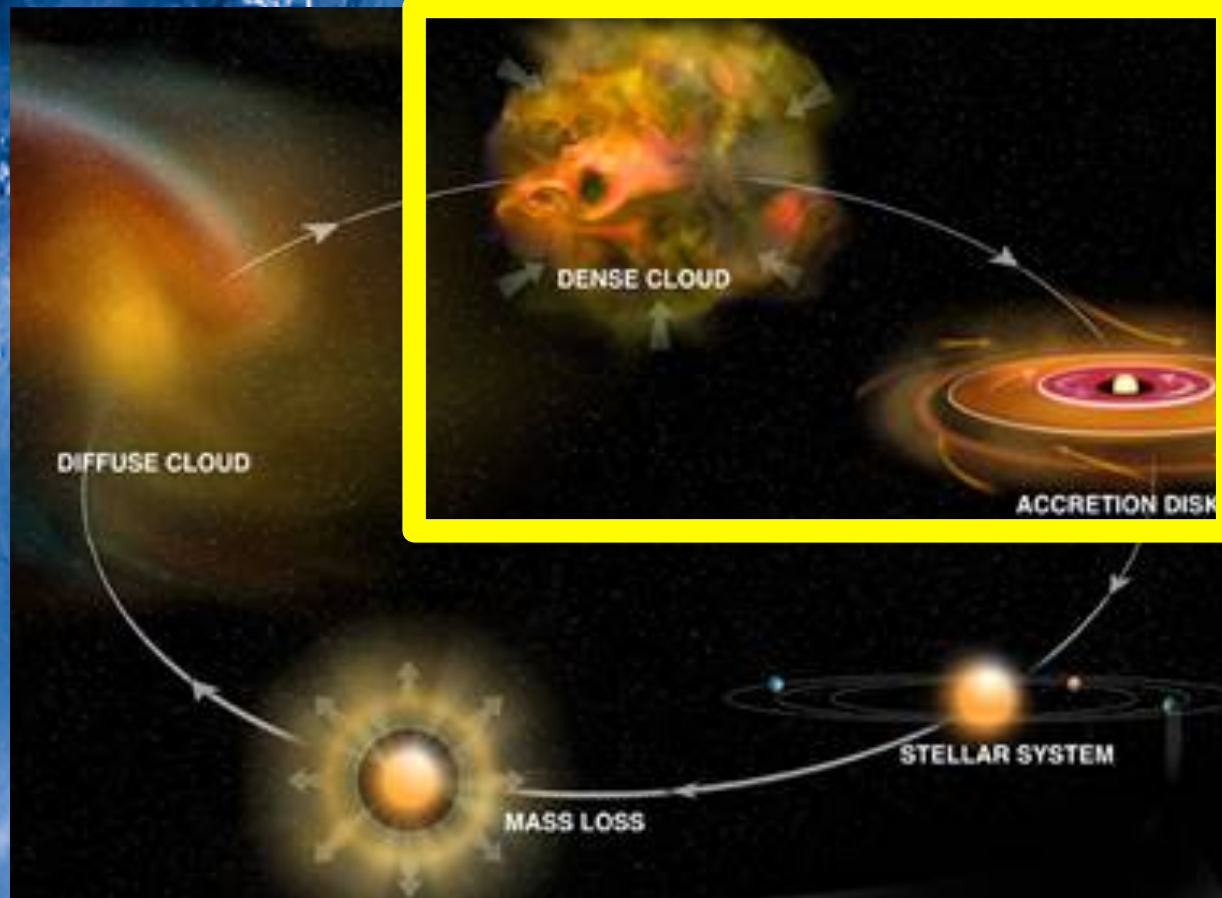
Formation and Evolution of Porous Water Ices

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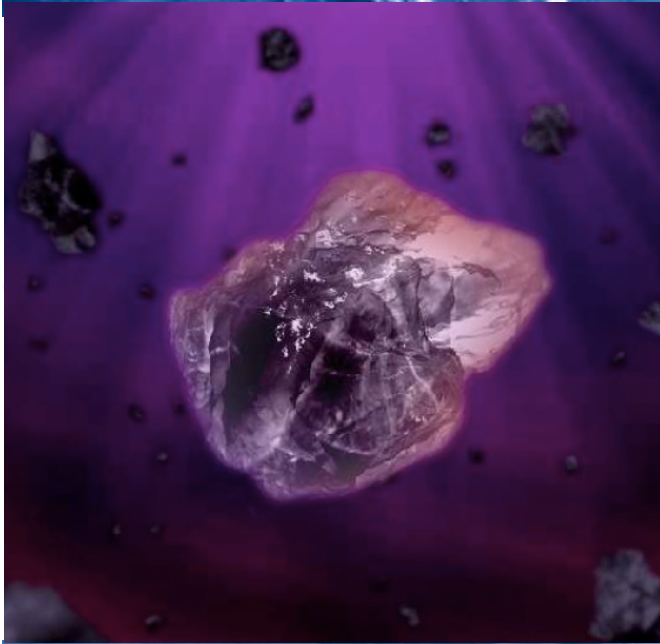
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Formation and evolution of ices



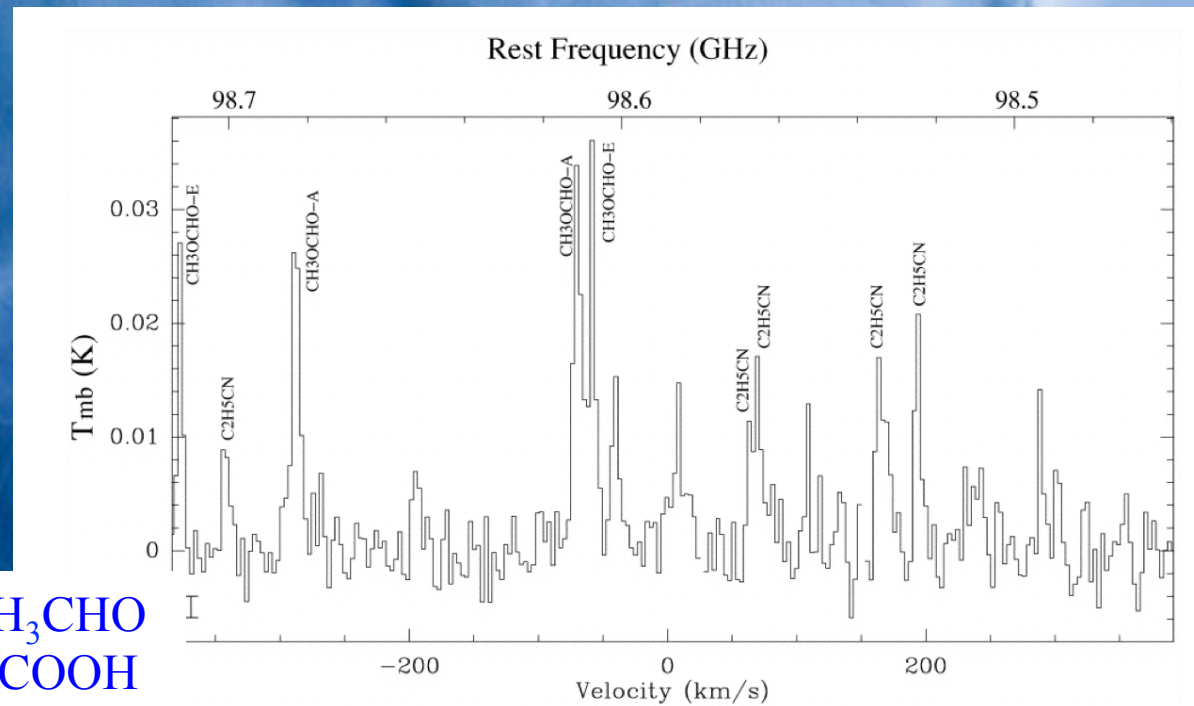
- During this circle → ices form onto dust
- Solid: ice composition in absorption
 - Gas phase: hot core/hot corino

Interstellar ices



B68 IRAM 30m;
Bergin et al. 2002
Extinction $A_V \sim 27$
 $C^{18}O$ J=1-0

Prestellar cores: CO depleted from gas
Bergin et al. 2002; Crapsi et al. 2004



CH_3CHO
 $HCOOH$
 CH_3CN
 C_2H_5CN
 CH_3OCHO

Hot corino: complex molecules
Cazaux et al. 2003

Interstellar ices

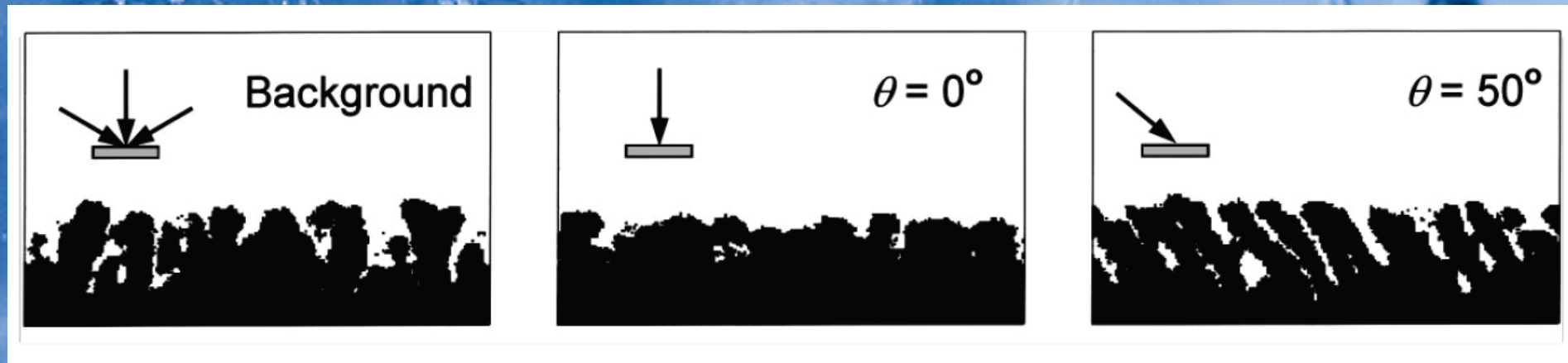
- ❑ Responsible for unique and rich chemistry
- ❑ ice composition → chemical history
- ❑ ice structure → accretion, desorption, segregation, and local radiation fields.

Ices morphology

- Frost of water in dense clouds → amorphous water ice +trapped impurities *Tielens & Allamandola 1987*
- Theory → amorphous and porous ices grown by a hit and stick mechanism *Cuppen & Herbst 2007*
- Laboratory → O+H = compact ices *Oba et al. 2009* but depend on the density of the gas *Garrod 2013*
- Ices porous in space? No observational evidence *Keane et al. 2001; Gibb et al. 2004*

Experiments

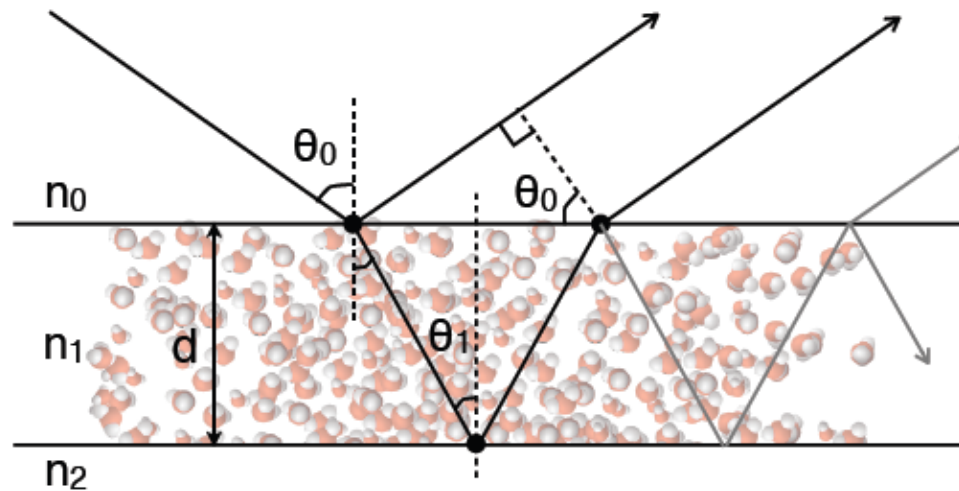
→ change of ice morphology under external influences: ion impact, VUV irradiation *Palumbo 2006; Raut et al. 2007*, H-atom bombardment, or during warming up



Ices created by deposition of water
Deposition sets porosity

Dohnálek et al. 2003

Experiments



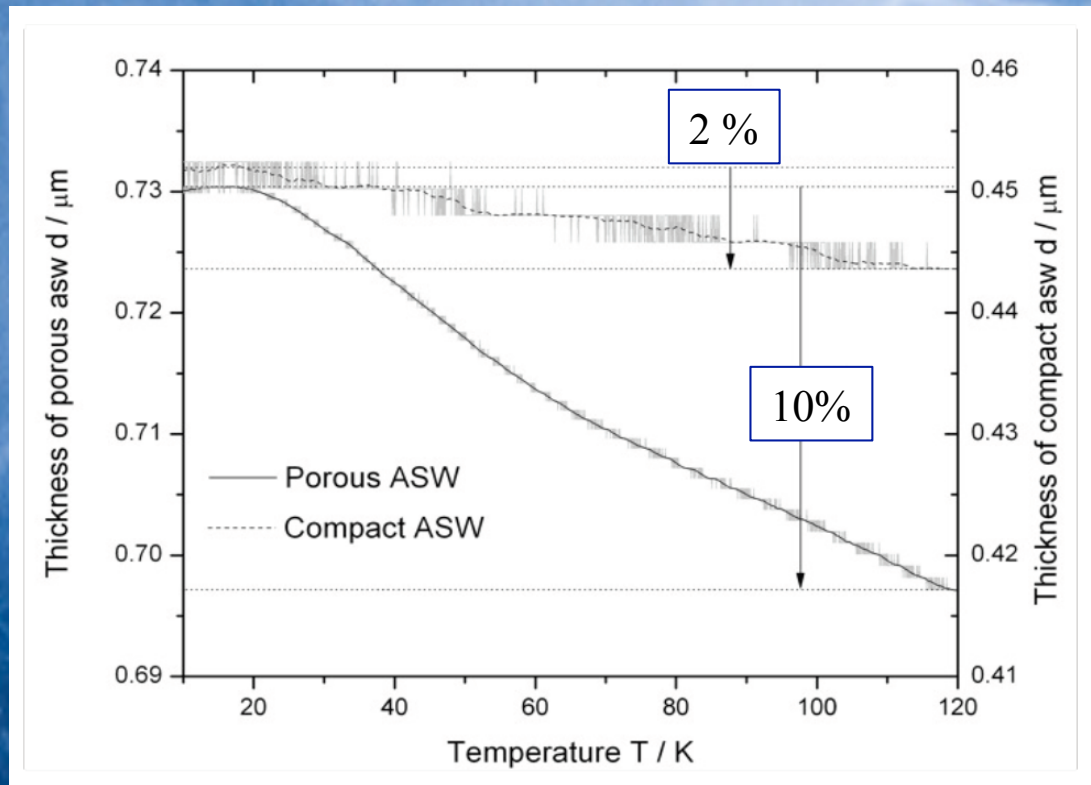
Bossa et al. 2012
Isokoski et al. 2014

- Leiden: Bossa, Isokoski, Linnartz, Tielens
- Optical interference technics (ice thickness)

Experiments

Exp. Show thickness decreases with T.
Density $\approx 0.61 \text{ g cm}^{-3}$
Porosity $\approx 32\%$

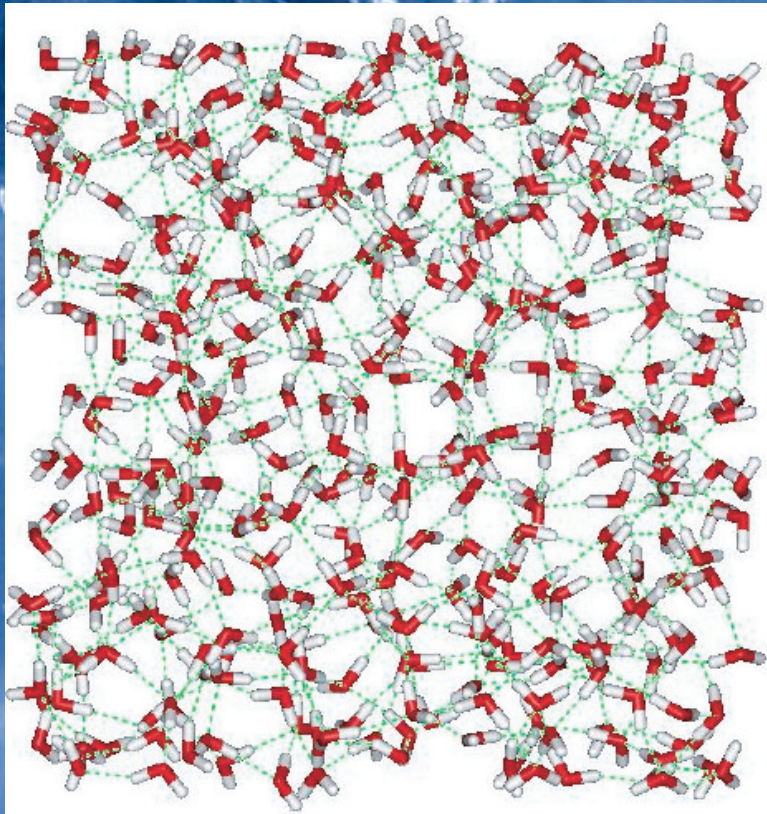
Bossa et al. 2012
Isokoski et al. 2014



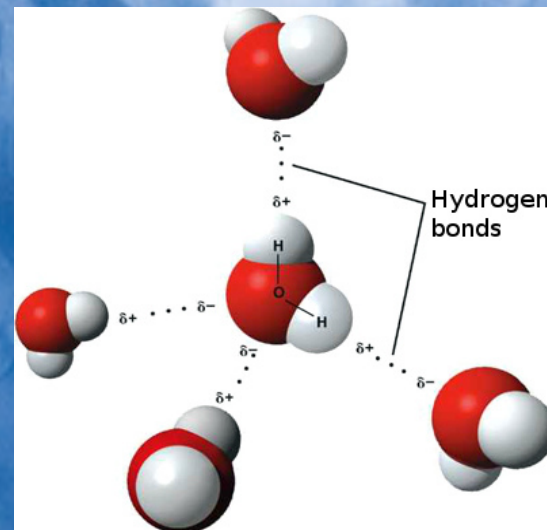
What are the physical processes involved in the decrease of ice thickness?

Model: Kinetic monte carlo simulations

Model

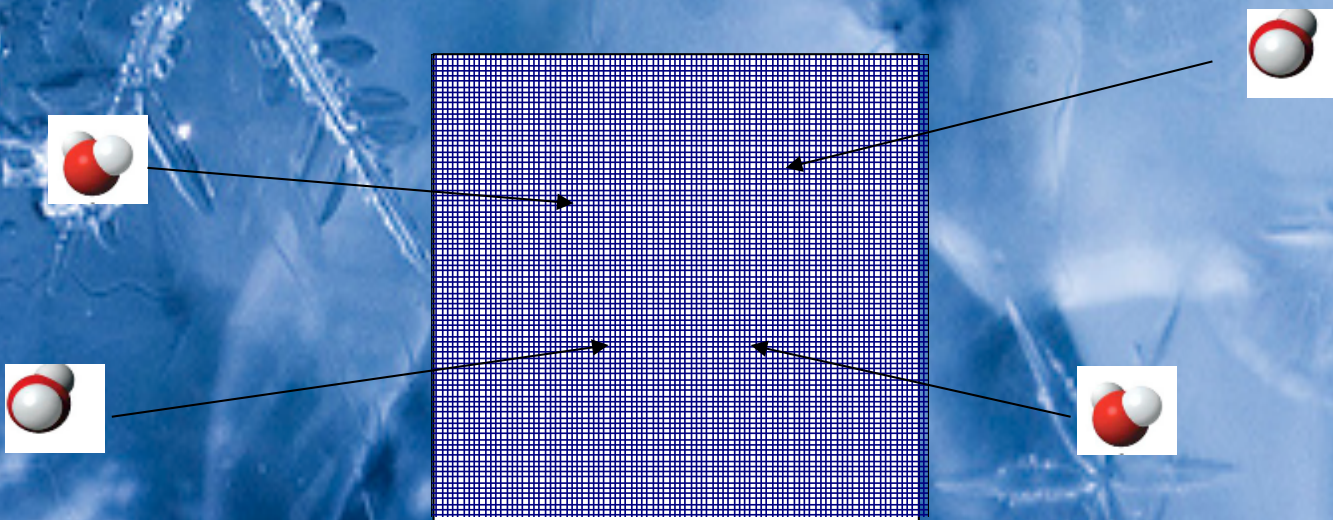


Amorphous ice
water molecules organized
Tetrahedron (4 neighbours)



Model

Kinetic monte carlo simulations:
hit and stick

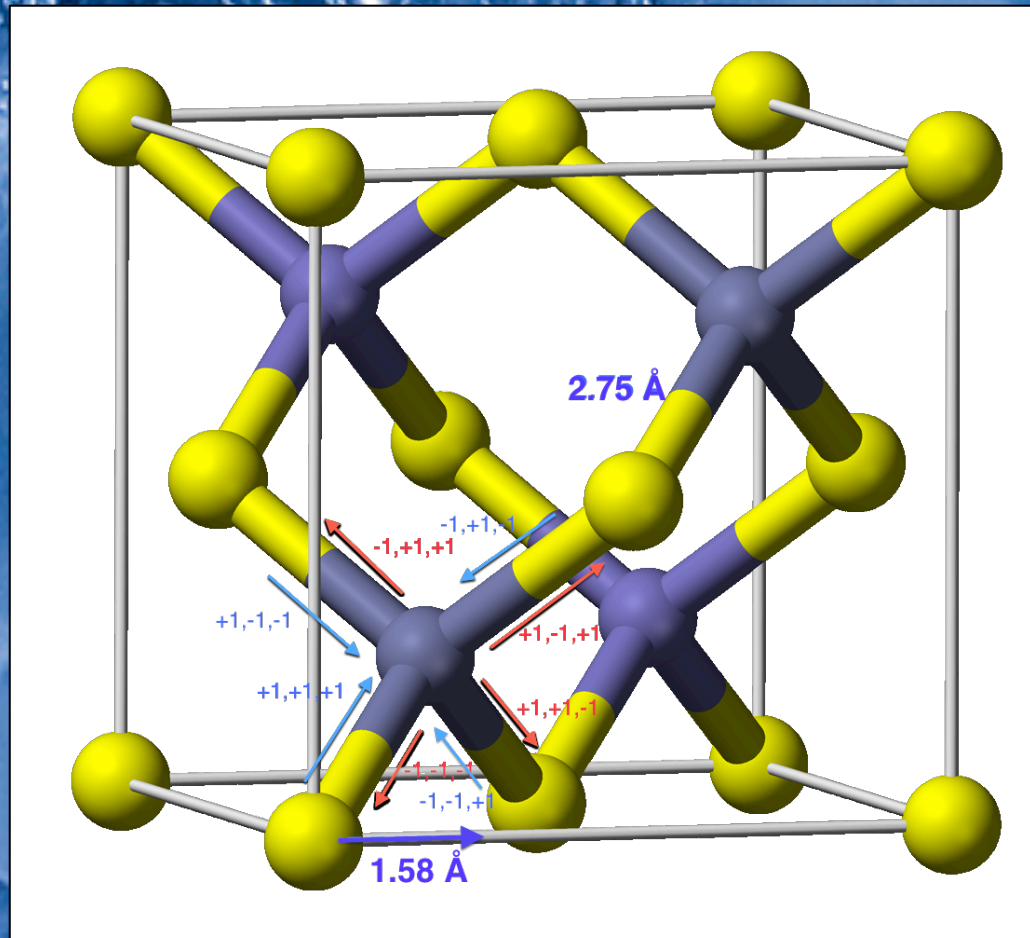


H_2O random
location and time

Grid=surface

Model

Kinetic monte carlo
simulations:
Position
Mobility

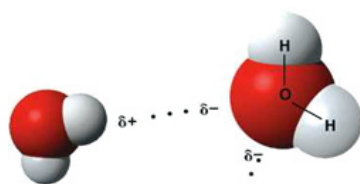


Model

- Binding energy is ~ 0.22 eV per hydrogen bond and increases with numbers of neighbours

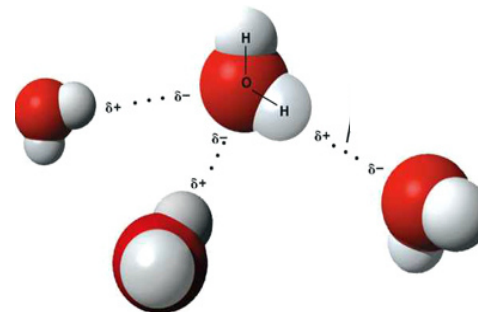
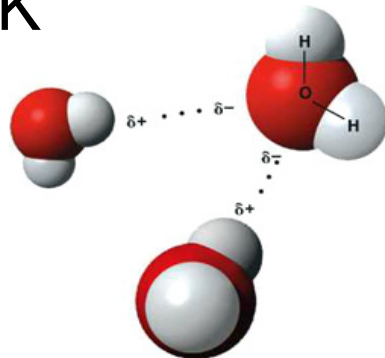
Brill & Tippe 1967; Isaacs et al. 1999; Dartois et al. 2013

- Barrier for diffusion $ED \sim nn^* \alpha^* EB$
- nn : number of neighbours and $\alpha \sim 0.4$



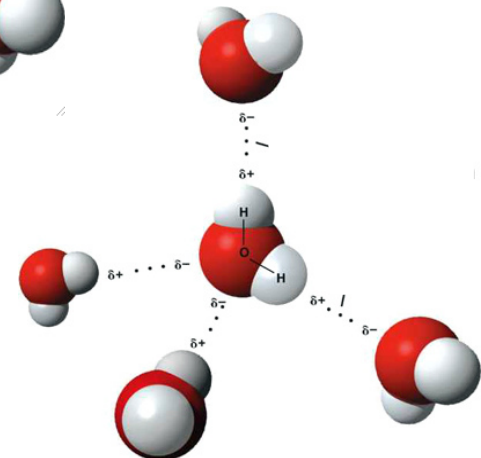
ED~1020K

ED~2040K

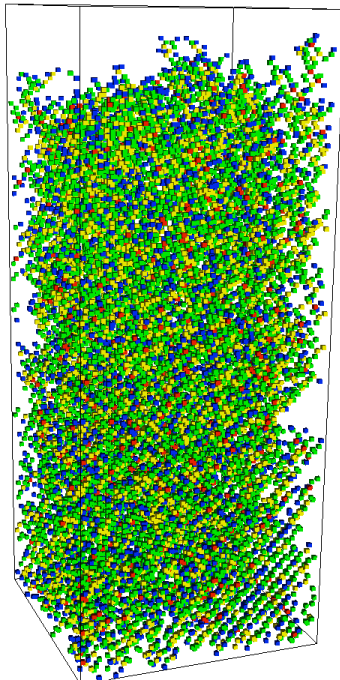
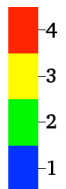


ED~3060K

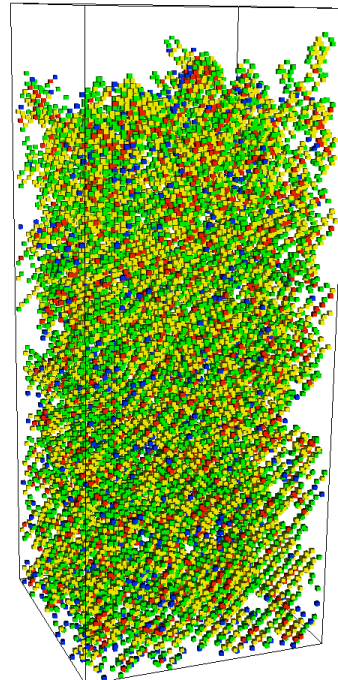
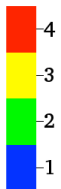
ED~4080K



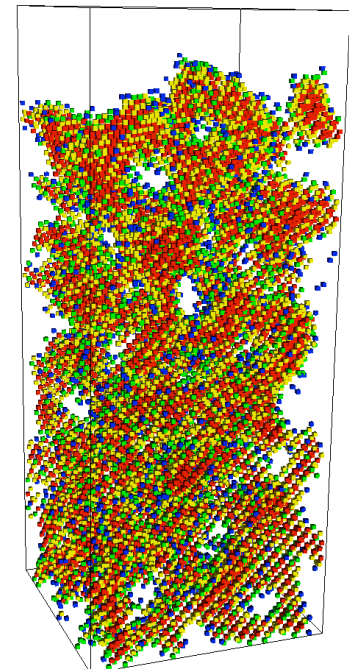
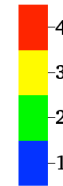
Ice morphology



$T = 10 \text{ K}$

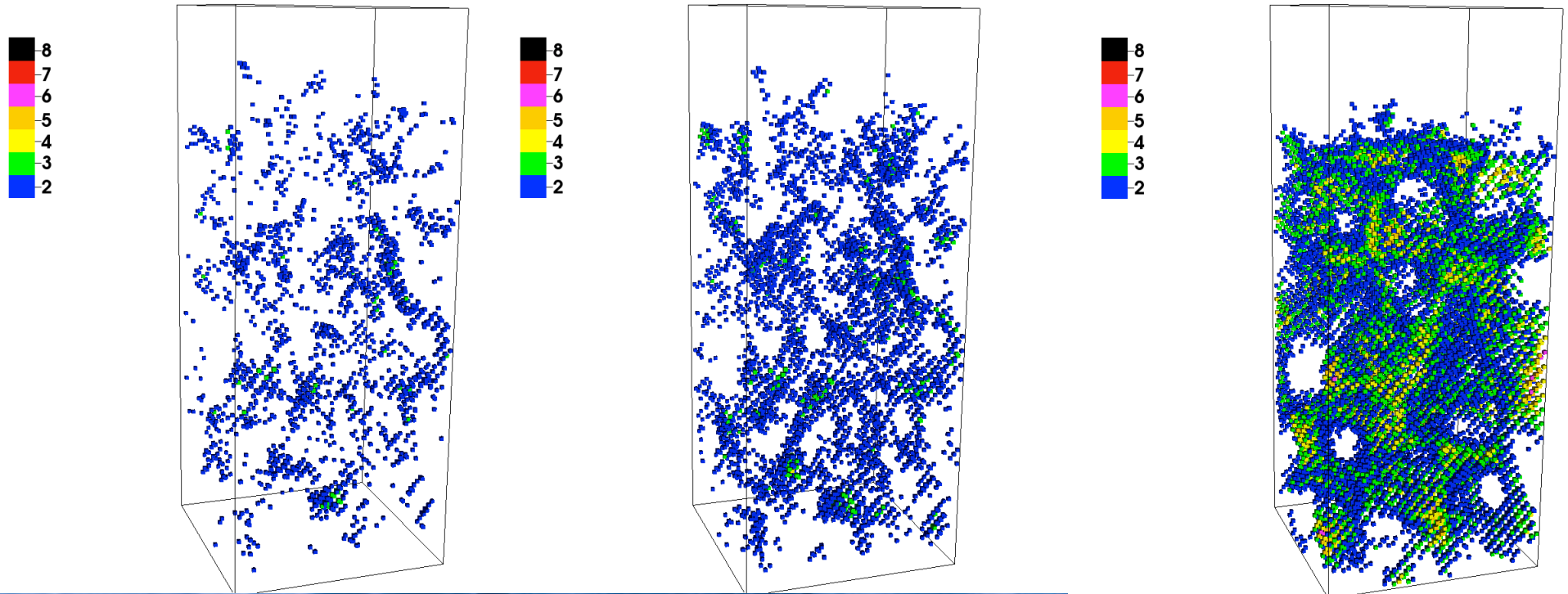


$T = 60 \text{ K}$



$T = 100 \text{ K}$

Ice porosity

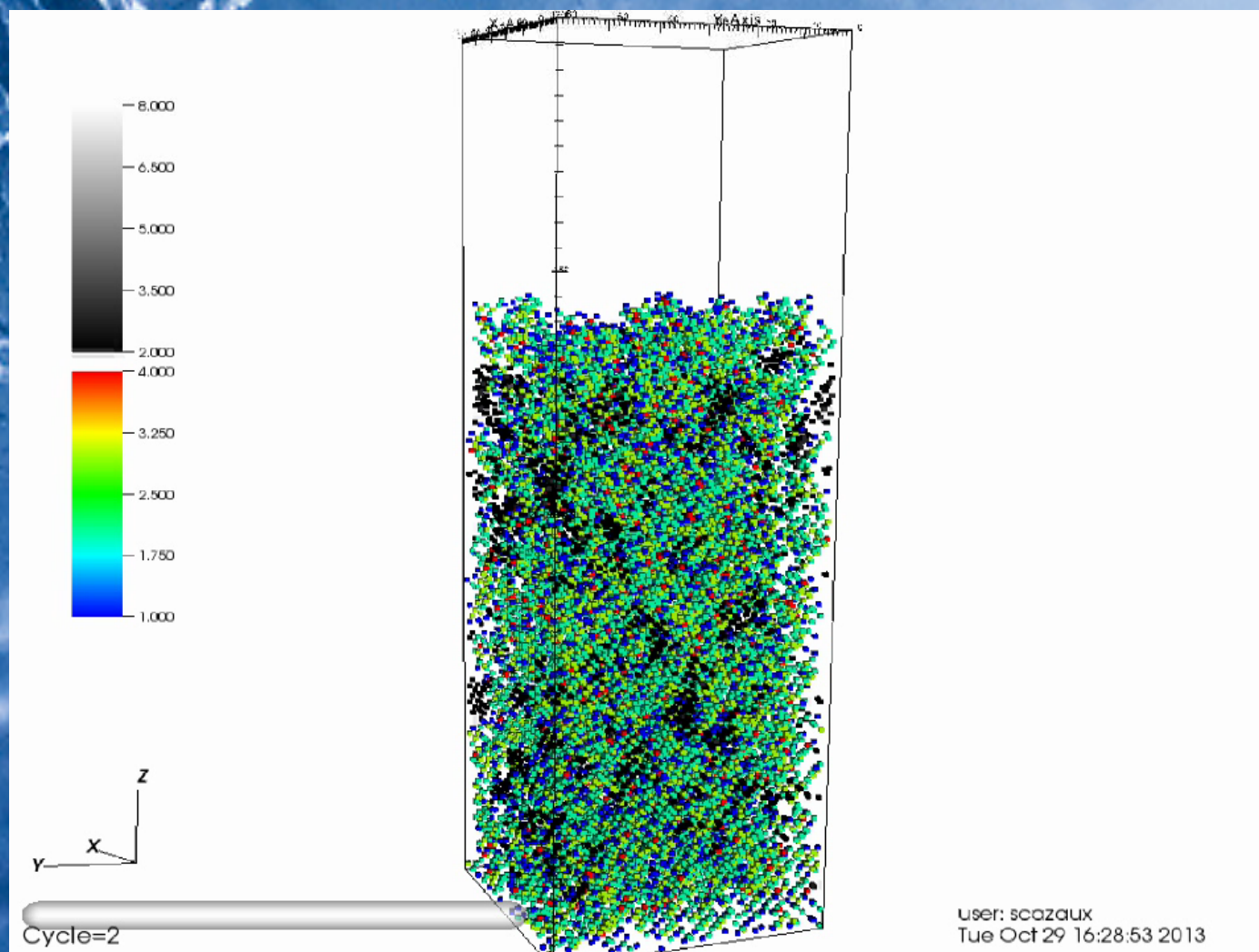


$T = 10 \text{ K}$

$T = 60 \text{ K}$

$T = 100 \text{ K}$

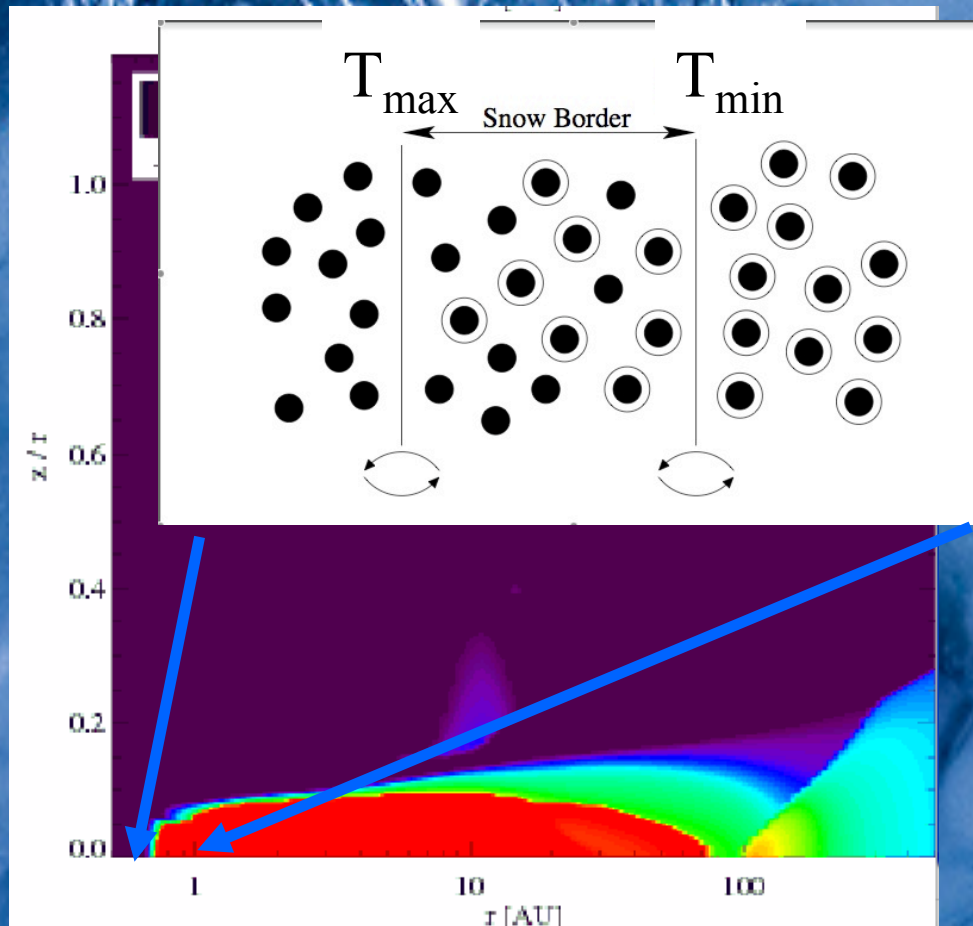
Evolution of water ice



Evolution of water ice

- We do not reproduce compaction with our Monte Carlo simulations (grid size)
- We find ices become more compact locally as T increases and pores grow
- Density ≈ 0.57 to 0.63 g cm^{-3}
Exp $\approx 0.61 \text{ g cm}^{-3}$
- Porosity $\approx 30\% - 40\%$
Exp $\approx 32 \%$

Formation of water ice in disks



Woitke et al. 2009 T-Tauri disk

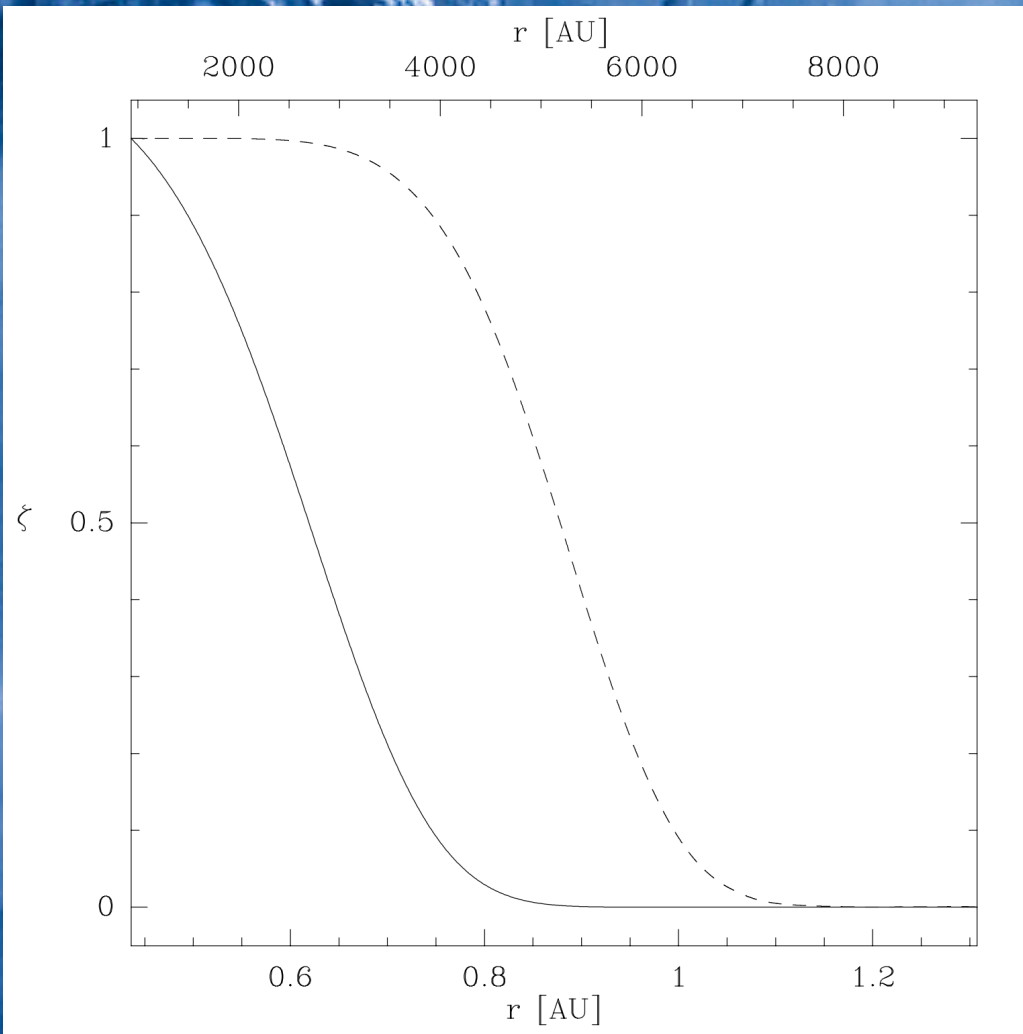
Water on carbon $E \approx 1400\text{K}$
Lin et al. 2005 \ll **water/ water**

T first layer $\ll T$ than ice

Evaporation and freeze-out do not occur at id T . *Papoular 2005*
 \rightarrow impact snowline?

- thermal velocity v_{θ}
- turbulent velocity $v_{\dagger} 0.1 \text{ km s}^{-1}$ *Pietu et 2003 HH star*
- accretion velocity v_{acc}
 $M \approx 10^{-6} M_{\odot} \text{ yr}^{-1}$ *Hueso & Guillot 2005*

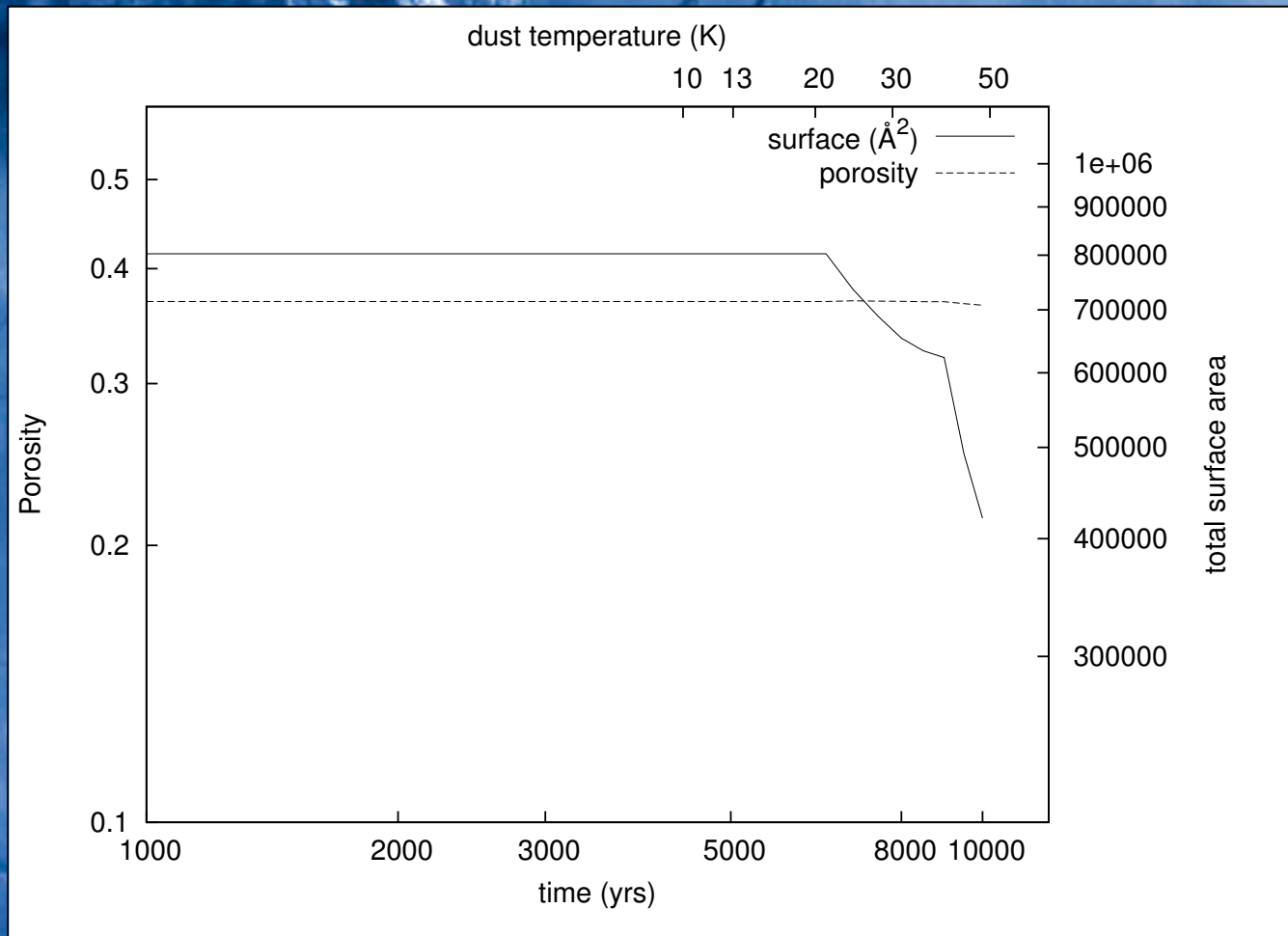
Formation of water ice in disks



- The snowline is actually a snow border (with a size of 0.4 AU).
- Impact on snowline locations
- planet formation \rightarrow coagulation of a mixture bare-icy grains to form planets?

Marseille & Cazaux 2011

Evolution of water ice

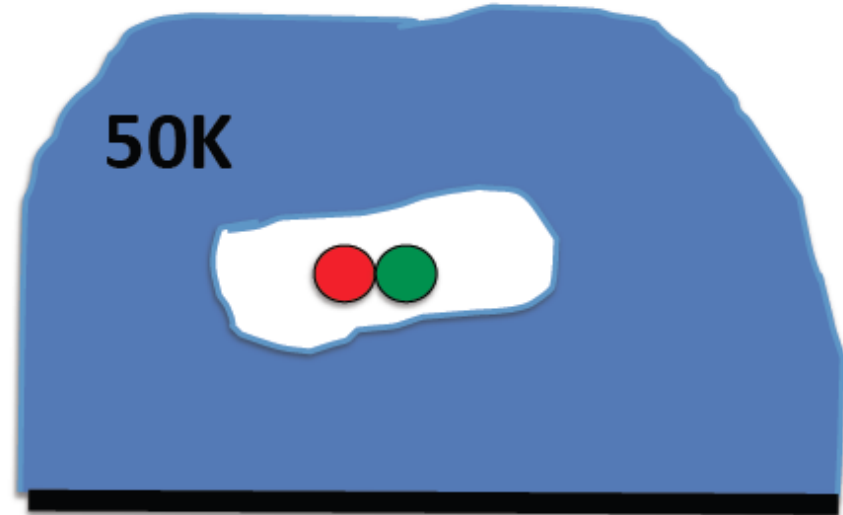
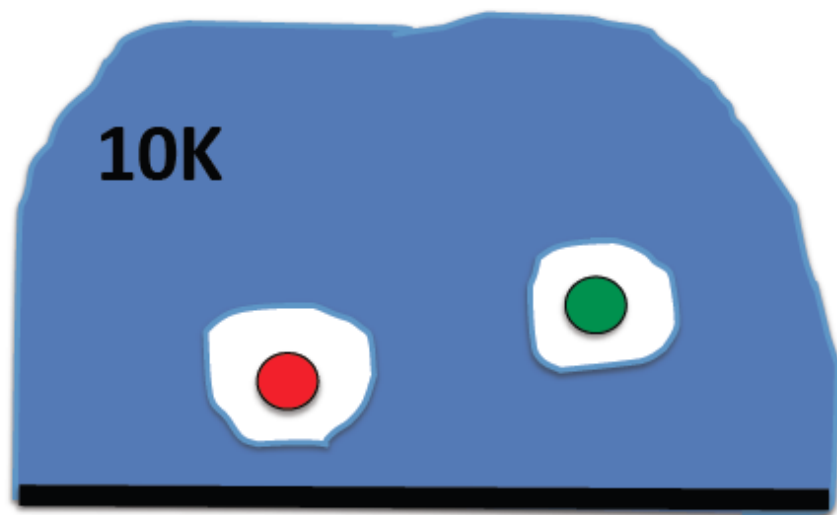


Star forming
Temperature of
gas and dust,
initially at 10 K,
reaches 200 K in
 5×10^4 years

Garrod & Herbst 2006

At $T \approx 30$ K,
which corresponds
to 8×10^3 years \rightarrow
restructuration

Pores boost reactivity?



New process to form molecules in space?

Conclusions

- Exp show → Porous ice become compact as T increases (10%)
- MC simulations show that ices become compact AND pores merge and grow.
- pore coalescence → new solid state process that may boost the formation of new molecules in space
- First layer of ice forms at lower T than evaporation → Snow border



Thank you

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