# Monte Carlo simulations on the formation of interstellar ice

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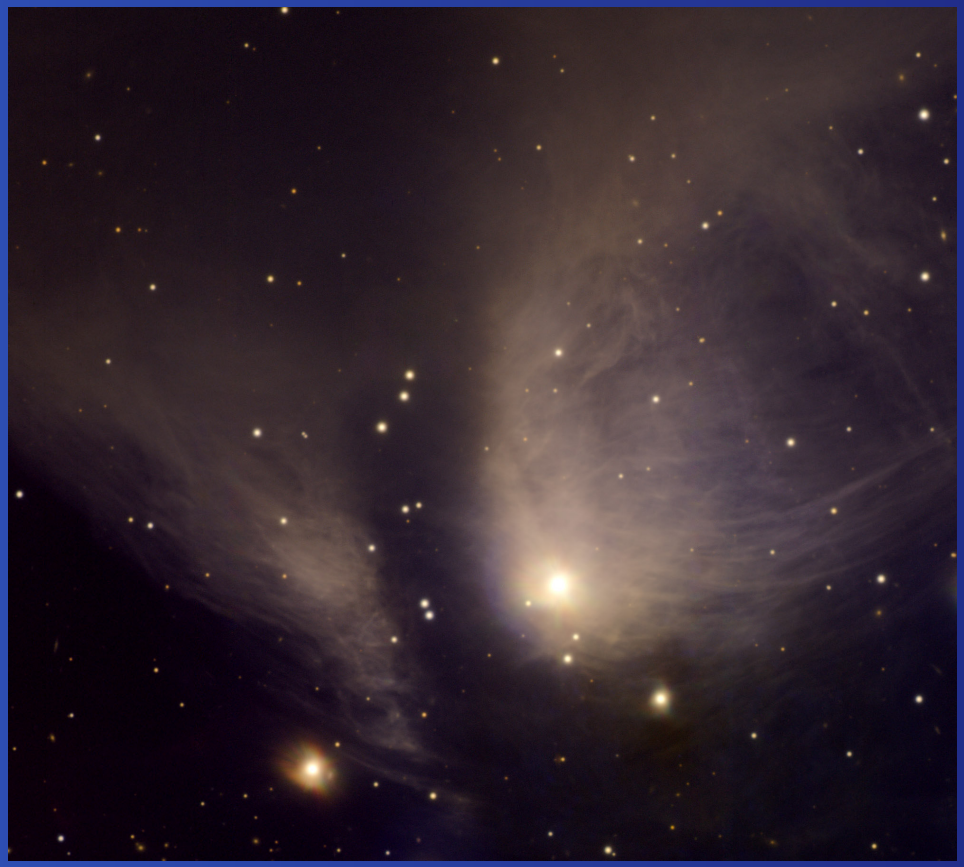
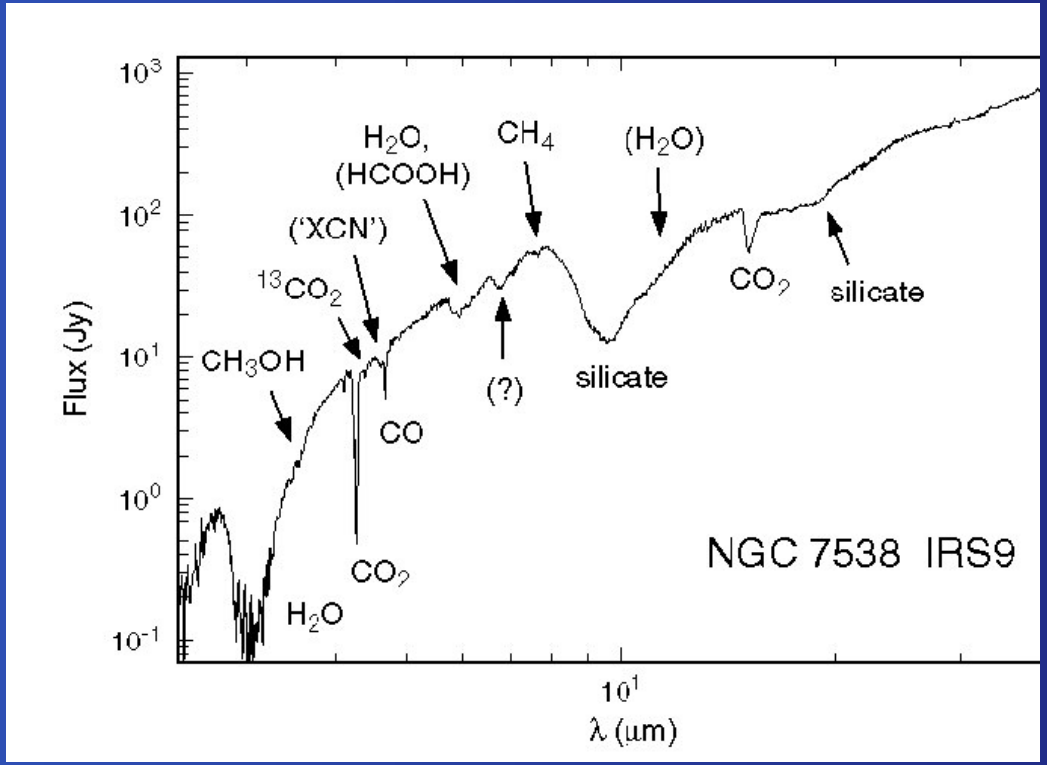
# Molecular Cloud



RY Tauri

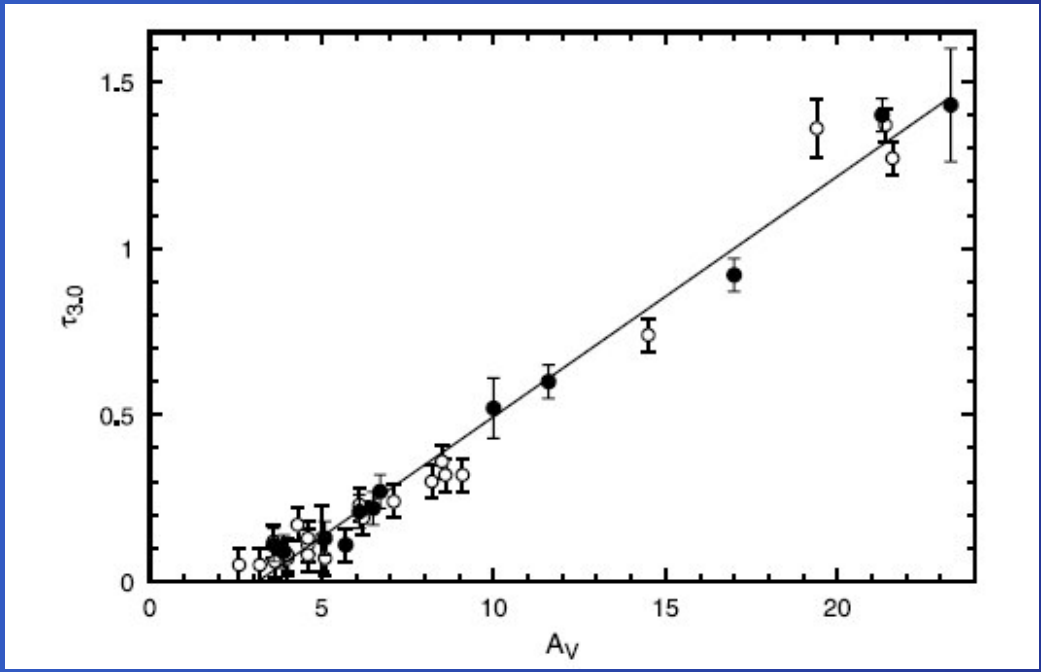
# IR spectrum towards a protostar




Dominant mantle species: water, $CO_2$, CO, $CH_3OH$

# Interstellar ice vs extinction

$$I_V(x) = I_V(0)10^{-A_V/2.5}$$




Whittet, ApJ (2001) 547, 872

Threshold value of $A_V = 3$

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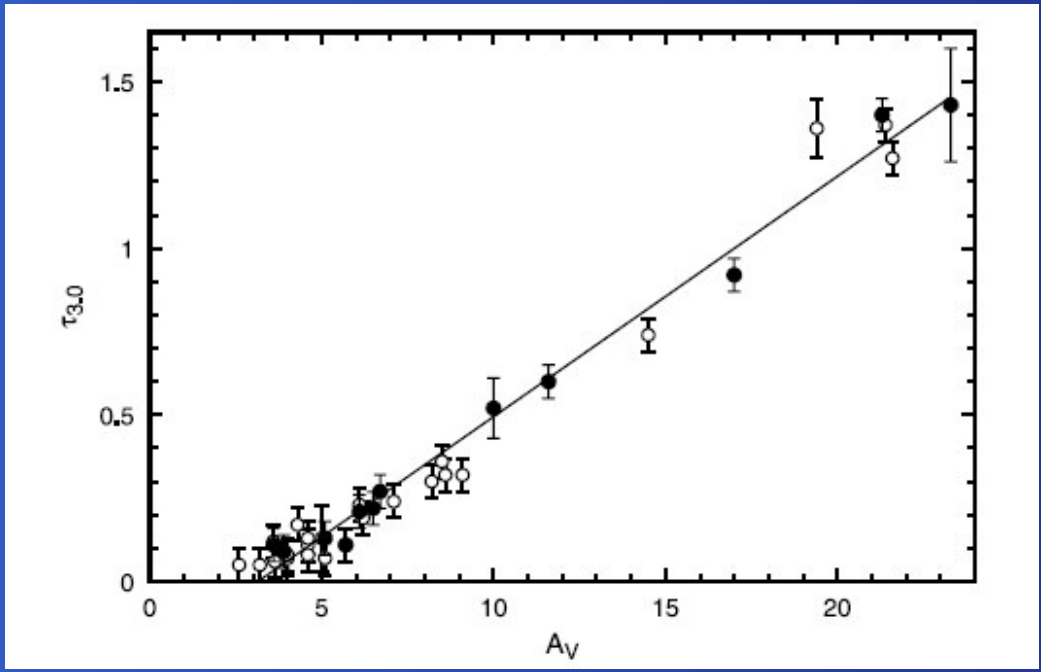


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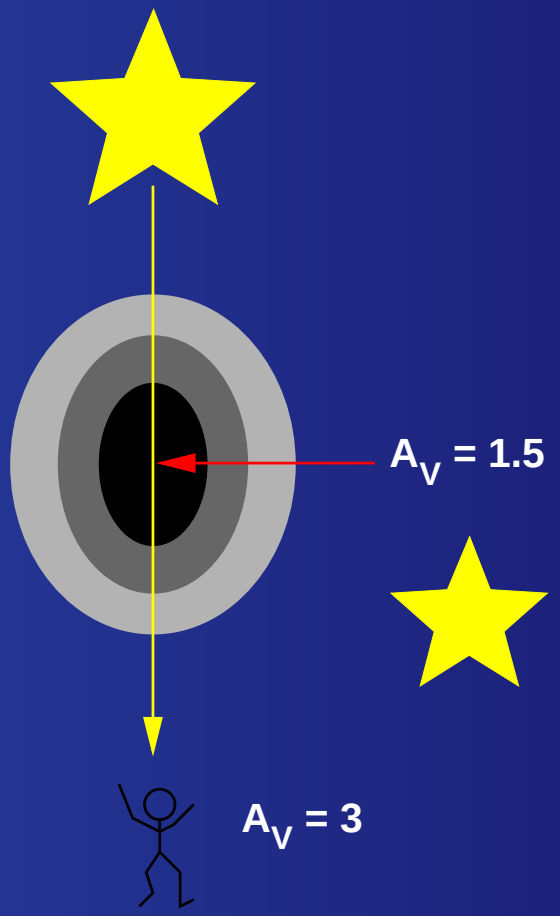
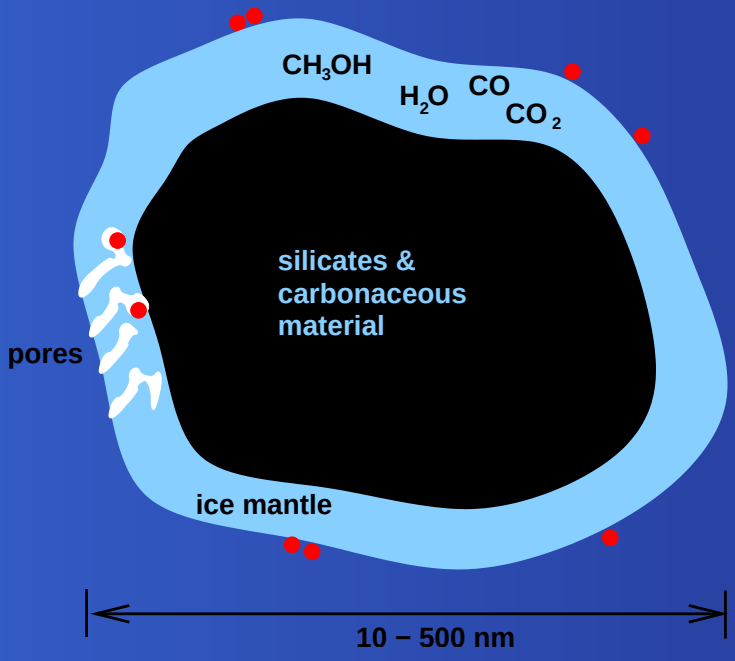
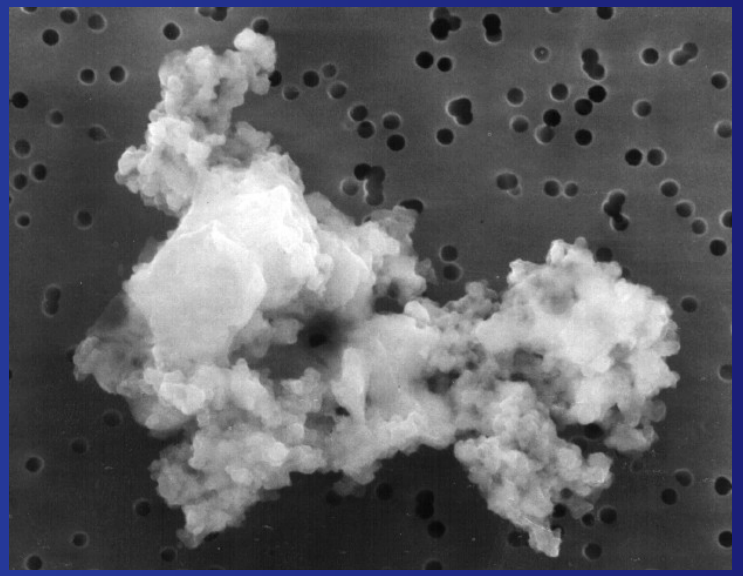


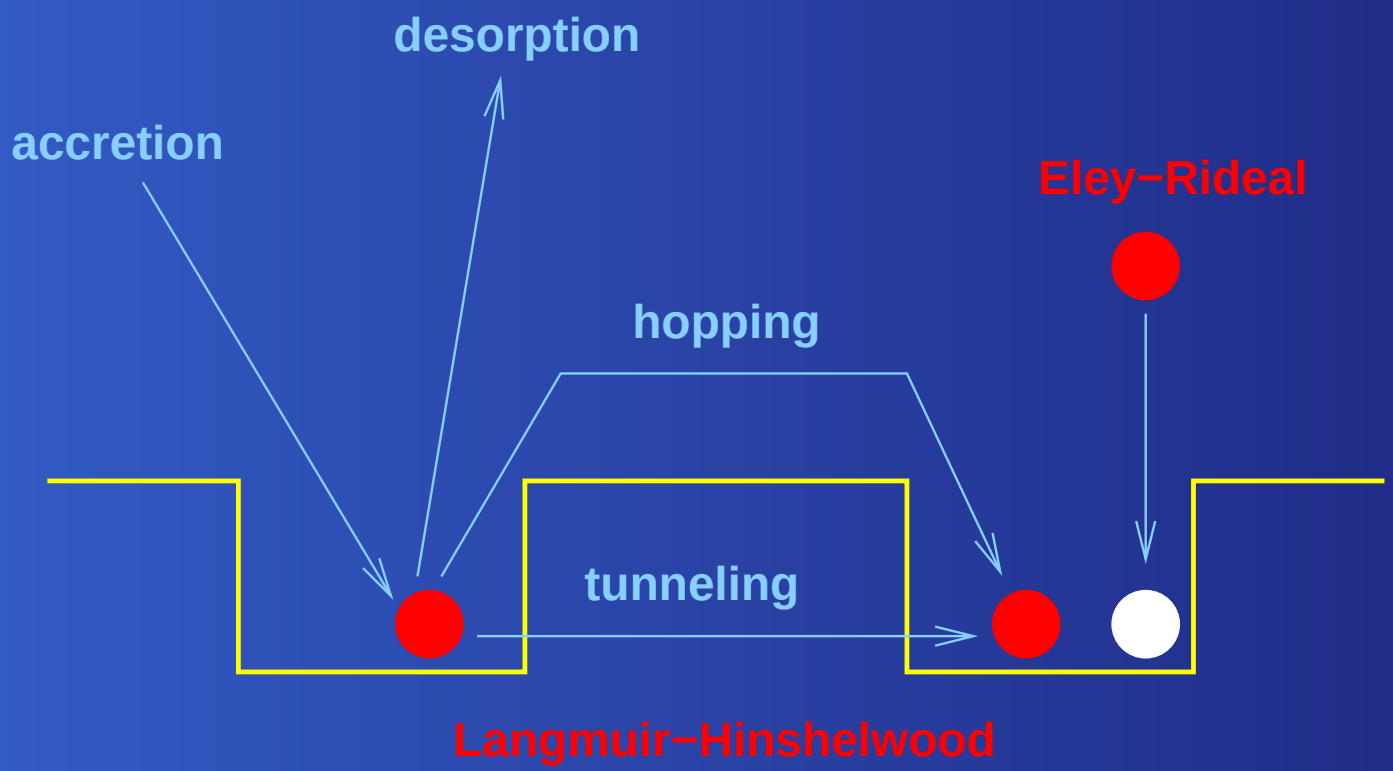
# Interstellar grains

- Ice present in dense and dark areas
  - Formed by surface reactions
  - Ice has porous character
- "Fluffy" shape



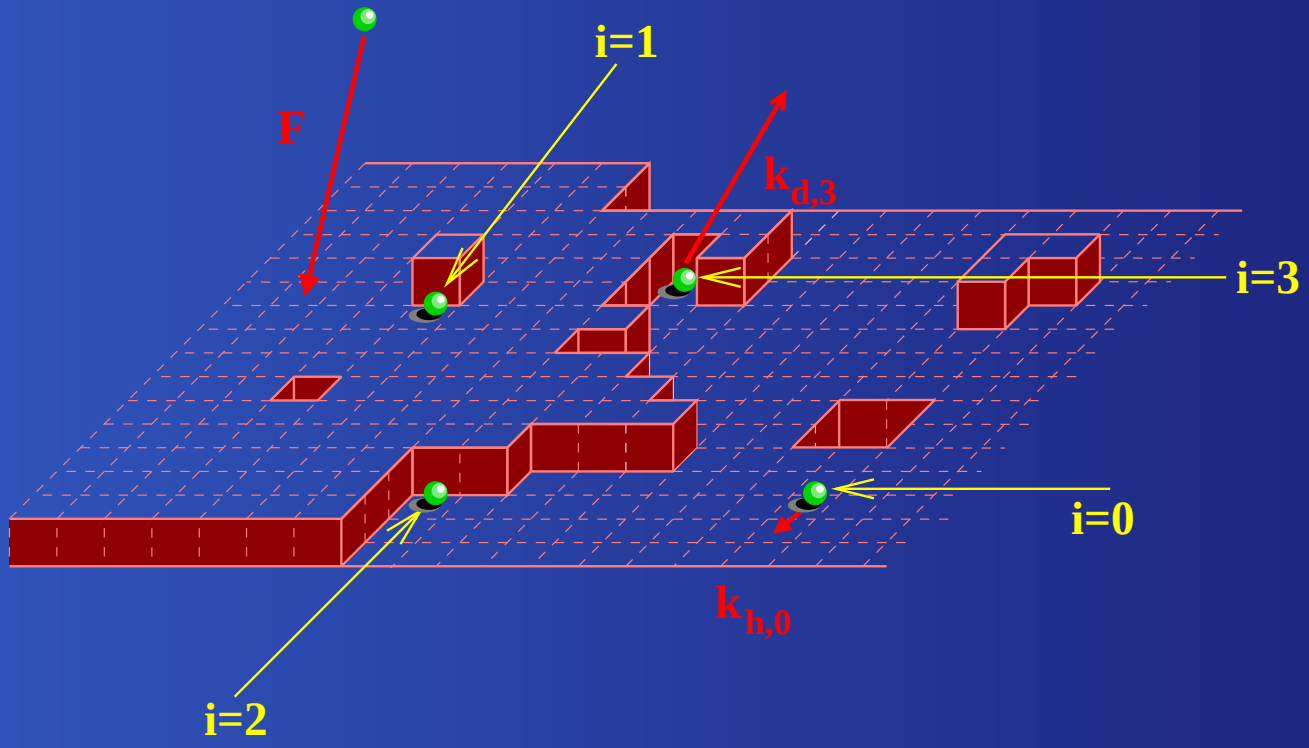
# Surface chemistry




"Physisorption"

"Flat"

# Monte Carlo simulations




- Surface structure can be included
- Different rates depending on the number of "surface" neighbors
- Individual atoms can be followed

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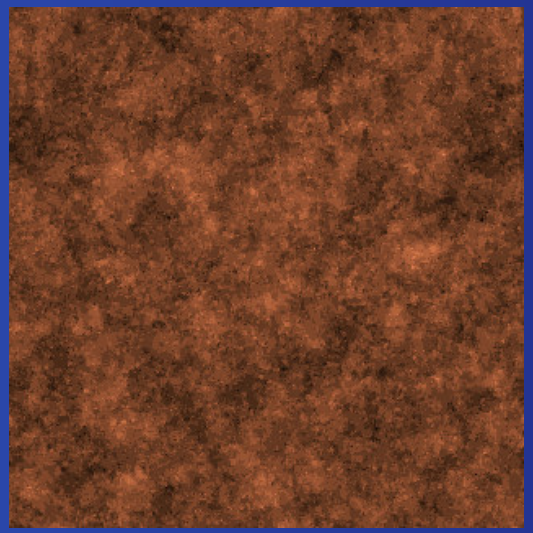
# Surface



$$k_{hop}^{\mathsf{A}} = \nu \exp\left(-\frac{0.78E^{\mathsf{A}} + \alpha i_c E_c^{\mathsf{A}} + \alpha i_{\mathsf{H_2O}} E_{\mathsf{H_2O}}^{\mathsf{A}}}{kT}\right)$$

$$k_{eva}^{\mathsf{A}} = \nu \exp\left(-\frac{E^{\mathsf{A}} + \alpha i_c E_c^{\mathsf{A}} + \alpha i_{\mathsf{H_2O}} E_{\mathsf{H_2O}}^{\mathsf{A}}}{kT}\right)$$

# Surface reactions

| Reaction | $\mu$[1] | $E_a$ (K) |
|---|---|---|
| $H + H \rightarrow H_2$ | 0.991 | 0 |
| $H + O \rightarrow OH$ | 0.991 | 0 |
| $H + OH \rightarrow H_2O$ | 0.991 | 0 |
| $O + O \rightarrow O_2$ | 0.991 | 0 |
| $H + O_2 \rightarrow O_2H$ | 0.991 | 1200 |
| $H + O_2H \rightarrow H_2O_2$ | 0.991 | 0 |
| $H + O_3 \rightarrow O_2 + OH$ | 1 | 450 |
| $H + H_2O_2 \rightarrow H_2O + OH$ | 1 | 1400 |
| $H_2 + OH \rightarrow H_2O + H$ | 1 | 2600 |
| $O + O_2 \rightarrow O_3$ | 0.991 | 0 |

[1] Kroes and Andersson, Proc. IAU symp 231, (2005) p. 427

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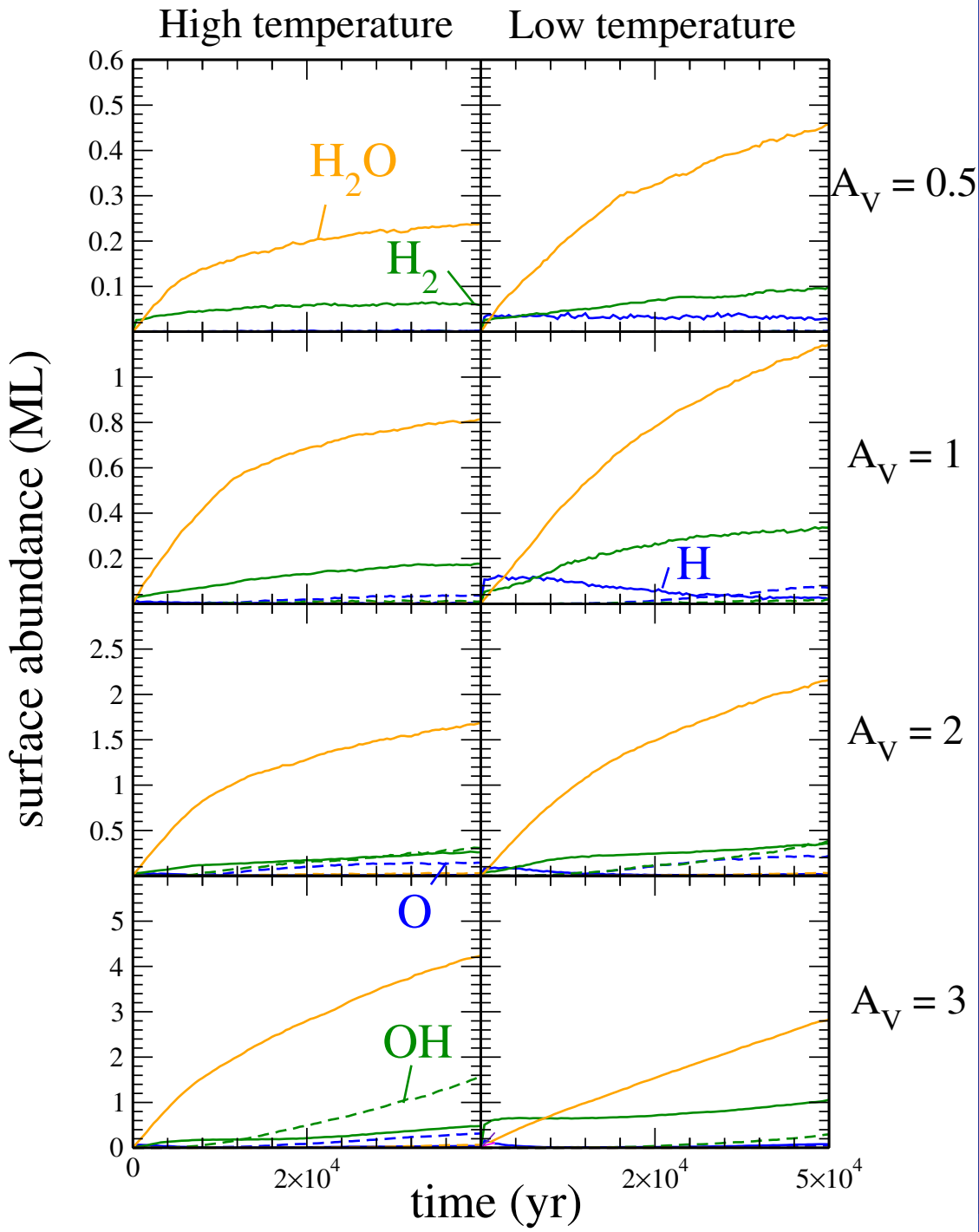
# Dissociation reactions

| Reaction | | | $\alpha_{photo}$ ($s^{-1}$) | $\gamma_{photo}$ | $\alpha_{CR}$ |
|---|---|---|---|---|---|
| OH | $\rightarrow$ O | + H | 1.68(-10) | 1.66 | 1.02(3) |
| $H_2O$ | $\rightarrow$ H | + OH | 3.28(-10) | 1.63 | 1.94(3) |
| $O_2$ | $\rightarrow$ O | + O | 3.30(-10) | 1.4 | 1.50(3) |
| $O_2H$ | $\rightarrow$ O | + OH | 0 | 0 | 1.50(3) |
| $O_2H$ | $\rightarrow$ H | + $O_2$ | 0 | 0 | 1.50(3) |
| $H_2O_2$ | $\rightarrow$ OH | + OH | 0 | 0 | 3.00(3) |

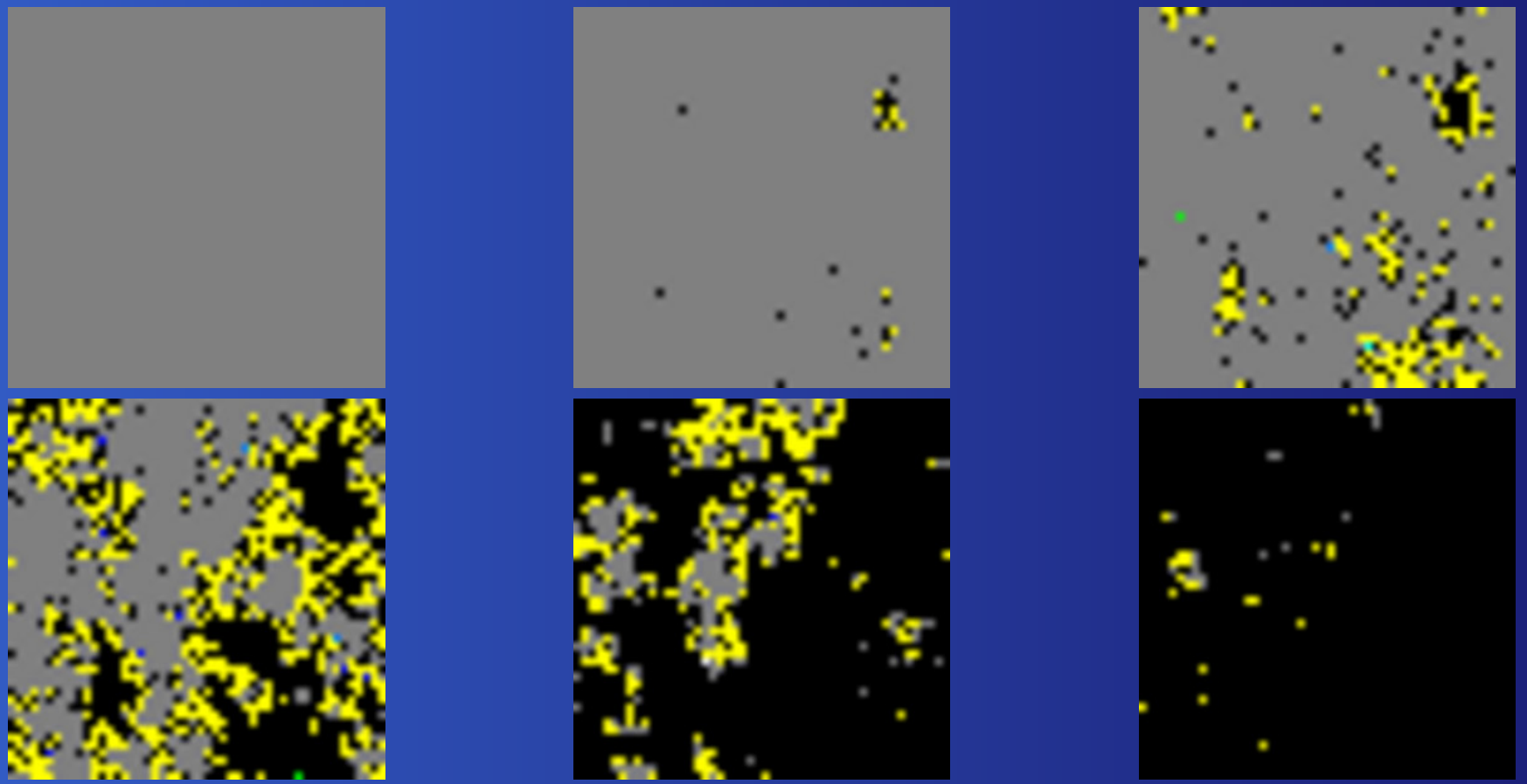



Diffuse regions

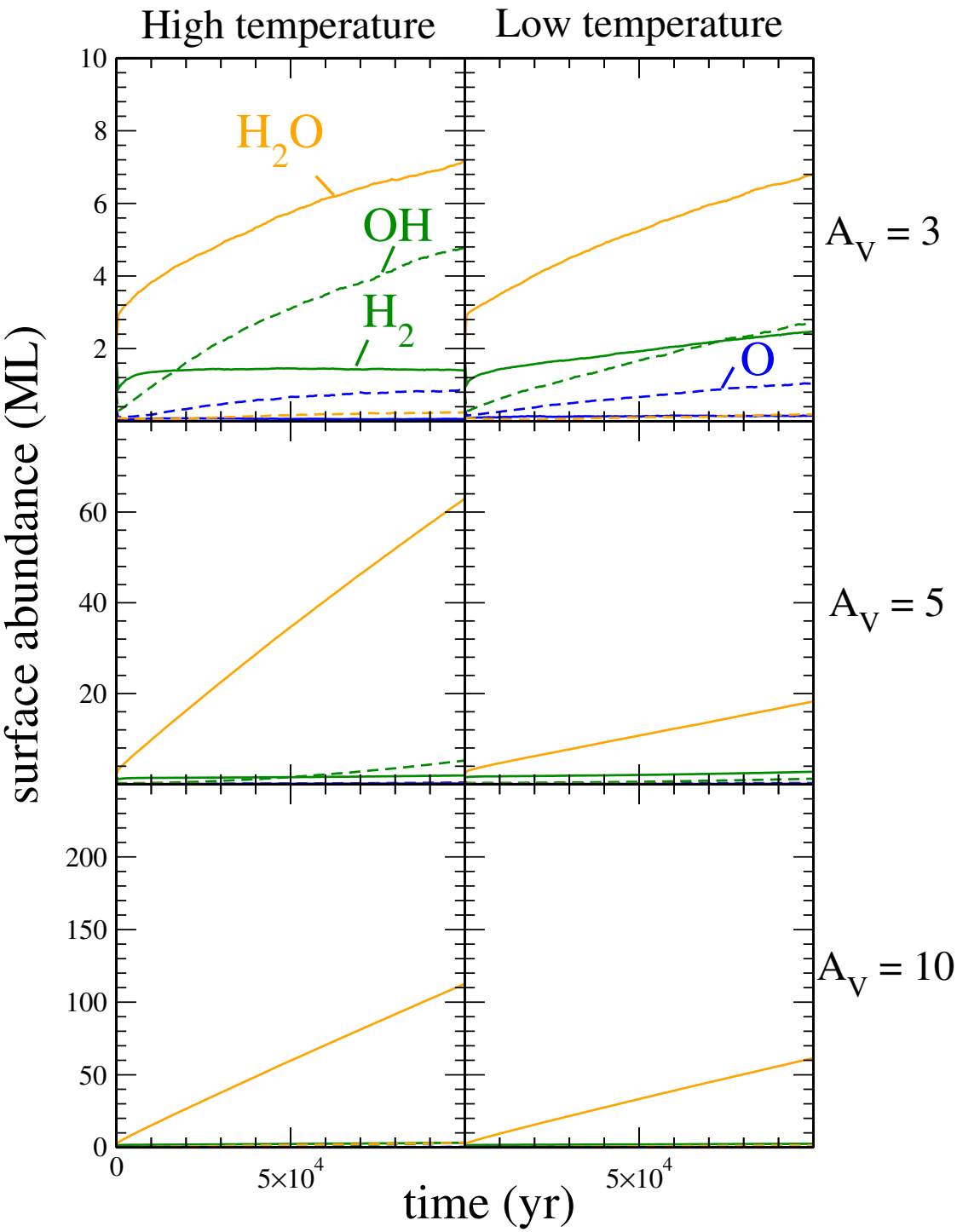
Threshold value

$A_V = 1.5$

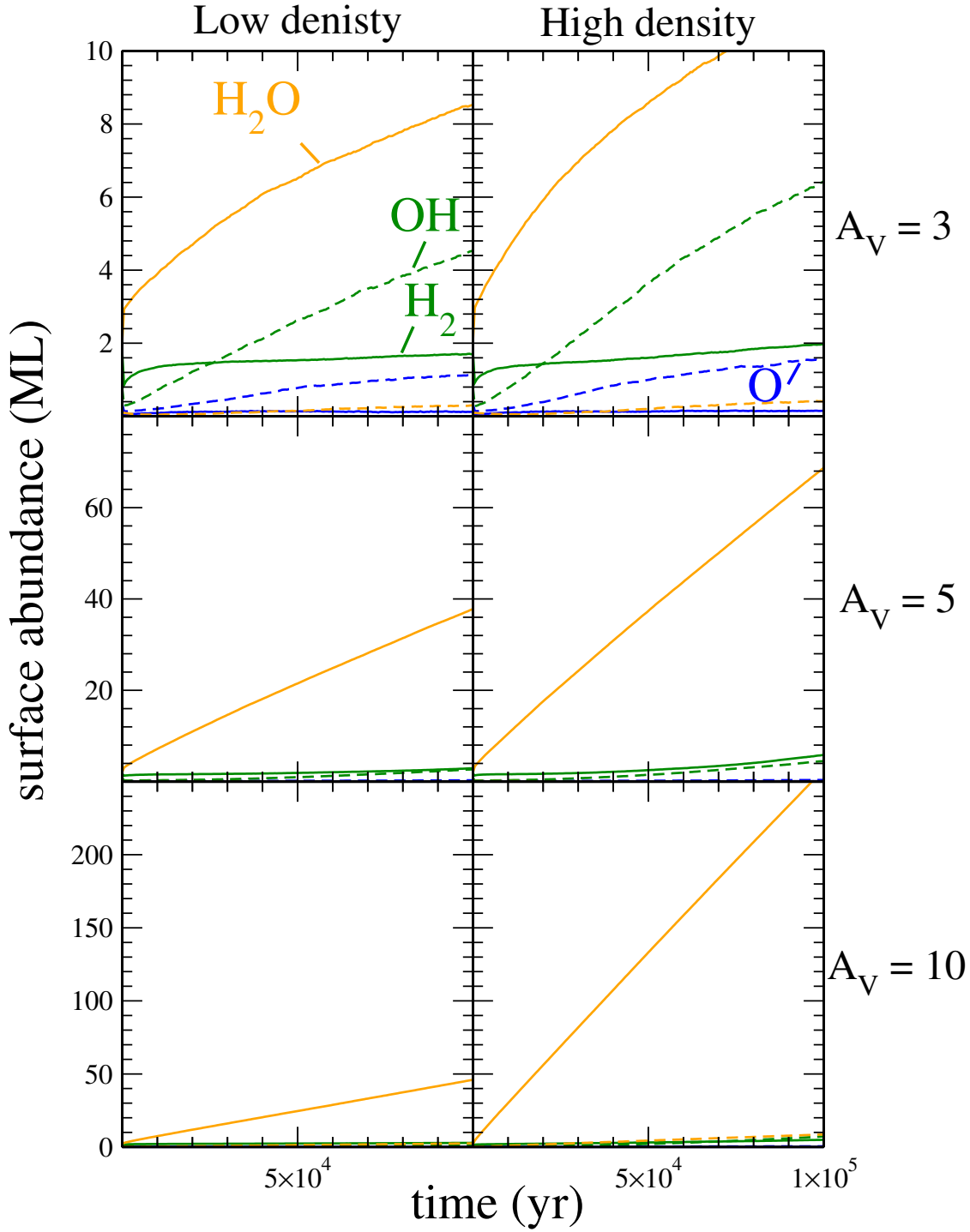
# Ice surfaces



carbonaceous grain; $H_2O$; ...; H; O; OH; $H_2$




Dense regions




Dense regions

# Conclusions

- Small surface coverage of ice in diffuse areas
- Ice function of temperature and density
- Ice mainly forms at surface steps
- Threshold value is in agreement
- $H_2$ blocks surface in dense areas

# Acknowledgments


- the Herbst group
- National Science Foundation for funding
- ... and you for your attention.

# Evaporation energies

| | Substrate | |
|---|---|---|
| Absorbate | carbon | $H_2O$ |
| H | 660 | 450 |
| O | 800 | 800 |
| OH | 1360 | 3500 |
| $H_2$ | 540 | 550 |
| $O_2$ | 1440 | 1000 |
| $H_2O$ | 2000 | 5640 |
| $O_3$ | 2240 | 1800 |
| $O_2H$ | 2100 | 1450 |
| $H_2O_2$ | 2760 | 1900 |