Monte Carlo simulations on the formation of interstellar ice

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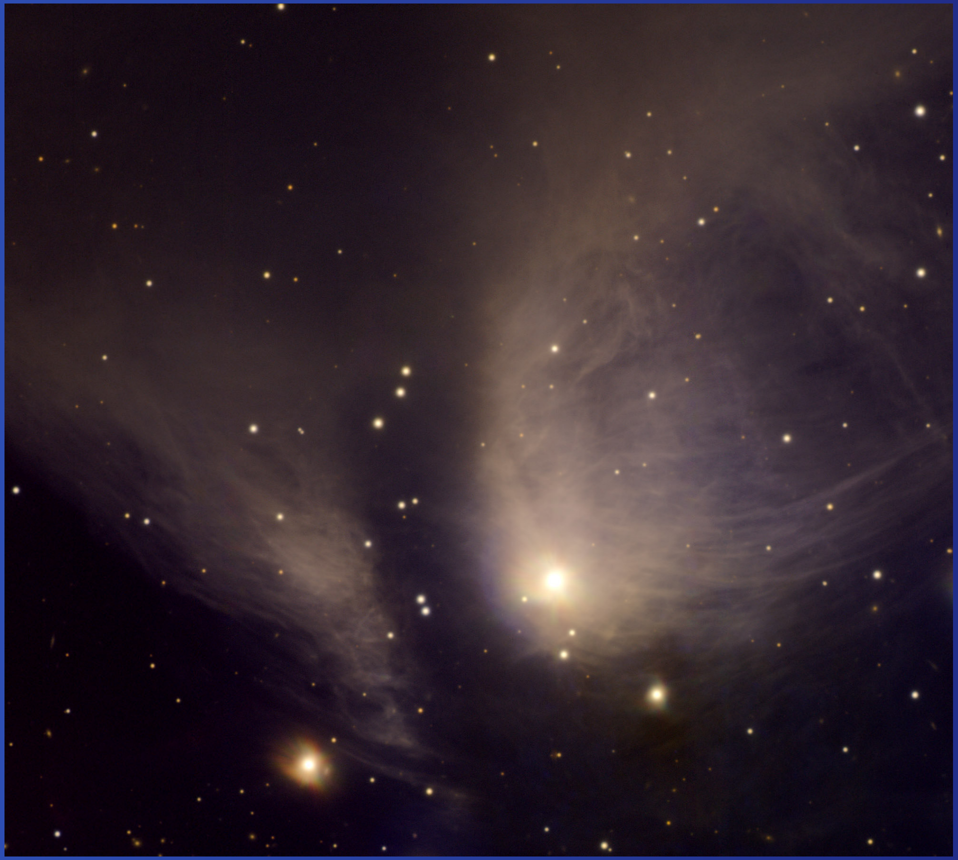
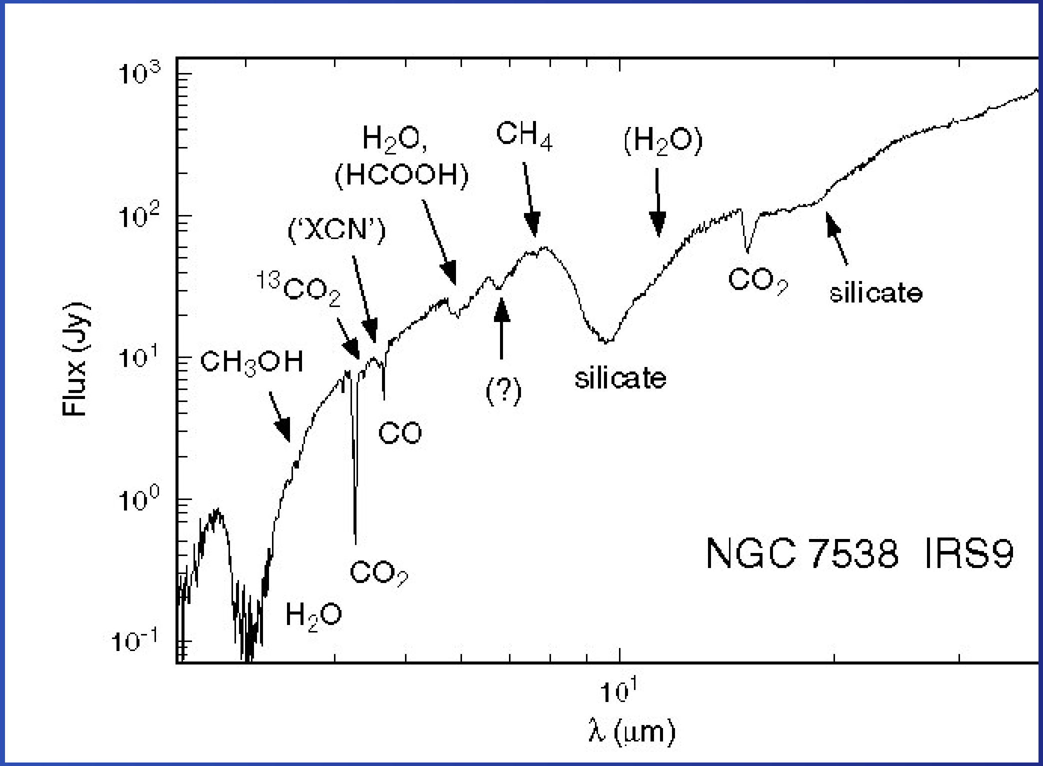
Molecular Cloud



RY Tauri

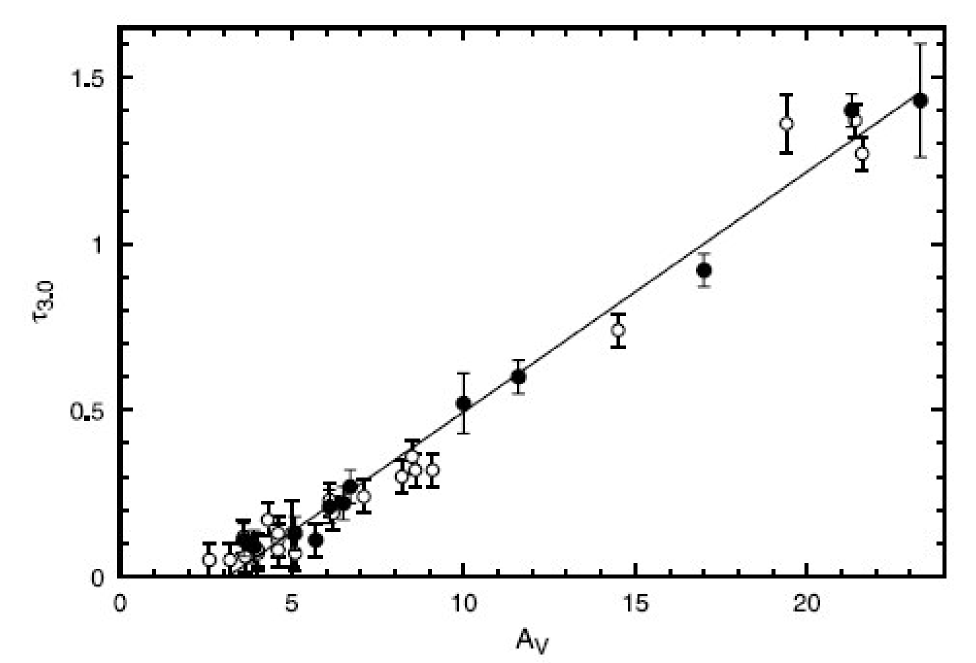
IR spectrum towards a protostar



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 $A_V = 3$

Interstellar ice vs extinction

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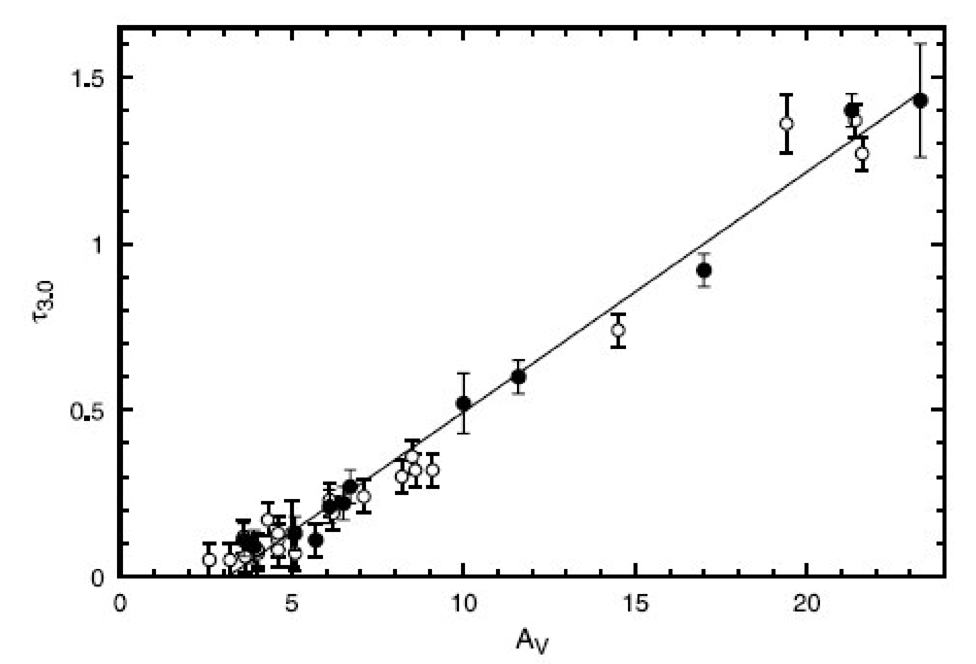

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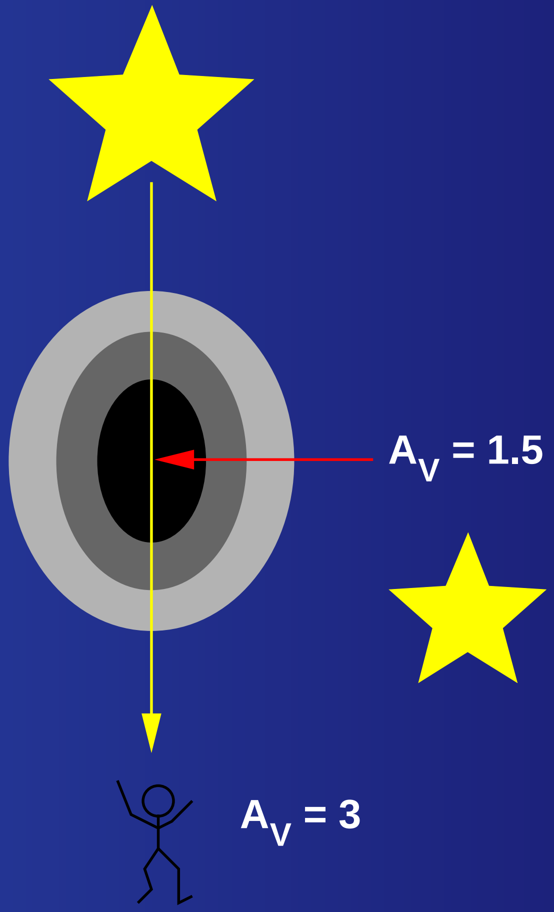
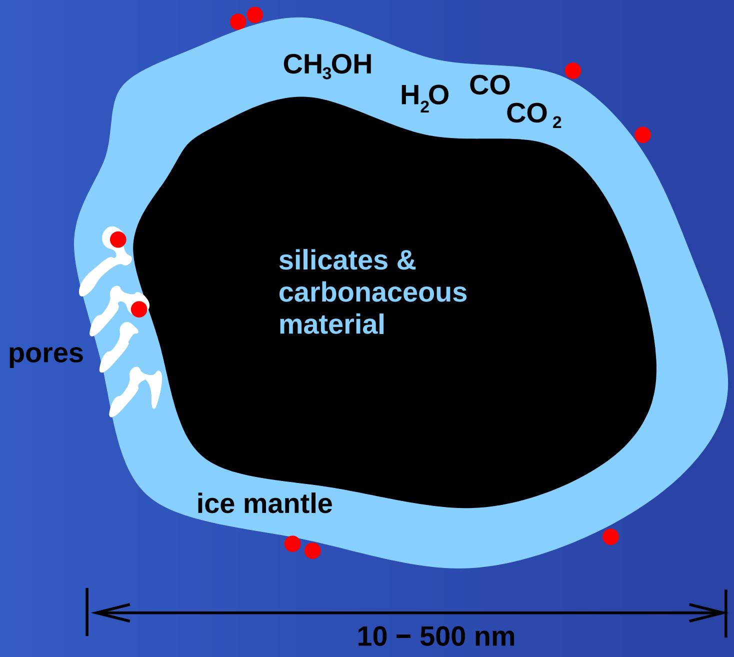


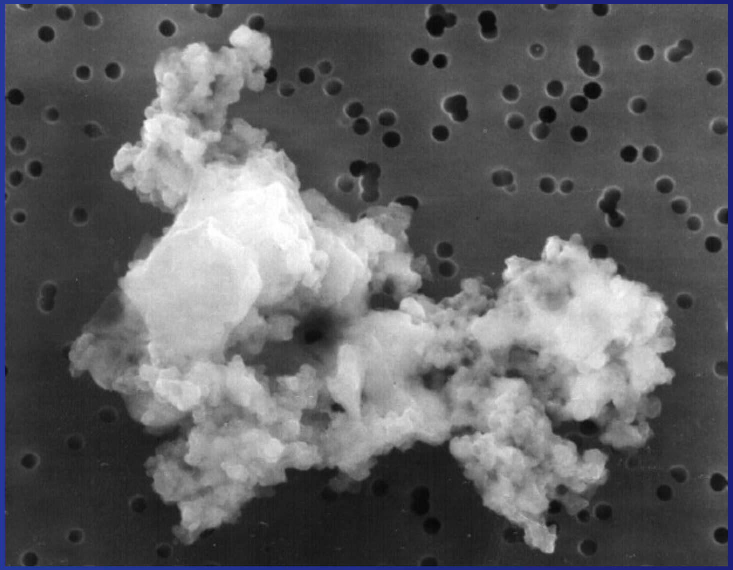
A_V = 1.5

A_V = 3

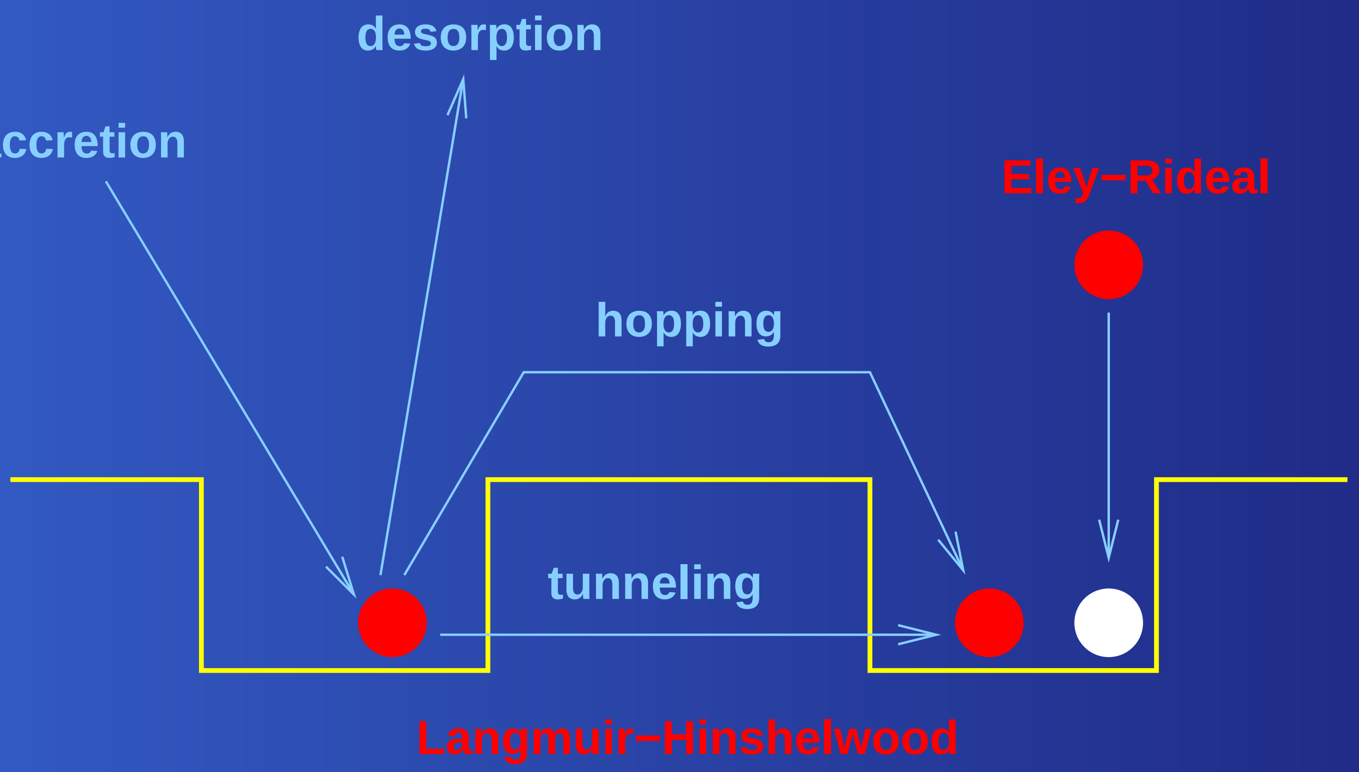
Interstellar grains

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





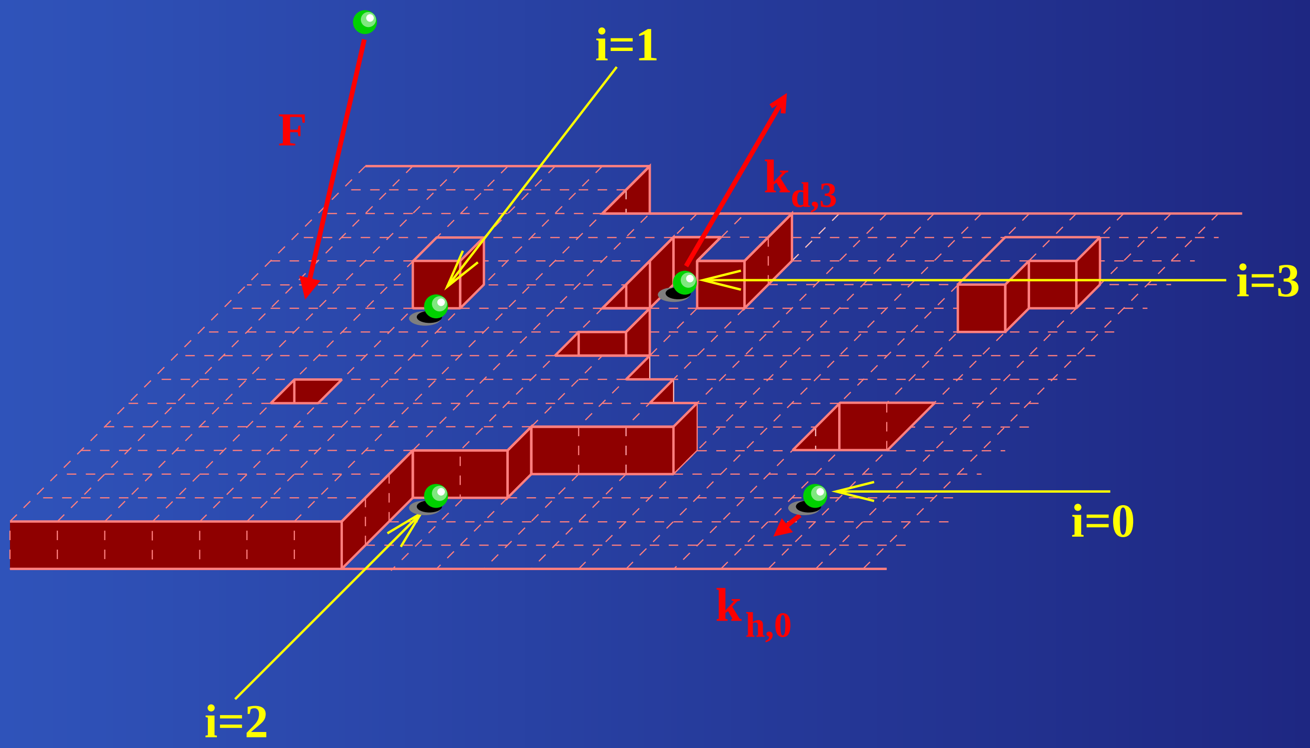
Surface chemistry



"Physisorption"

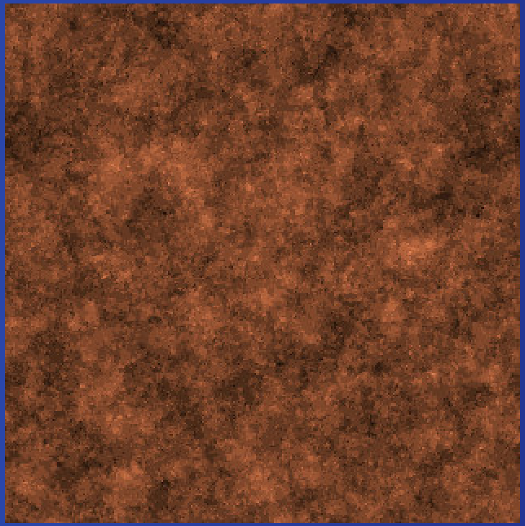
"Flat"

Monte Carlo simulations



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

Surface



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

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Surface reactions

Reaction				μ[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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$H + O_2H \rightarrow H_2O_2$	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
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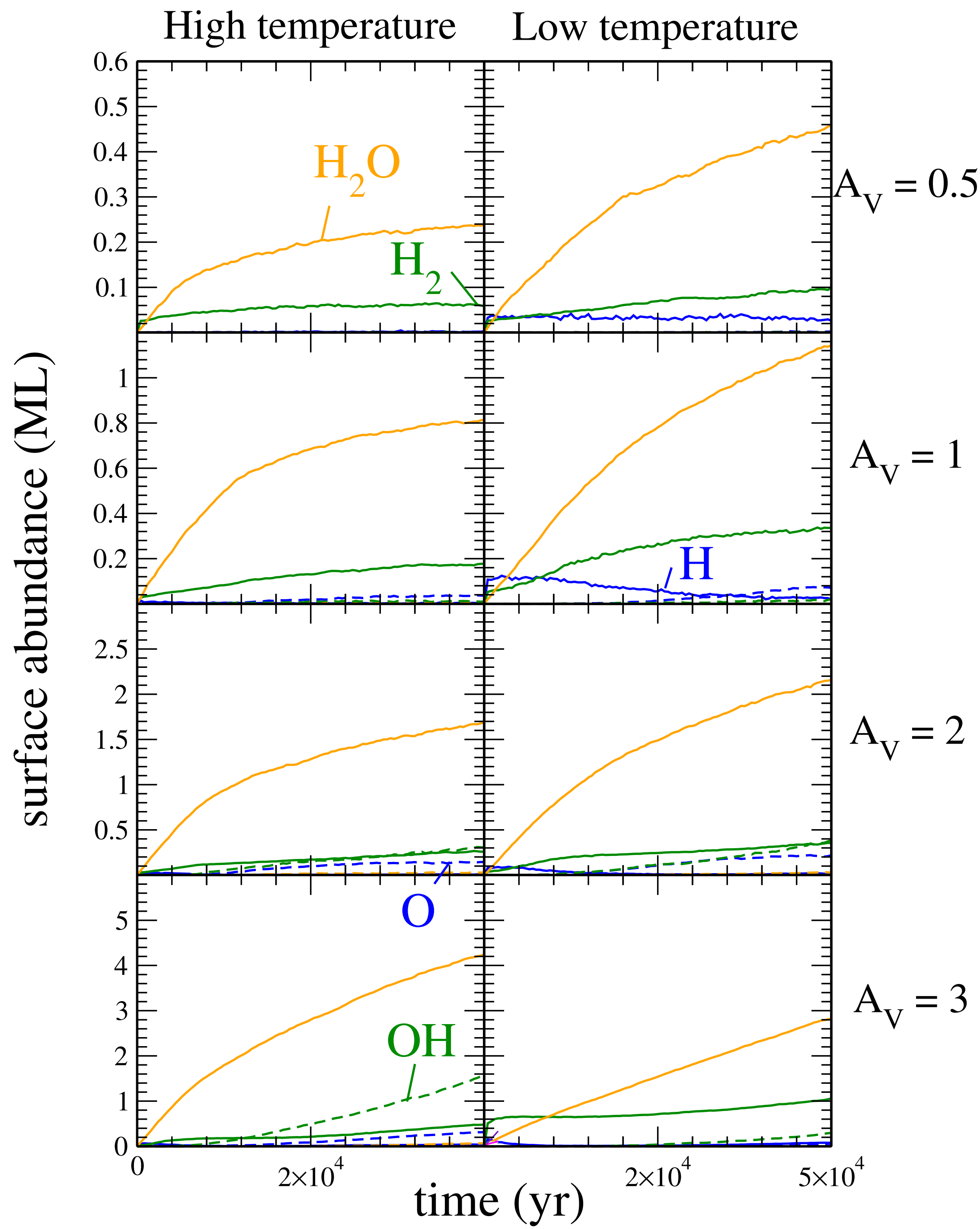
Dissociation reactions

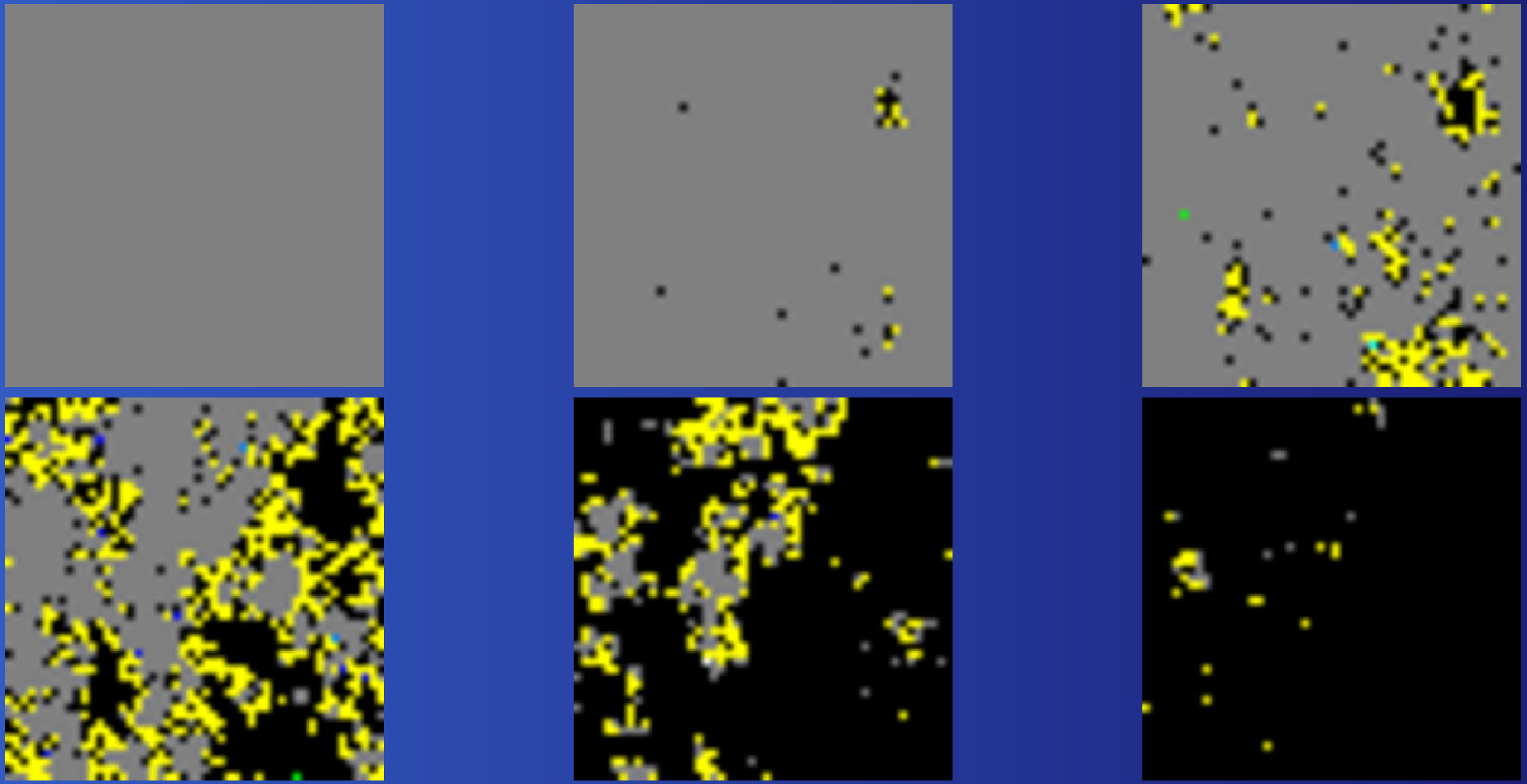
Reaction	α_{photo} (s^{-1})	γ_{photo}	α_{CR}
$OH \longrightarrow O + H$	1.68(-10)	1.66	1.02(3)
$H_2O \longrightarrow H + OH$	3.28(-10)	1.63	1.94(3)
$O_2 \longrightarrow O + O$	3.30(-10)	1.4	1.50(3)
$O_2H \longrightarrow O + OH$	0	0	1.50(3)
$O_2H \longrightarrow H + O_2$	0	0	1.50(3)
$H_2O_2 \longrightarrow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



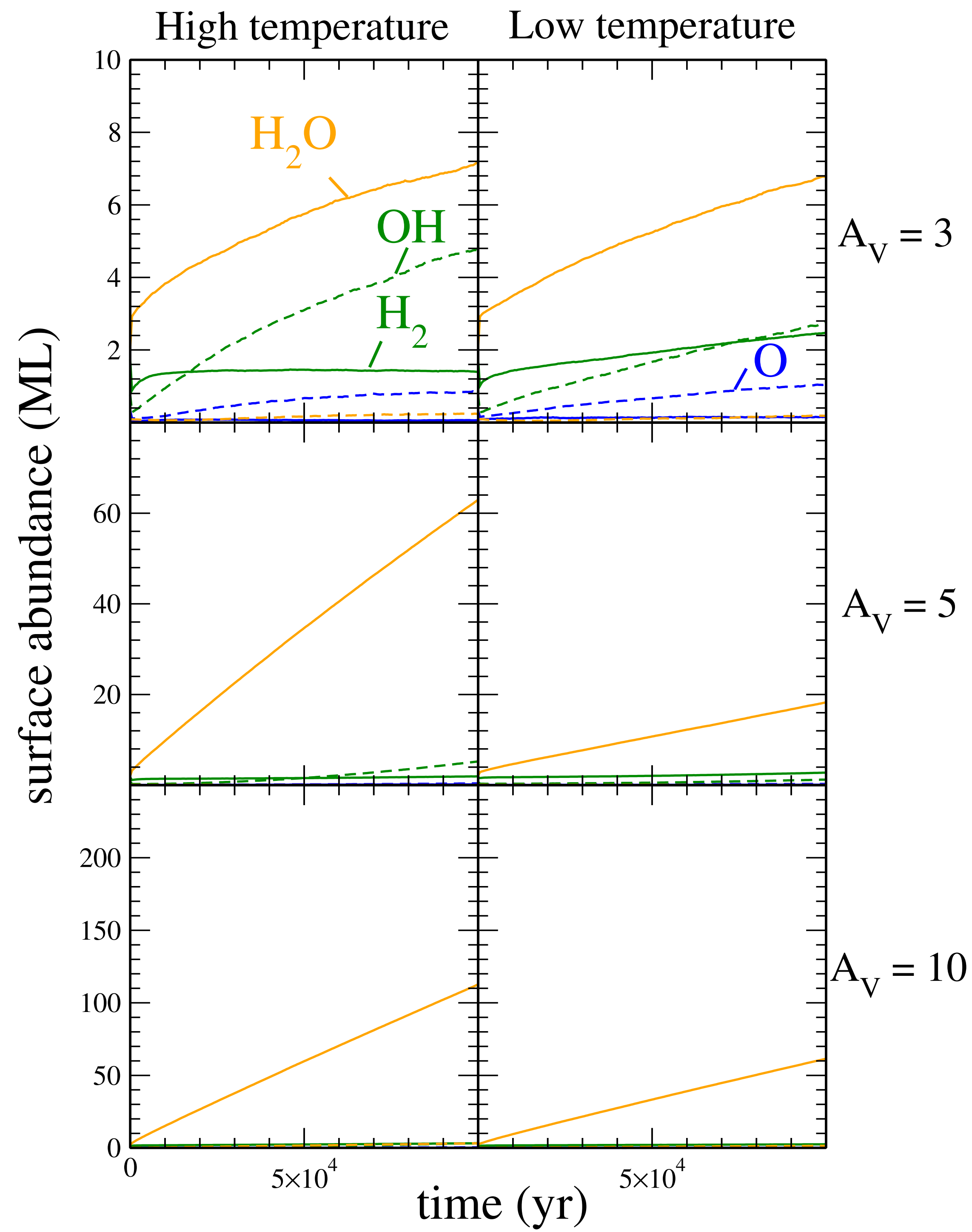
Diffuse regions

Threshold value $A_V = 1.5$

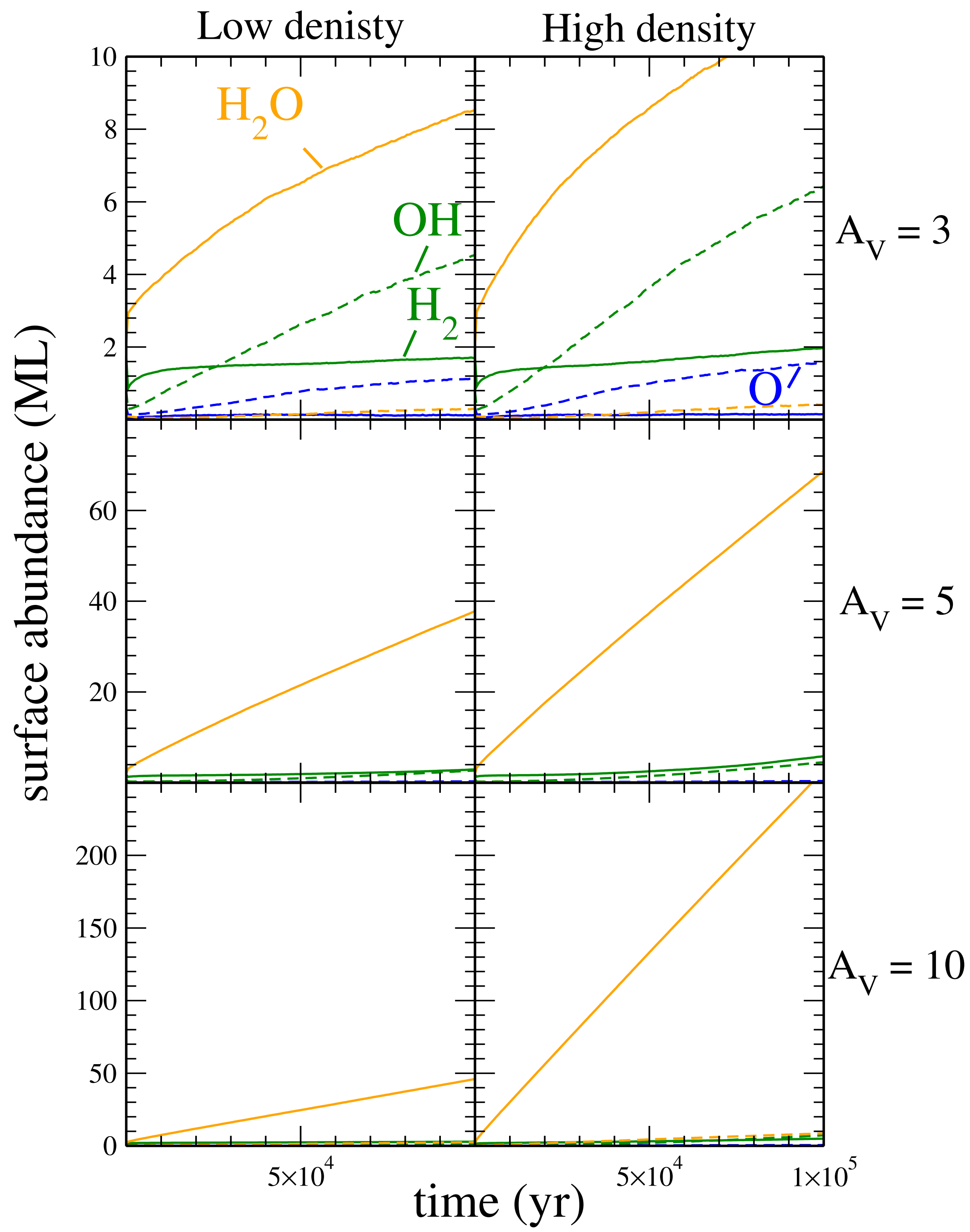
Ice surfaces



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