Water in protoplanetary disks: D/H ratio

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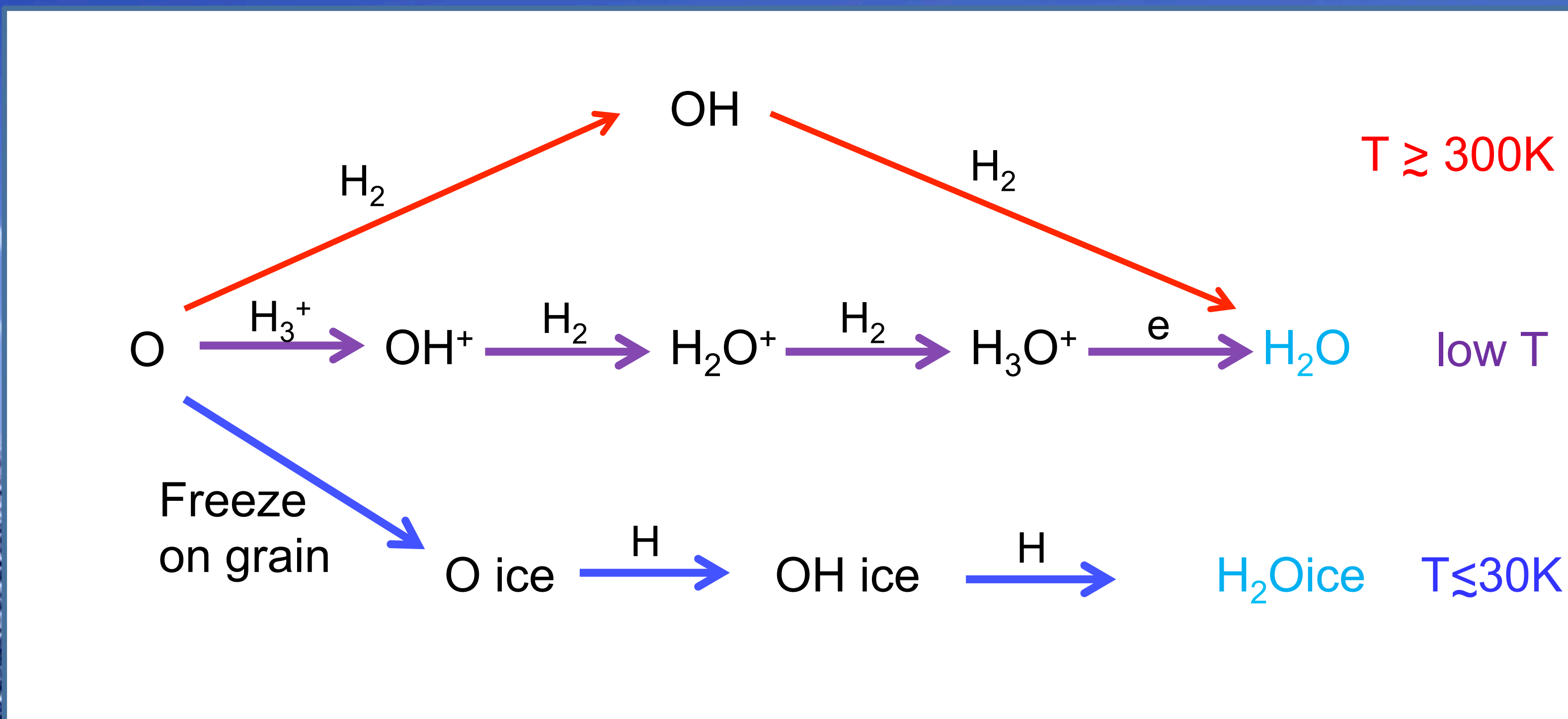
Water

- Major Oxygen reservoire

- Major ice (+ other volatiles as impurities)
  … raw material for { outer planets, atmosphere, ocean }

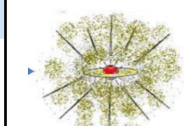
- 3 formation paths of water in ISM

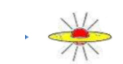


Water in star-forming regions

Evolutionary stage	Water vapor $n(H_2O)/n_H$	Water ice column density [cm^{-2}]
Starless core	~10^{-9}	~10^{18} cm^{-2} 10% of elemental O
Protostellar core (Class 0--I):		
Outer envelope (T < 100 K)	10^{-9} –10^{-8}	~10^{18} cm^{-2}
Inner envelope (T > 100 K)	10^{-6} –10^{-5}	---
Cavity wall by outflow	10^{-5} –10^{-4}	---
Circumstellar disk (Class II):		
Outer disk (>100 AU)	<10^{-7}	~10^{18} cm^{-2}
Inner disk (< 3 AU)	1.3 [relative to CO]	---


分子雲コア


原始星 / ガス円盤


中心星 /
原始惑星系円盤

Ref. Whitet & Duley (1991); Terada et al. (2007); Najita & Carr (2008); Honda et al. (2009); Kristensen et al. (2010, 2012); Hogerheijde et al. (2011); Caselli et al. (2012); Coutens et al. (2012)

Water is everywhere!

⟶ Does water in disks & planetary systems originate in ISM?

HDO/H_2O ratio

- Probe of formation site of H_2O

  formation at lower temperature → Higher HDO/H_2O ratio

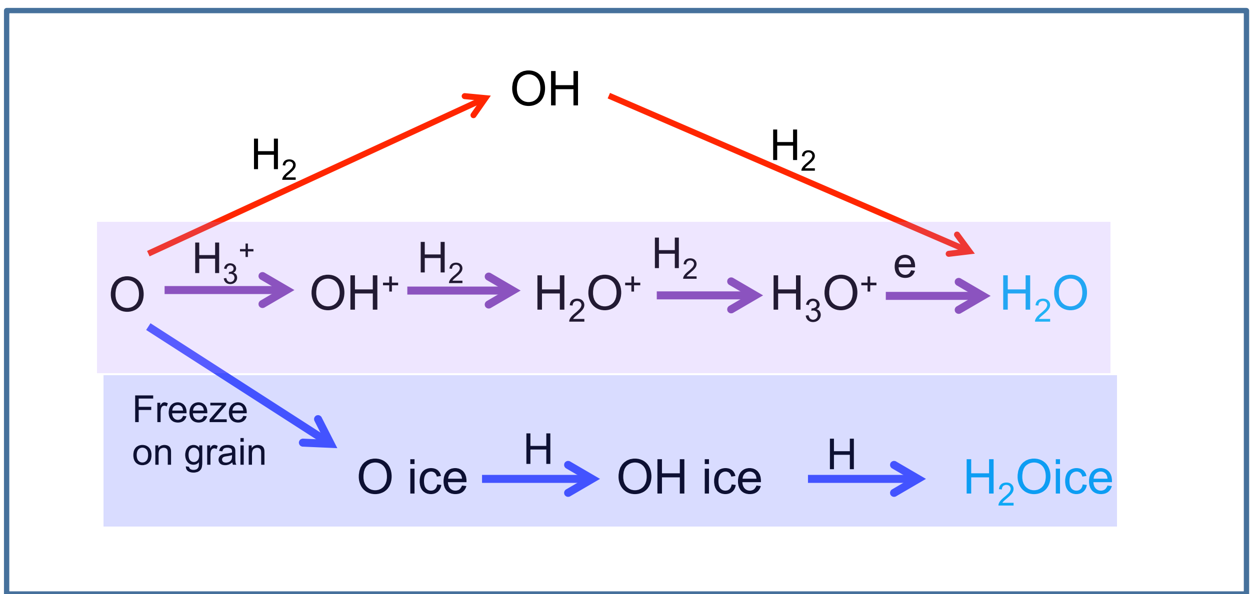
Exothermic Exchange Reactions

$$H_3^+ + HD \rightleftarrows H_2D^+ + H_2 + 230\ \mathrm{K}$$

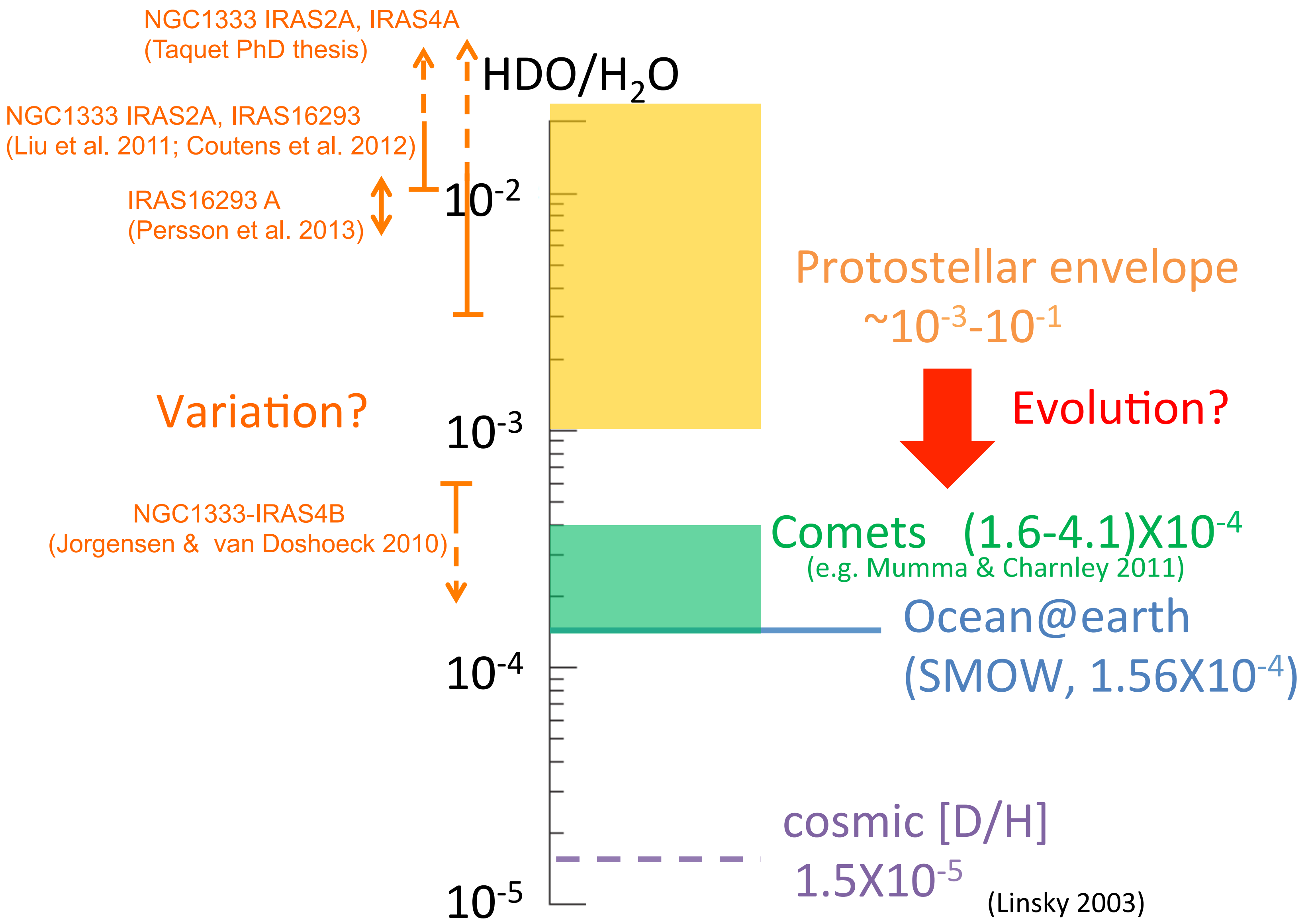
- high H_2D^+/H_3^+

(e.g. Millar, Bennet & Herbst 1989)

- $H_2D^+ + e \rightarrow H_2 + D$ → high atomic D/H



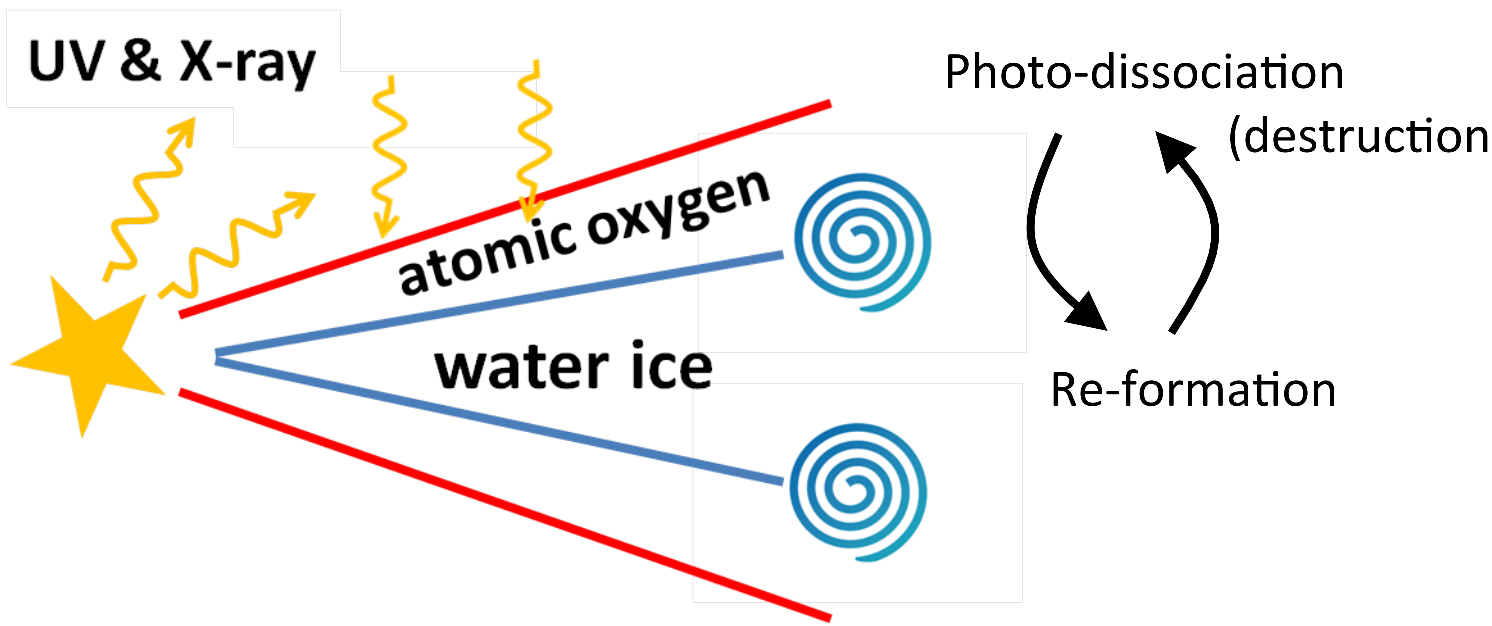
HDO/H_2O in comets and protostellar cores



This Work

- Can water be destroyed and re-formed in disks?
  → Does HDO/H_2O ratio change?

- Effect of vertical mixing by turbulence



(cf. Lyons & Young 2005)

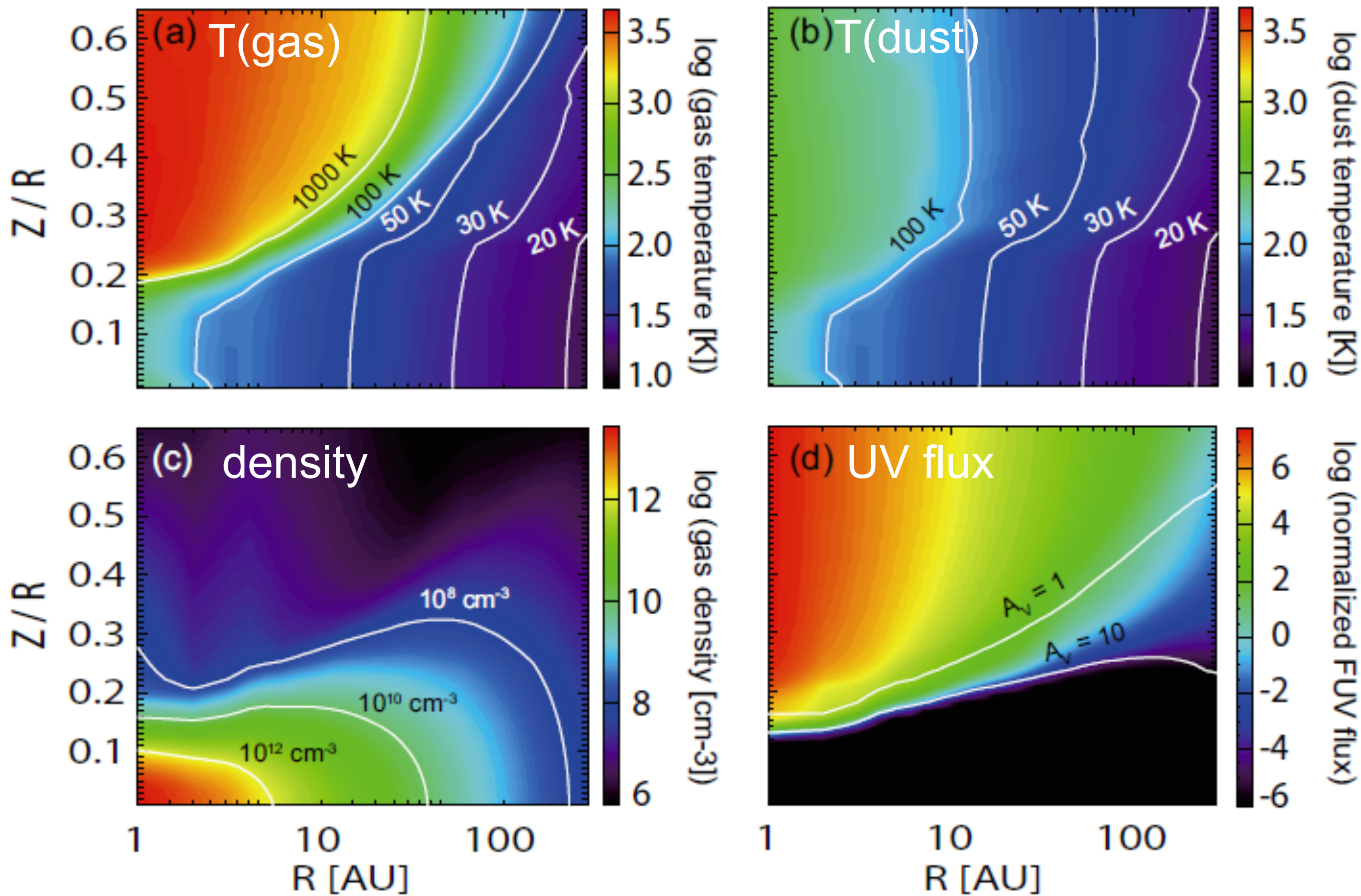
Model

- Disk model (Nomura et al. 2007)
  - Small dust (i.e. large surface area) well-mixed with gas
  - Stellar, interstellar, and induced UV
  - Stellar X-ray

$M_* = 0.5\ M_\odot$

$L_* = 0.87 L_\odot$

$M_\mathrm{d} = 2.4 \times 10^{-2}\ M_\odot$



Model

- Chemical model

  \# Gas – Grain network of Garrod & Herbst (2006)
  + mono- & multi-Deuteration (Aikawa et al. 2012; Talukdar et al. 1996; Bergin et al. 1999; UMIST07)
  + high T reactions (Harada et al. 2010)

  \# Photodesorption & photodissociation of ice
  (Oberg et al. 2007; Andersson & van Dishoeck 2008; Mason et al. 2006)

  - Desorption yield ~10^{-3}
  - Dissociation is allowed only in the surface 2 layers

- Basic equation (e.g. Xie et al. 1995; Willacy et al. 2006)

$$\frac{\partial n_i}{\partial t} - \underbrace{\frac{\partial}{\partial z}\left[n D_z \frac{\partial}{\partial z}\left(\frac{n_i}{n}\right)\right]}_{\text{diffusion(vertical)}} = \underbrace{P_i - L_i}_{\text{Chemistry}}$$

n_i : num density of species i

$D_z = \alpha_z c_s h$: diff coef

grain radius: 0.1μm

α_z = 0, 10^{-3}, 10^{-2}

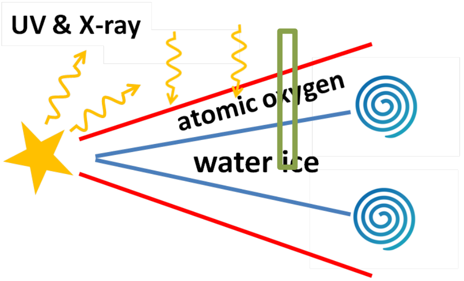


Photo-desorption

Andersson & van Dishoeck (2008)

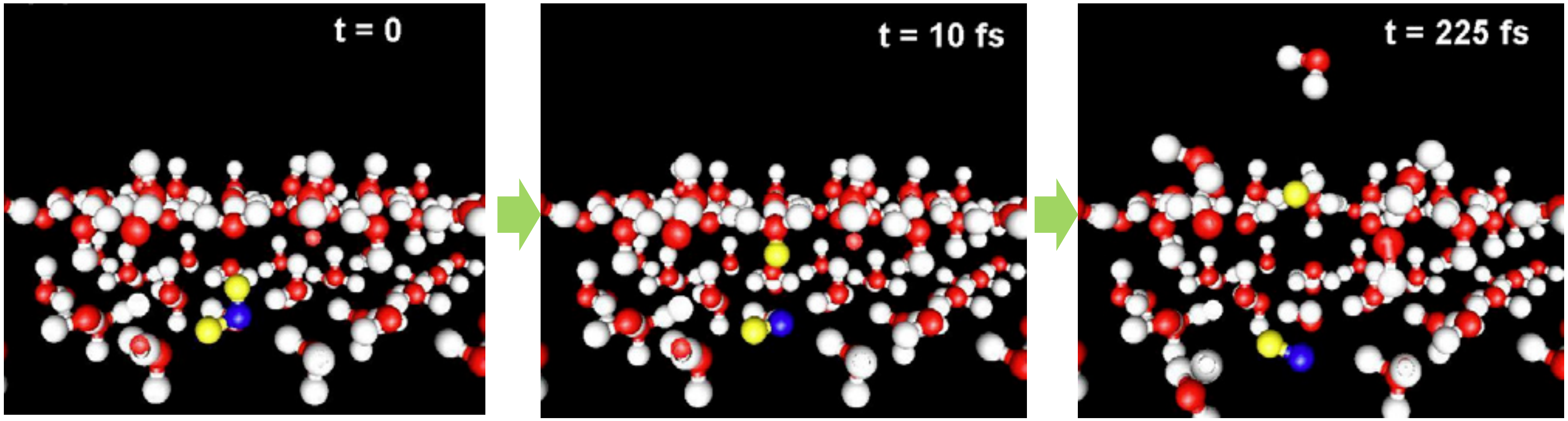
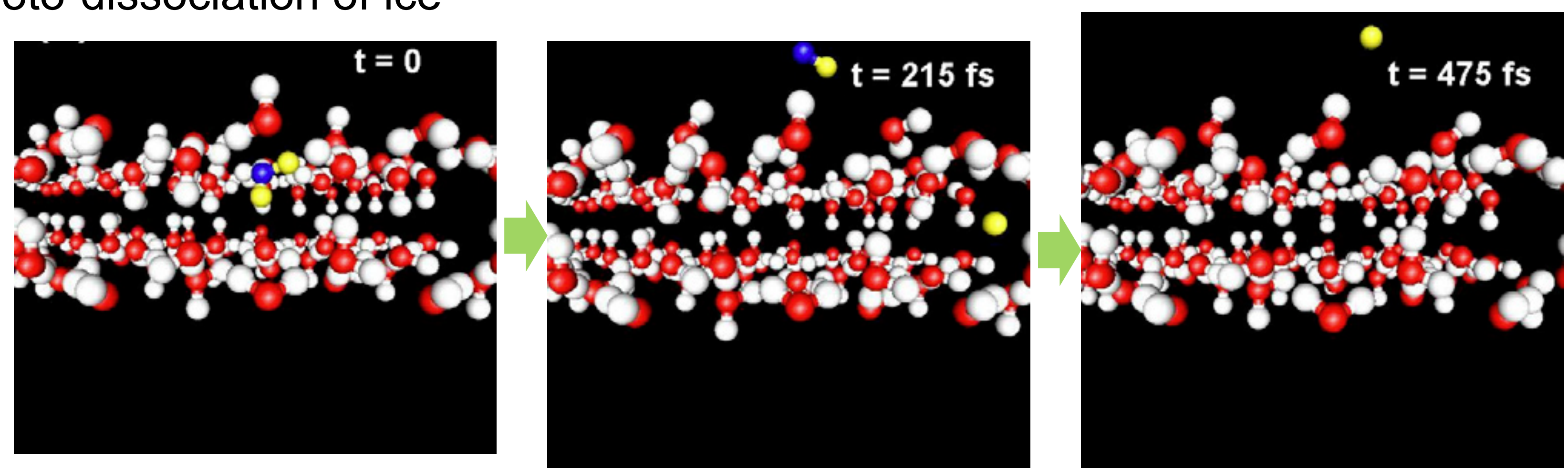
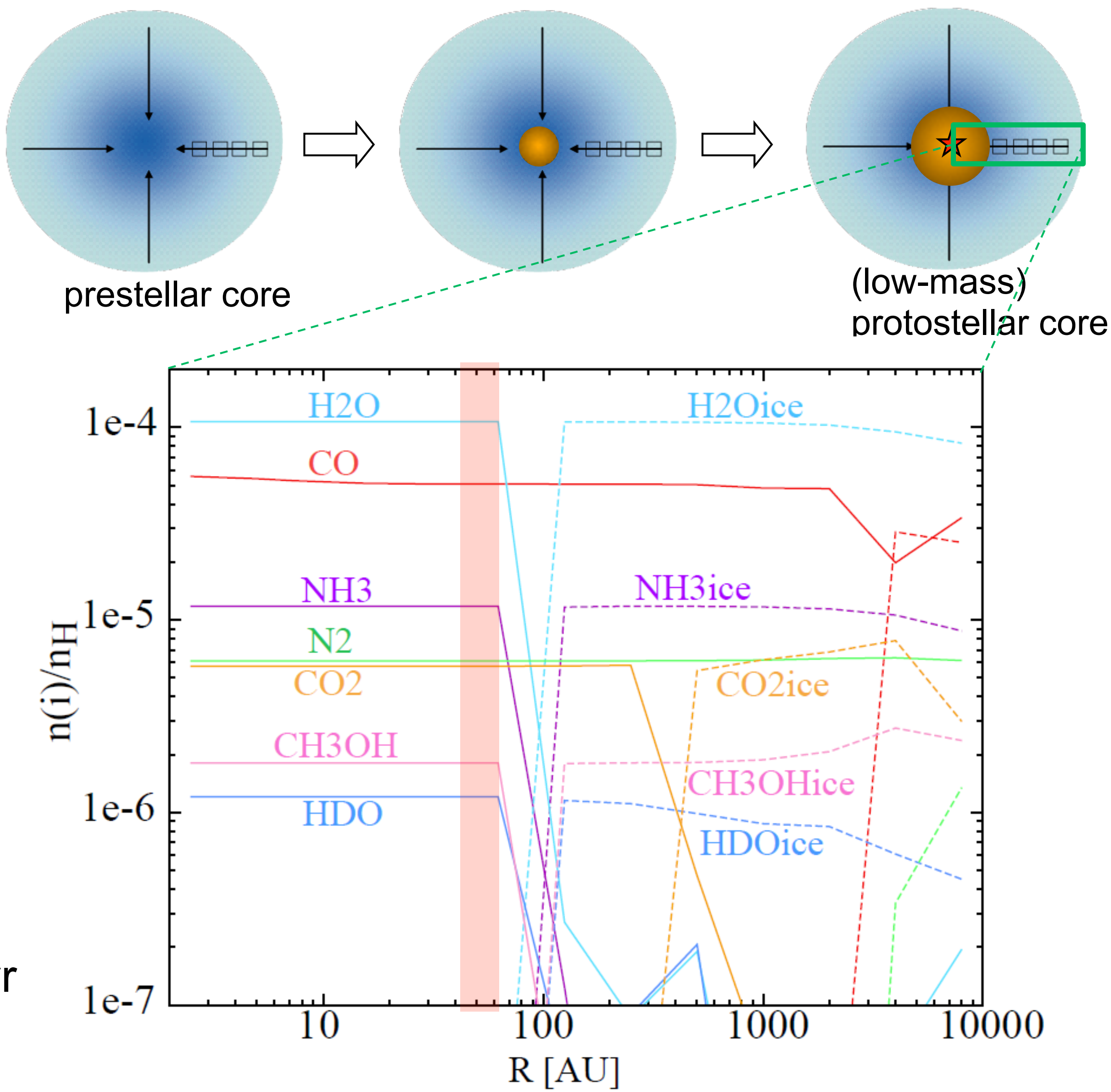


Photo-dissociation of ice



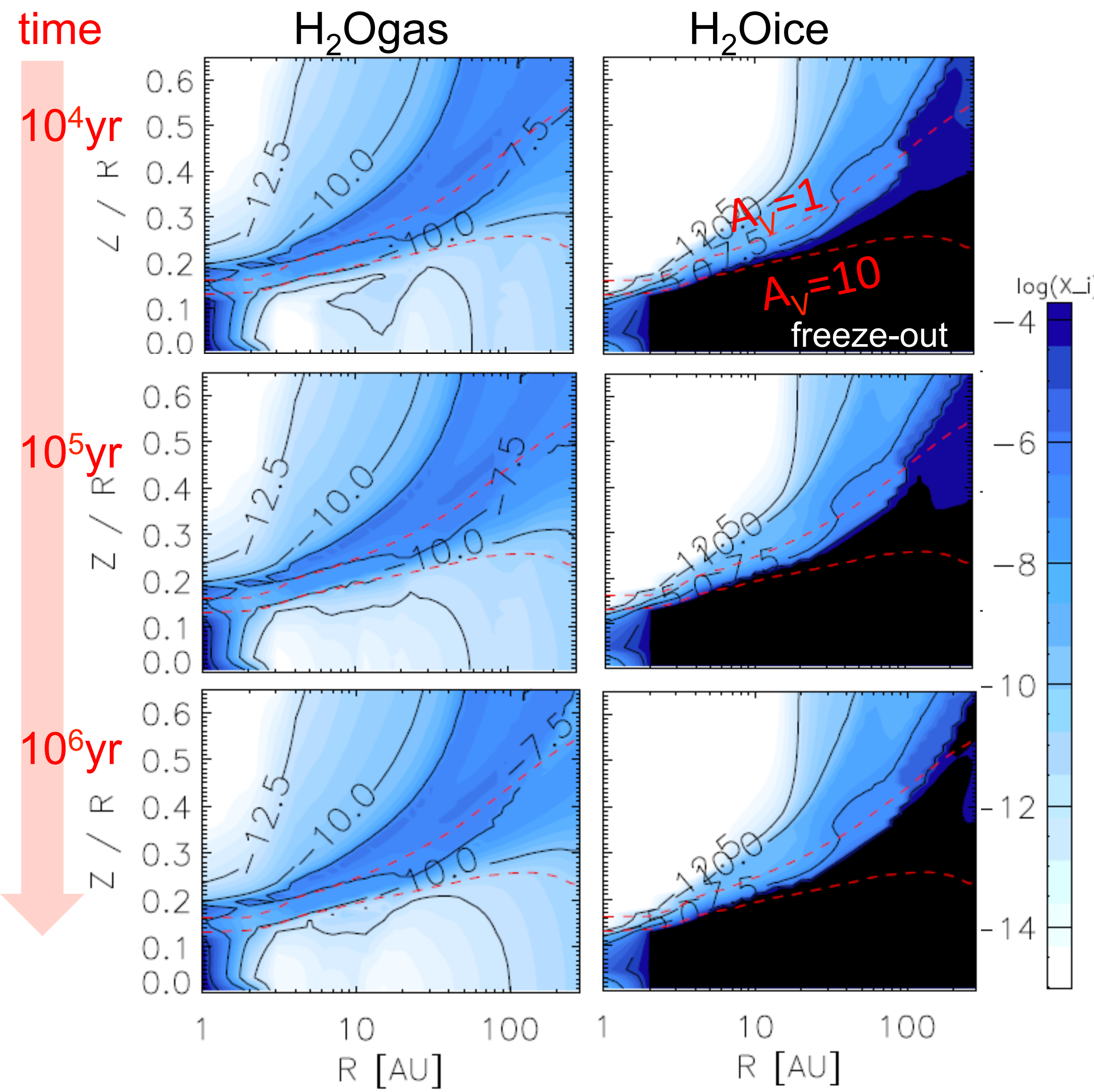
- Initial Abundances
  - Collapsing star-formation core (Aikawa et al. 2012)
  - H_2O is the major O carrier
  - $HDO/H_2O \sim 10^{-2}$

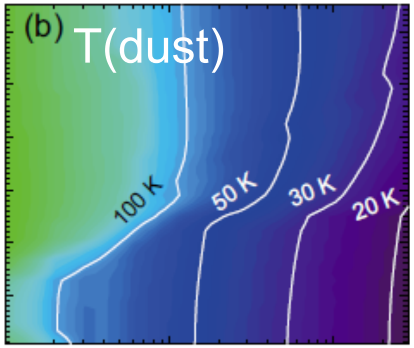


@9.3x10^4 yr

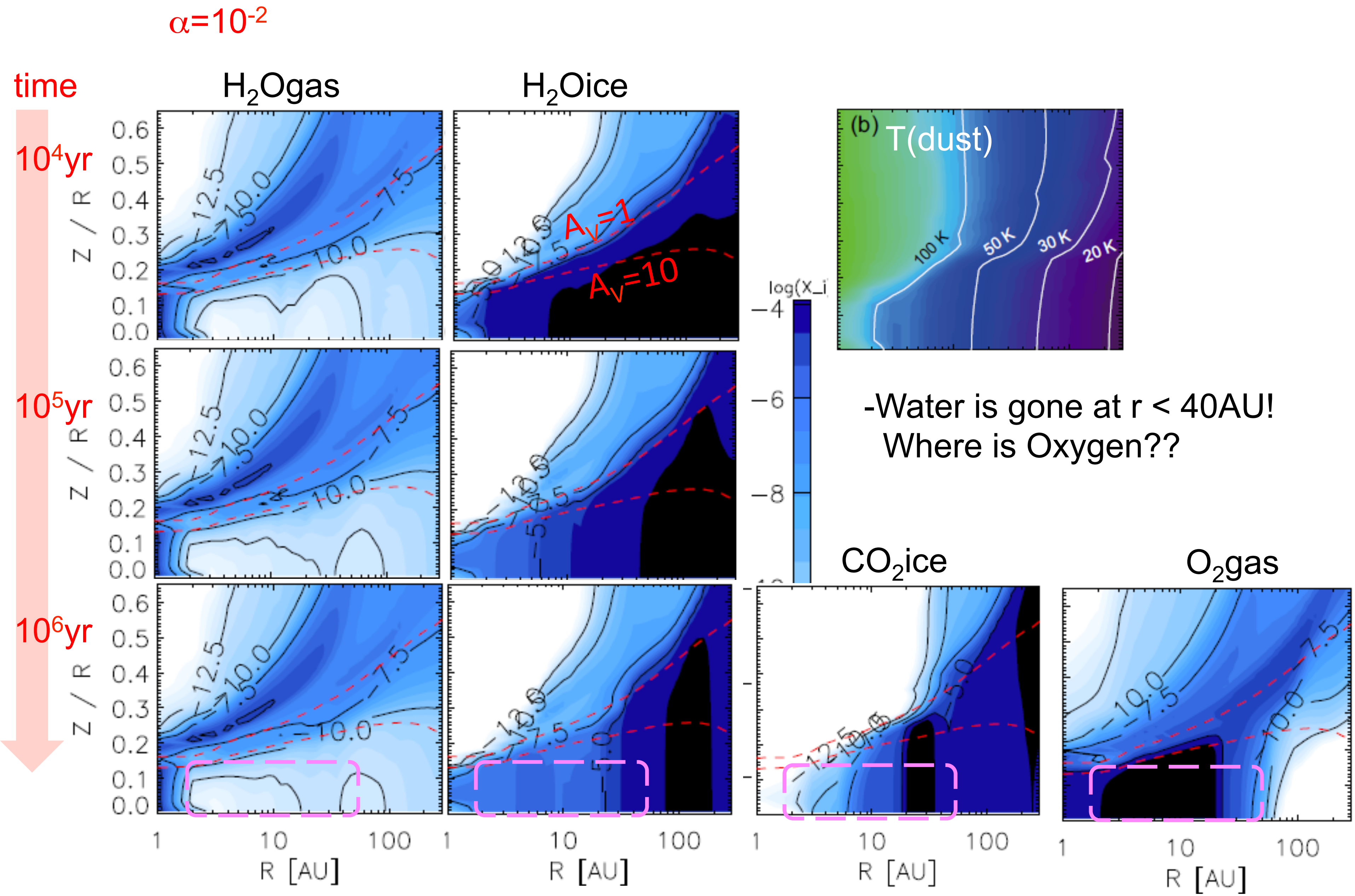
Result: H_2O abundances

α=0: no diffusion





Result: H_2O abundances

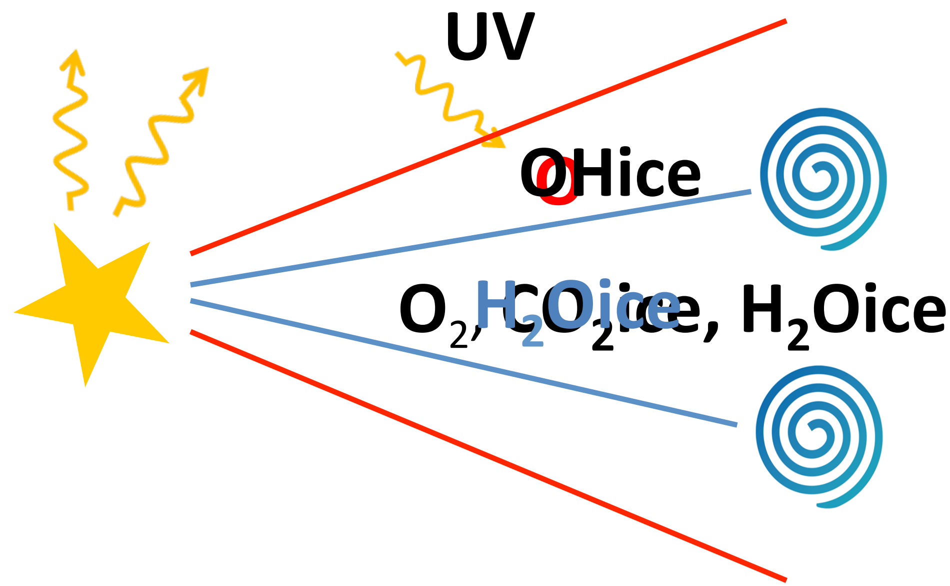


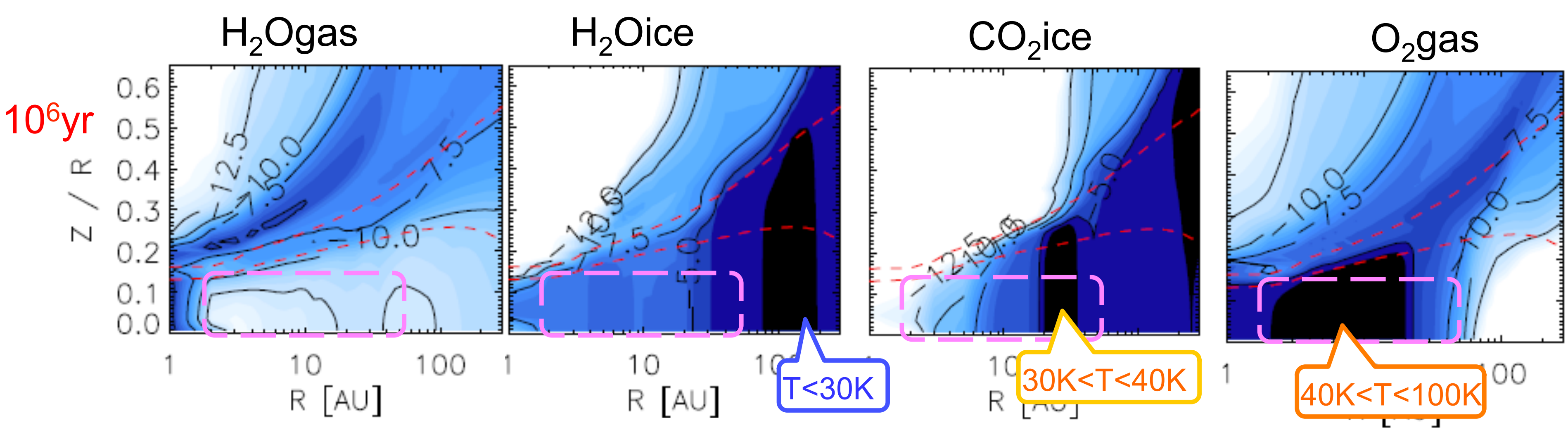
-Water is gone at r < 40AU!
Where is Oxygen??

Result: Oxygen chemistry

- H_2Oice
  Transported to disk surface
  → photodissociation

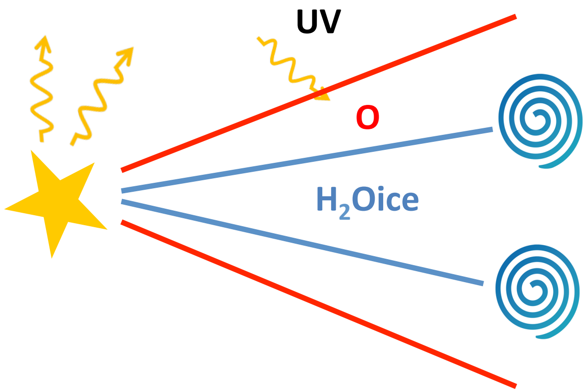
- O atom
  Transported to deeper layers
  @ T_d <30K
  H_2O ice is re-formed
  @ T_d >30K
  H_2O formation is inefficient
  → O is converted to O_2 & CO_2ice

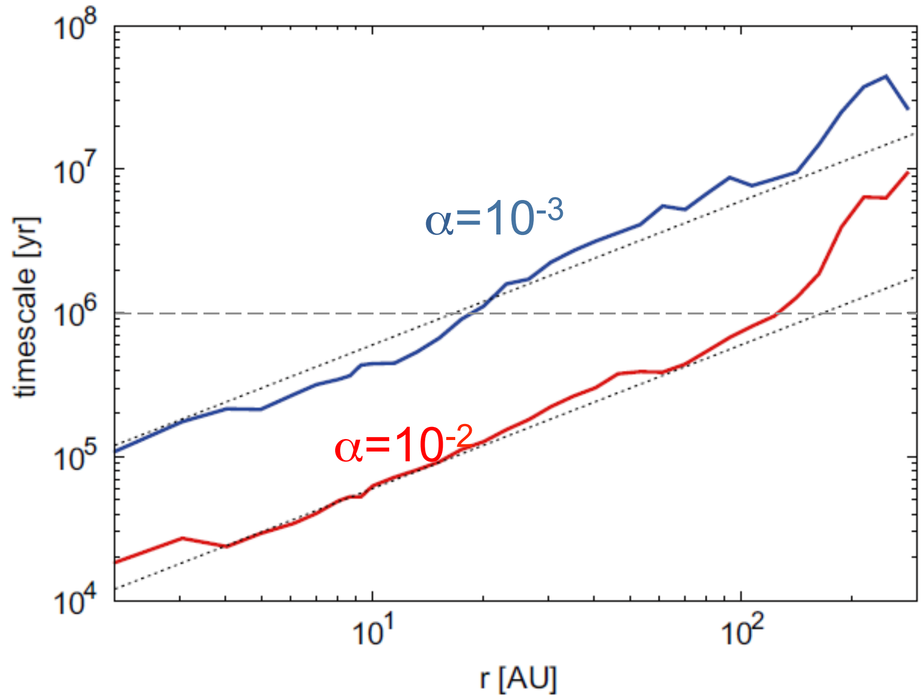


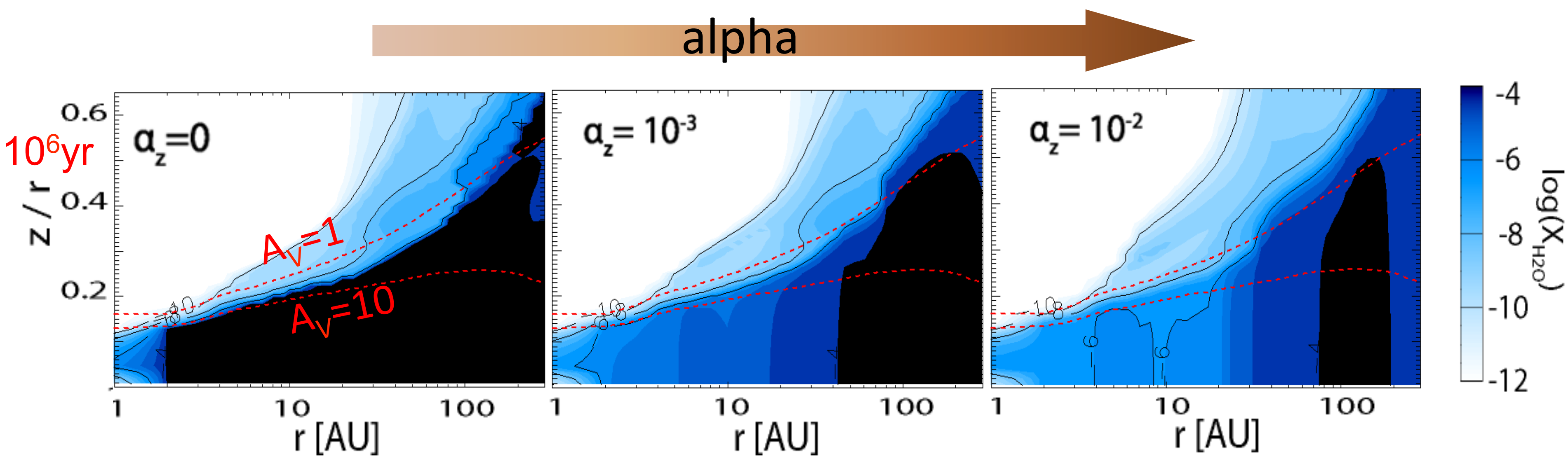


Result: Timescale of H_2O destruction

$$\tau \approx \frac{N_{\mathrm{H2Oice}}}{\text{flux @ H}_2\text{O - Oatom boundary}} \propto r$$







Result: HDO/H_2O ratio

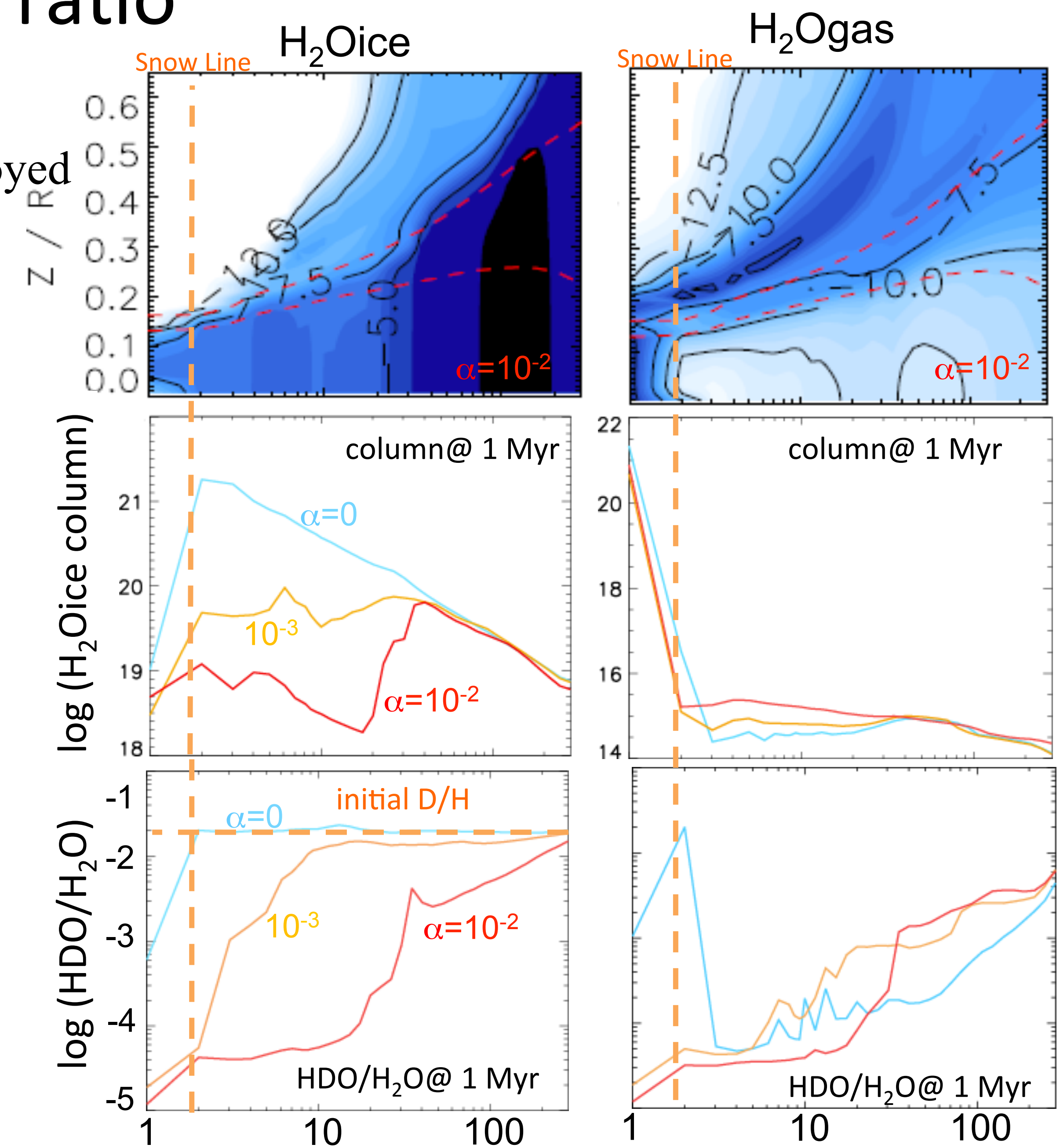
- HDO/H_2O ice ratio decreases ONLY when H_2O ice is destroyed significantly

- H_2O gas is abundant at
  - disk surface
  - inside snow line

- $\left(\frac{HDO}{H_2O}\right)_{gas} < \left(\frac{HDO}{H_2O}\right)_{ice}$

←Reformation in gas phase

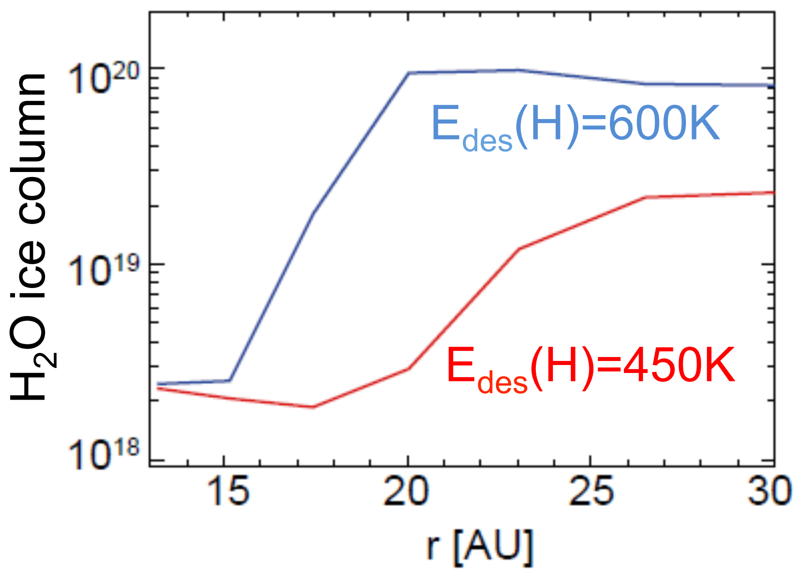
(see also Willacy & Woods 2009)

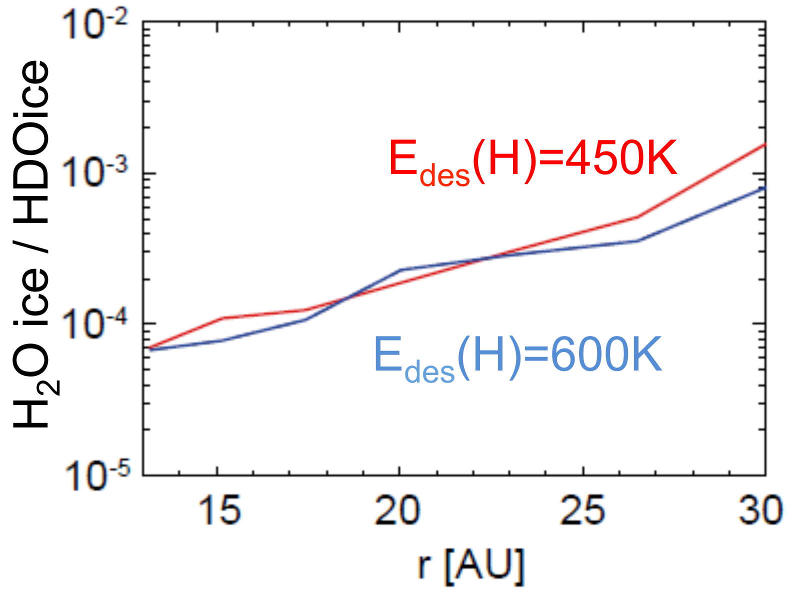


Discussion: Dependence on E_{des}(H)

- H_2O reformation is inefficient, because H atom is easily desorbed
  So far, we assumed E_{des}(H)=450K

- E_{des}(H) ~ 600 K on amorphous ice
  (Al-Halabi & van Dishoeck 2007; Watanabe et al 2010; Hama et al. 2012)
  → H_2O can be reformed at <u>higher temperature</u>!
  → Abundant H_2O ice with low D/H ratio ~10^{-4}





Summary on H_2O & Implications

- H_2O ice is photo-desorbed & dissociated at disk surface and
  - reformed at T< ~~30K~~ 40K
    - $HDO/H_2O \sim$ ~~10^{-3}-10^{-2}~~ 10^{-4}-10^{-3} — if $E_{des}(H)$=600K
  - converted to CO_2 at 30K < T <40K
  - converted to O_2 at 40K < T < 100K

→ Sedimentation of large grains (while small grains are stirred up) will protect H_2Oice. (cf. Hogerheijde et al. 2011)

→ But then $(HDO/H_2O)_{ice}$ does not change

- $HDO/H_2O \sim 10^{-4}$ in comets could be set in turbulent disk

- $(HDO/H_2O)_{gas} \sim 10^{-4}$-$10^{-3}$

$$\left(\frac{HDO}{H_2O}\right)_{gas} < \left(\frac{HDO}{H_2O}\right)_{ice}$$

cf. $(HDO/H_2O)_{gas} = 6\times10^{-4}$ @NGC1333 IRAS4B (Jorgensen & van Dishoeck 2010)