# Physical and Chemical Evolution of Hydrides in Protoplanetary Disks

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The Hydride Toolbox,
*Universite Pierre et Marie Curie*
Paris, France December 15, 2016

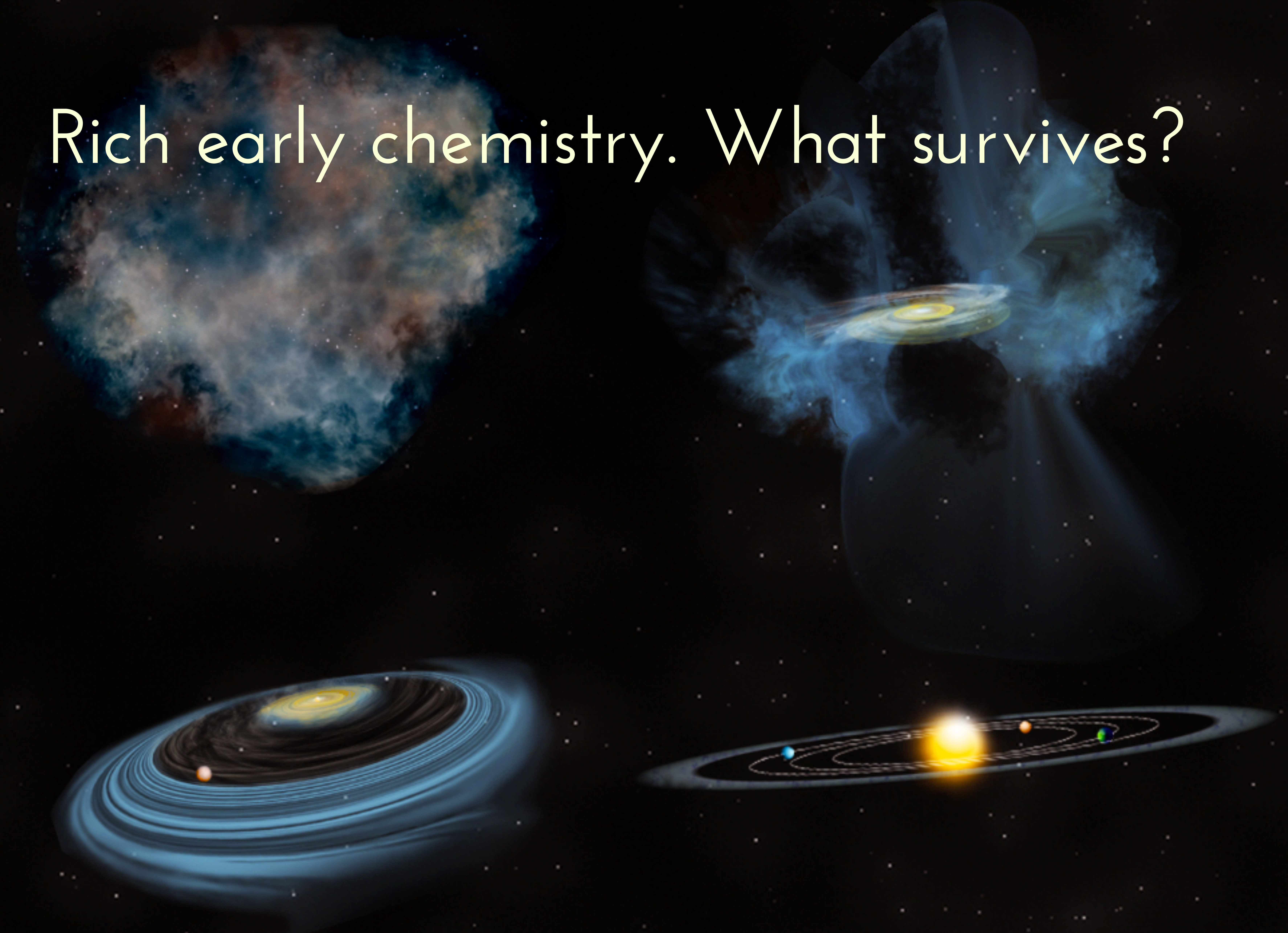
## Hydrides are a starting point of prebiotic chemistry

Laboratory irradiation of “astrophysically large” molecules in a $NH_3$ and $H_2O$ mixture has been shown to form biologically interesting molecules including cytosine, urea, and glycine (e.g., Nuevo, Milam et al. 2013).

## Hydrides provide insight into key question of inheritance vs. reprocessing during star formation

High binding energies result in key hydrides ($NH_3$ and $H_2O$) being largely in the ice phase under dense ISM conditions. Sensitive to extreme energetic events, like forming a star!

# Rich early chemistry. What survives?



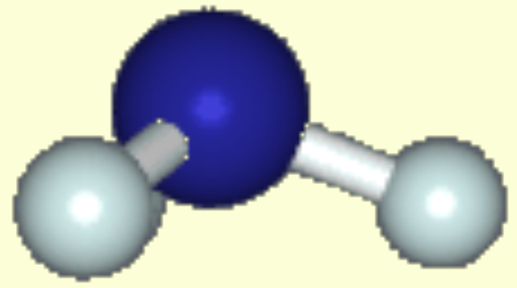
Credit: Bill Paxton modified by I. Cleeves

# Detected Disk Hydrides

## $CH_4$

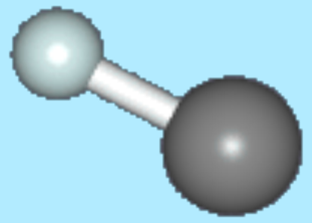
One source, GV Tau N (Gibb et al. 2013)

## $NH_3$



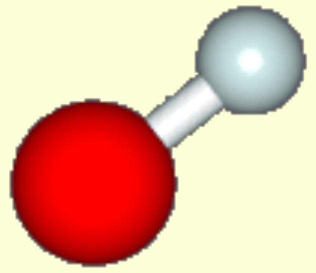
One source, TW Hya (Salinas et al. 2016)

## $CH^+$



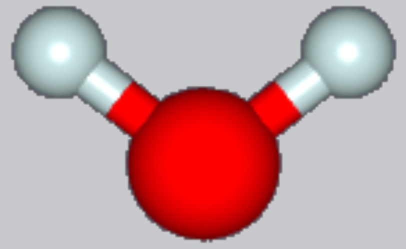
One source, HD 100546 (Thi et al. 2011)

## OH

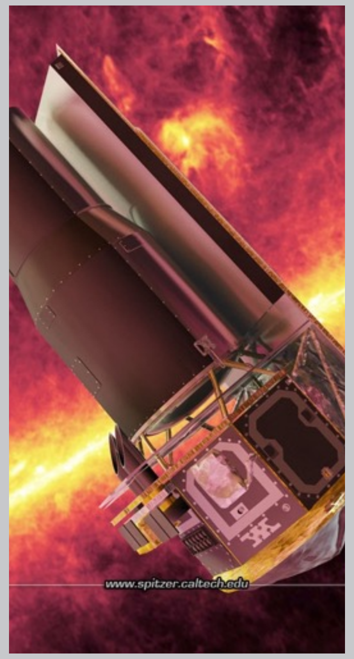


*Herschel:* Sturm et al. 2010, Fedele et al. 2012, Bergin, et al. 2013,
*Spitzer:* e.g., Pontoppidan et al. 2010
*Ground:* Mandel+08, Lisowsky+12

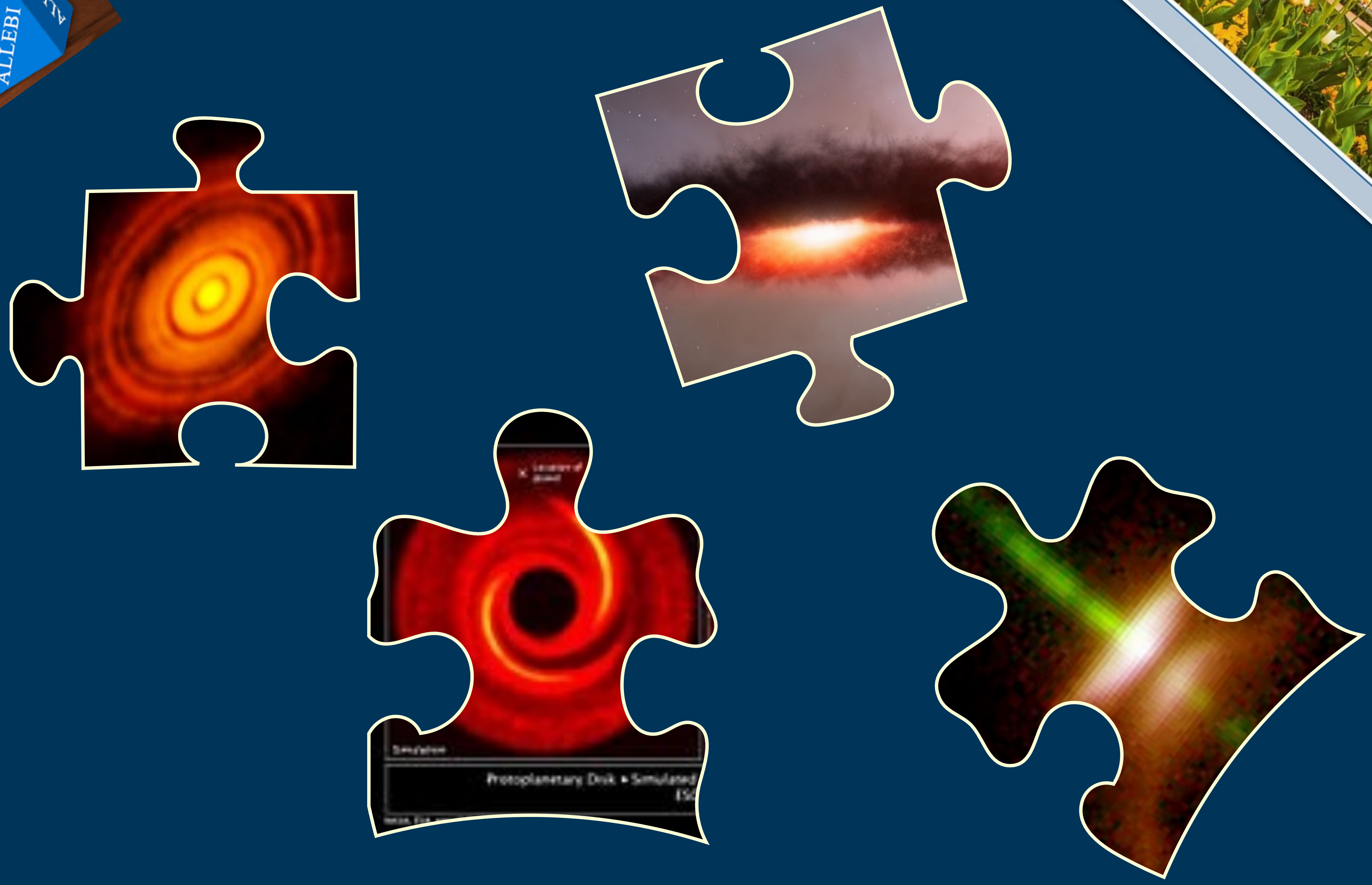
## $H_2O$



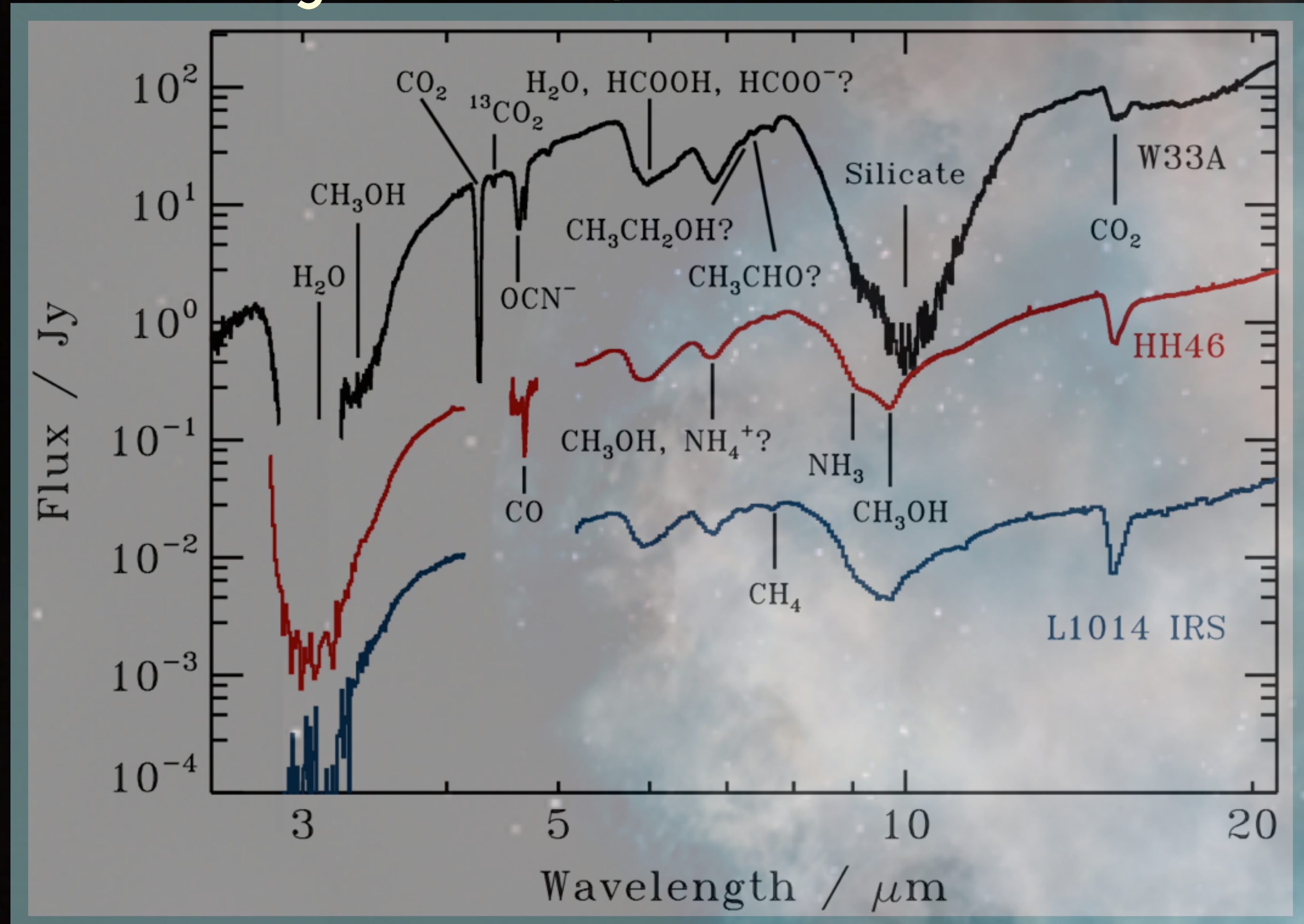
Pontoppidan+10, +11, Bergin+10, Sturm+10, Hogerheijde+11, Du+16, Fedele+12, Banzatti+16
Hot $H_2O$: Sample ~ 120 disks, 60-80% detection
Cold (<100 K) $H_2O$: ~15%



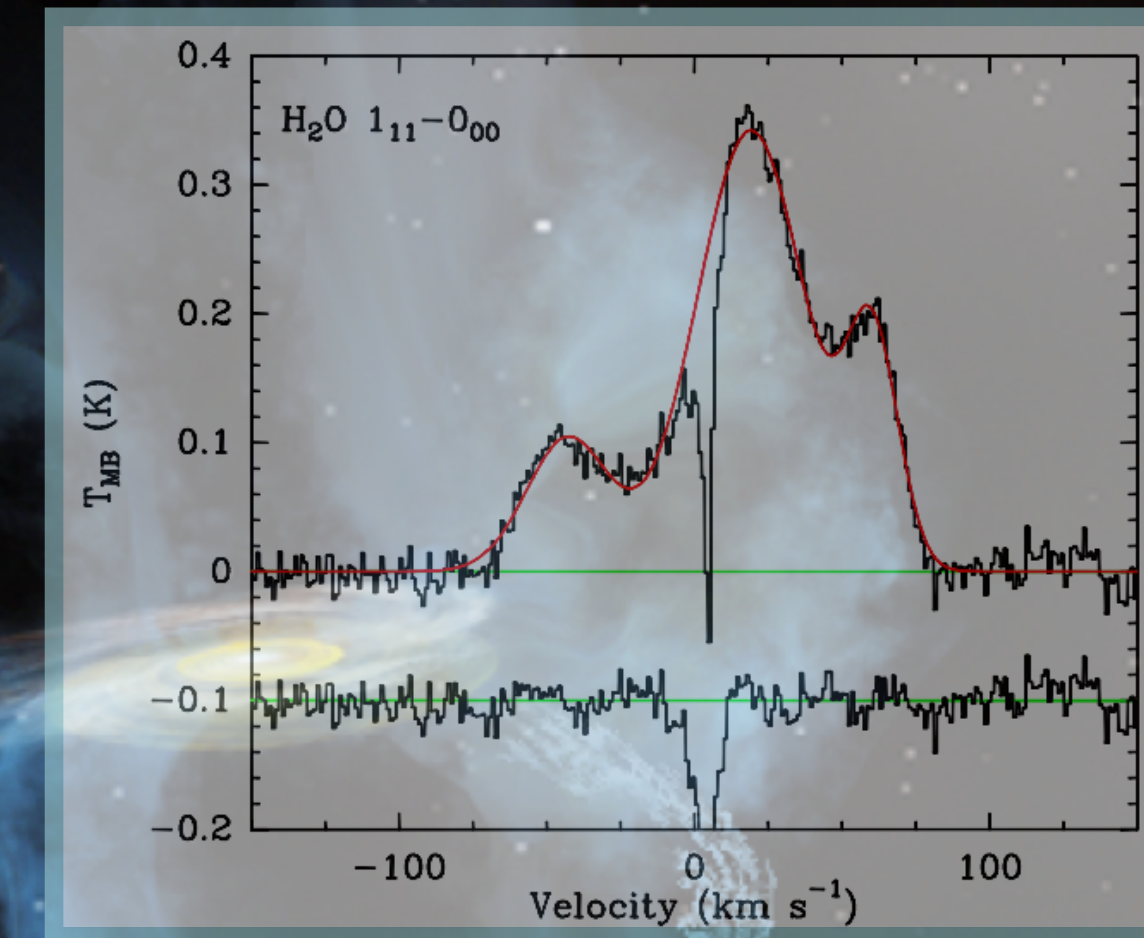
# Measuring pieces of the puzzle, but from all different boxes.

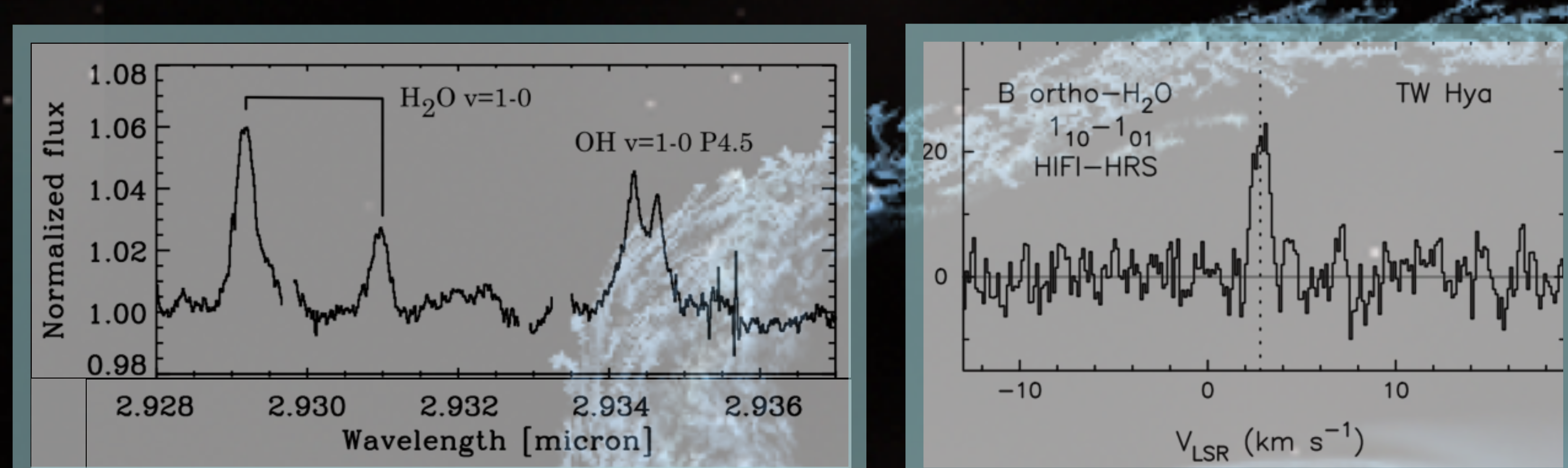



*Ice:* Öberg et al 2011, *Gas:* Caselli et al. 2012

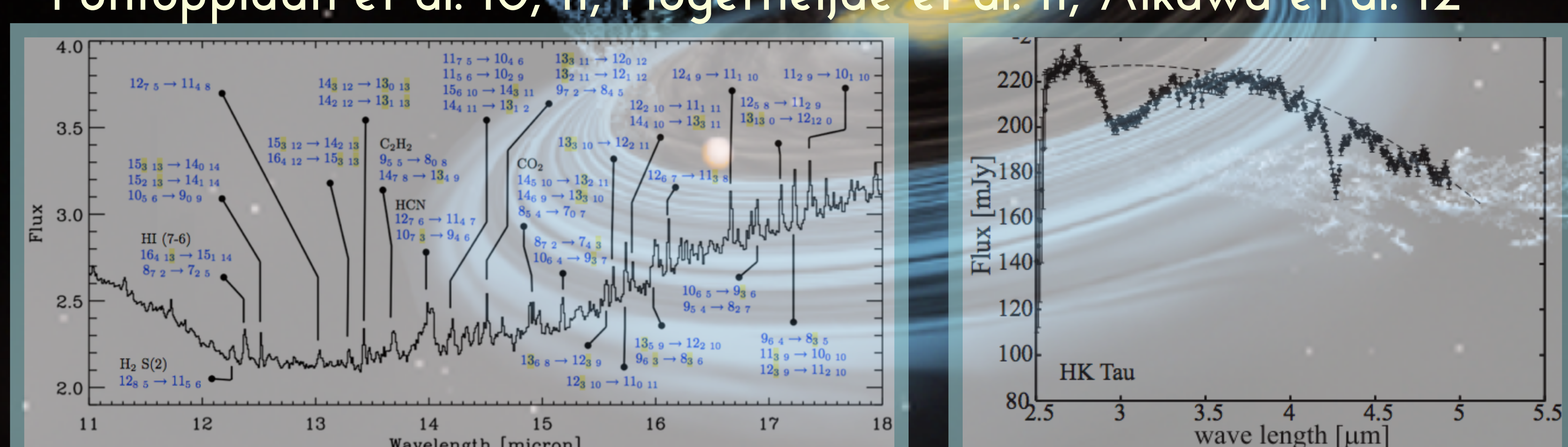



Kristensen et al. 2011 (and many others)



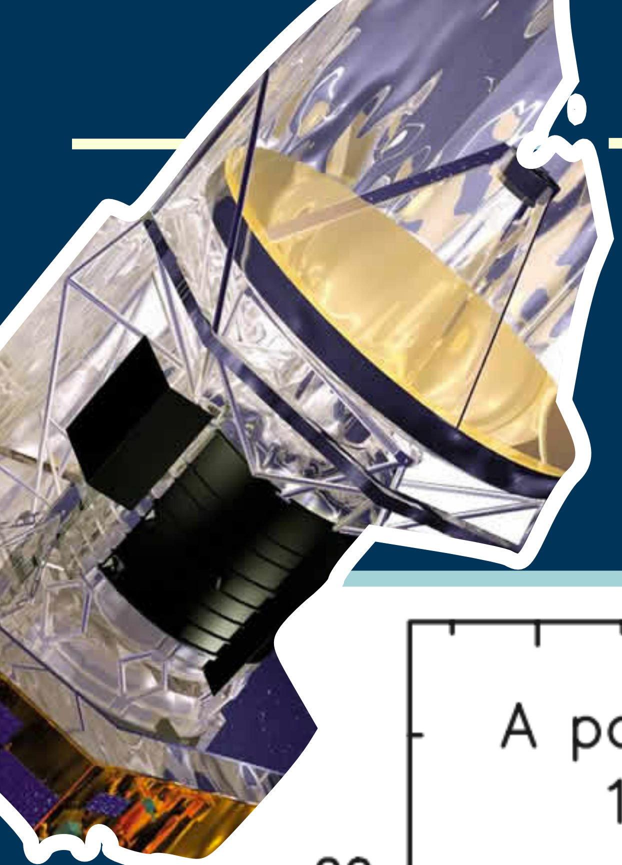



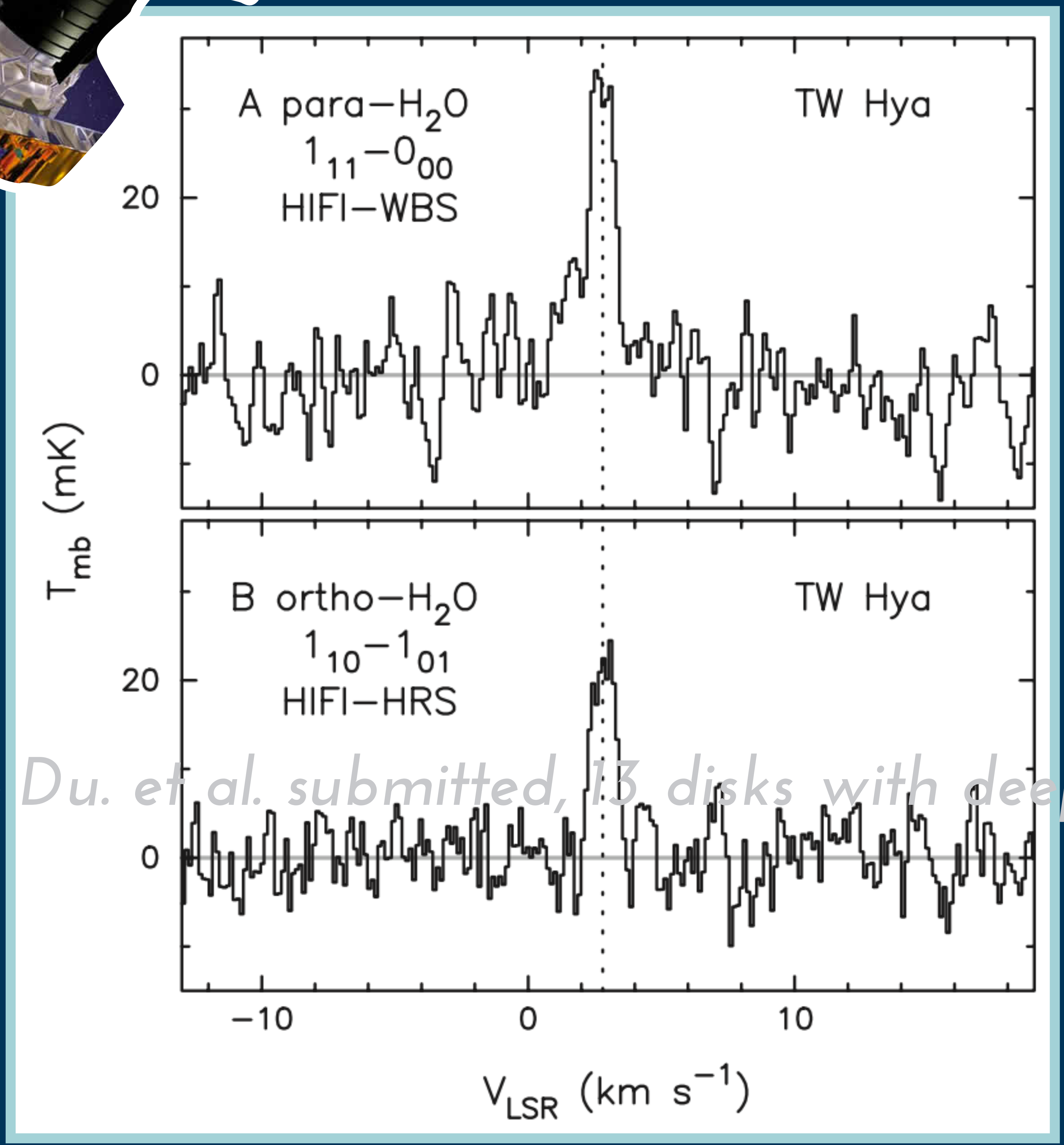

Pontoppidan et al. 10, 11, Hogerheijde et al. 11, Aikawa et al. 12




Biver et al. 2015

# Cold Water in Protoplanetary Disks

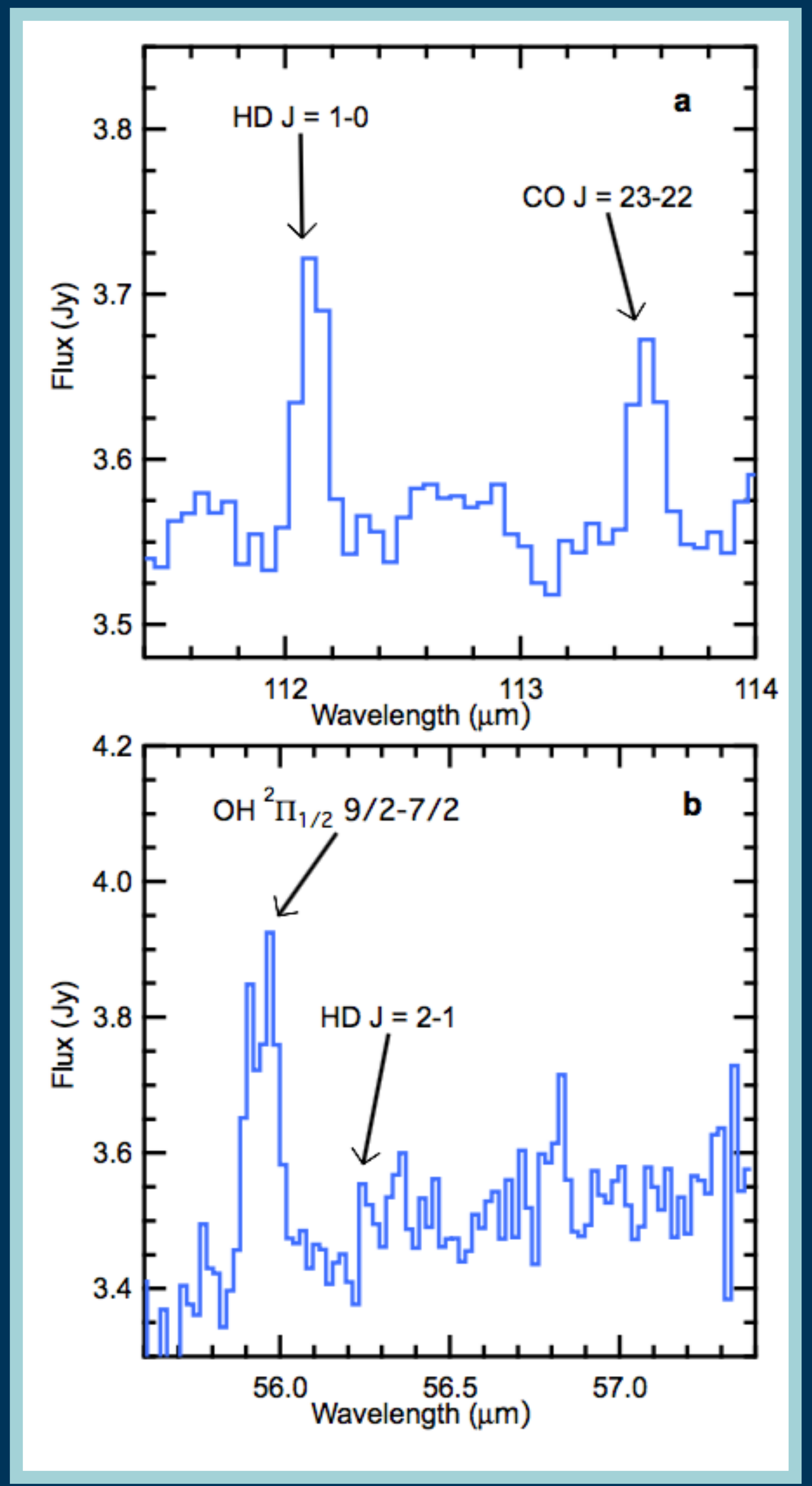





Cold water detected with *Herschel* (and opr), Hogerheijde et al. 2011.

also Du. et al. submitted, 13 disks with deep integrations, non-detections!

HD detected with *Herschel*, Bergin et al. 2013. Mass unambiguous, water depleted.



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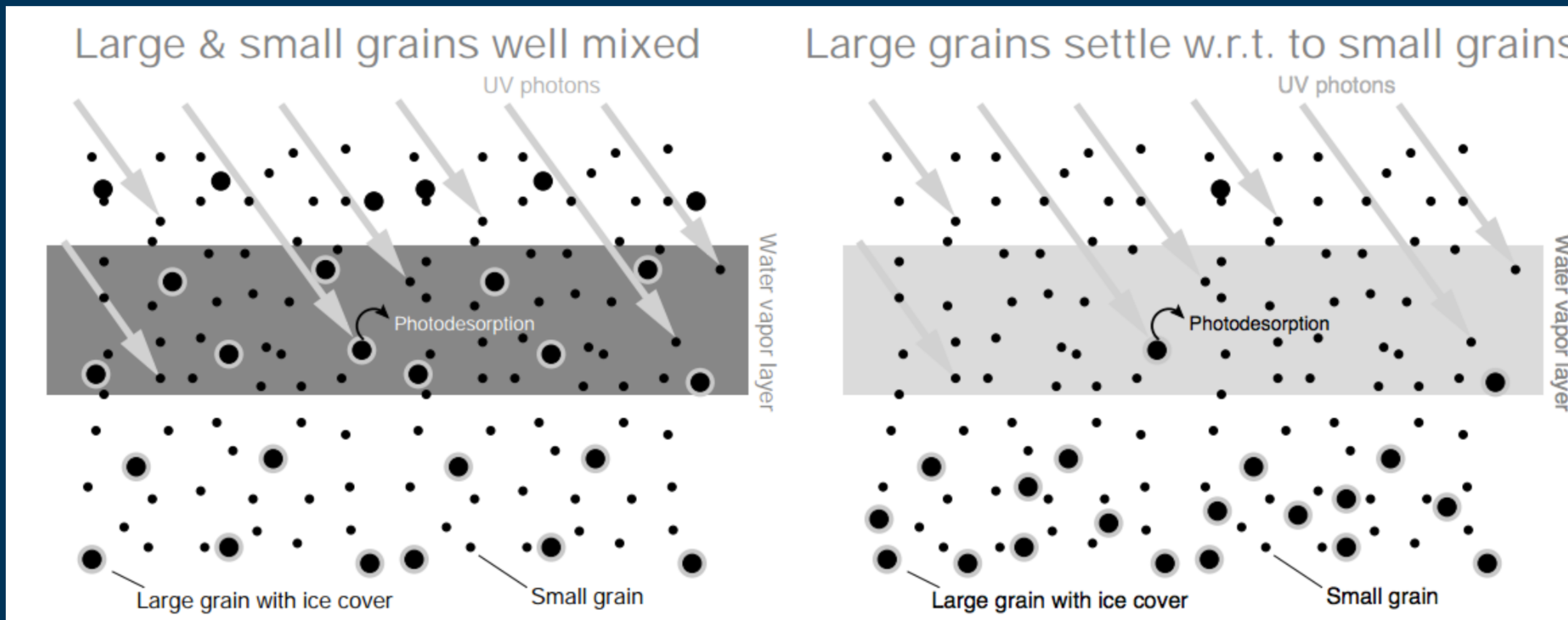
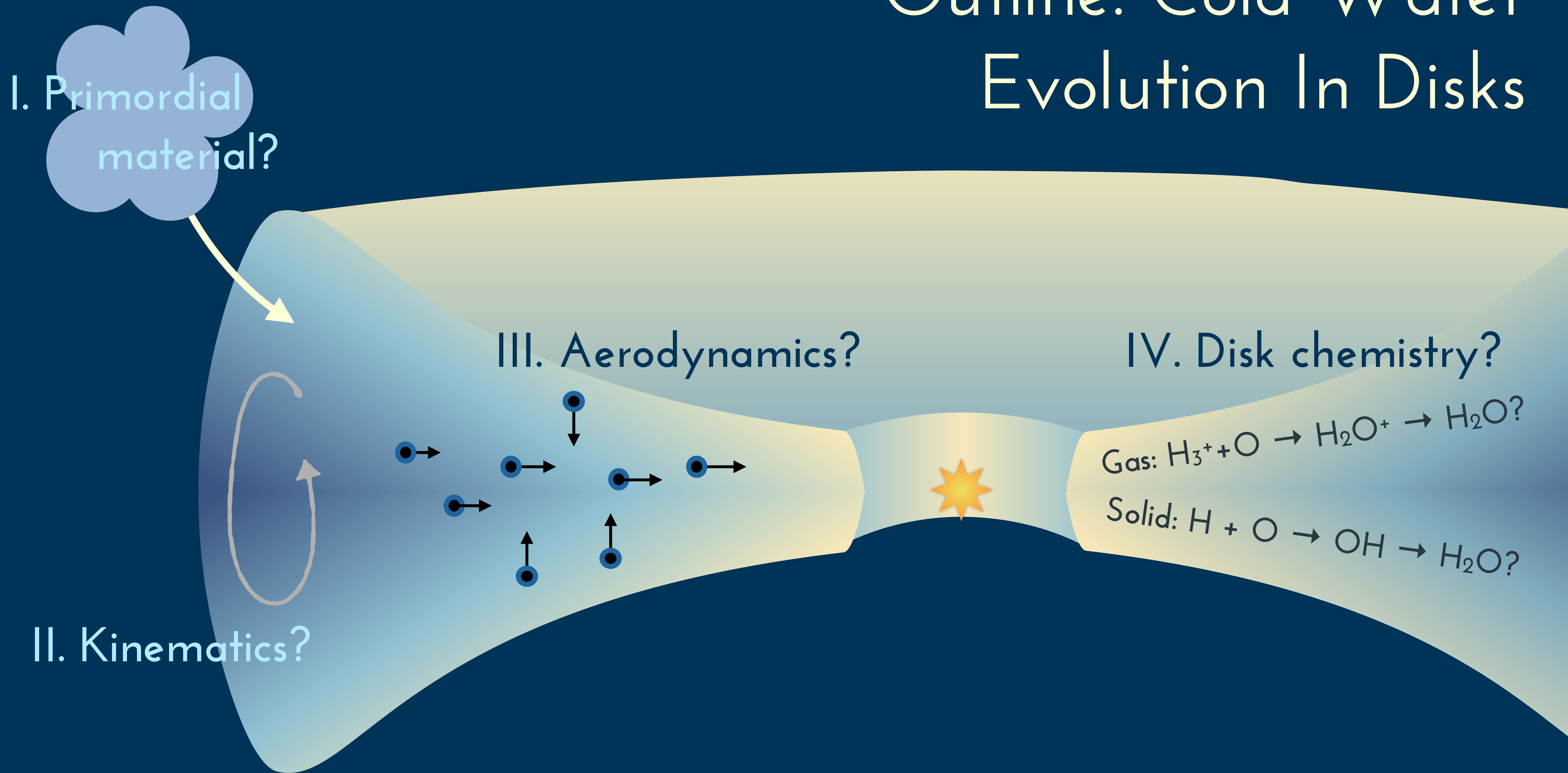
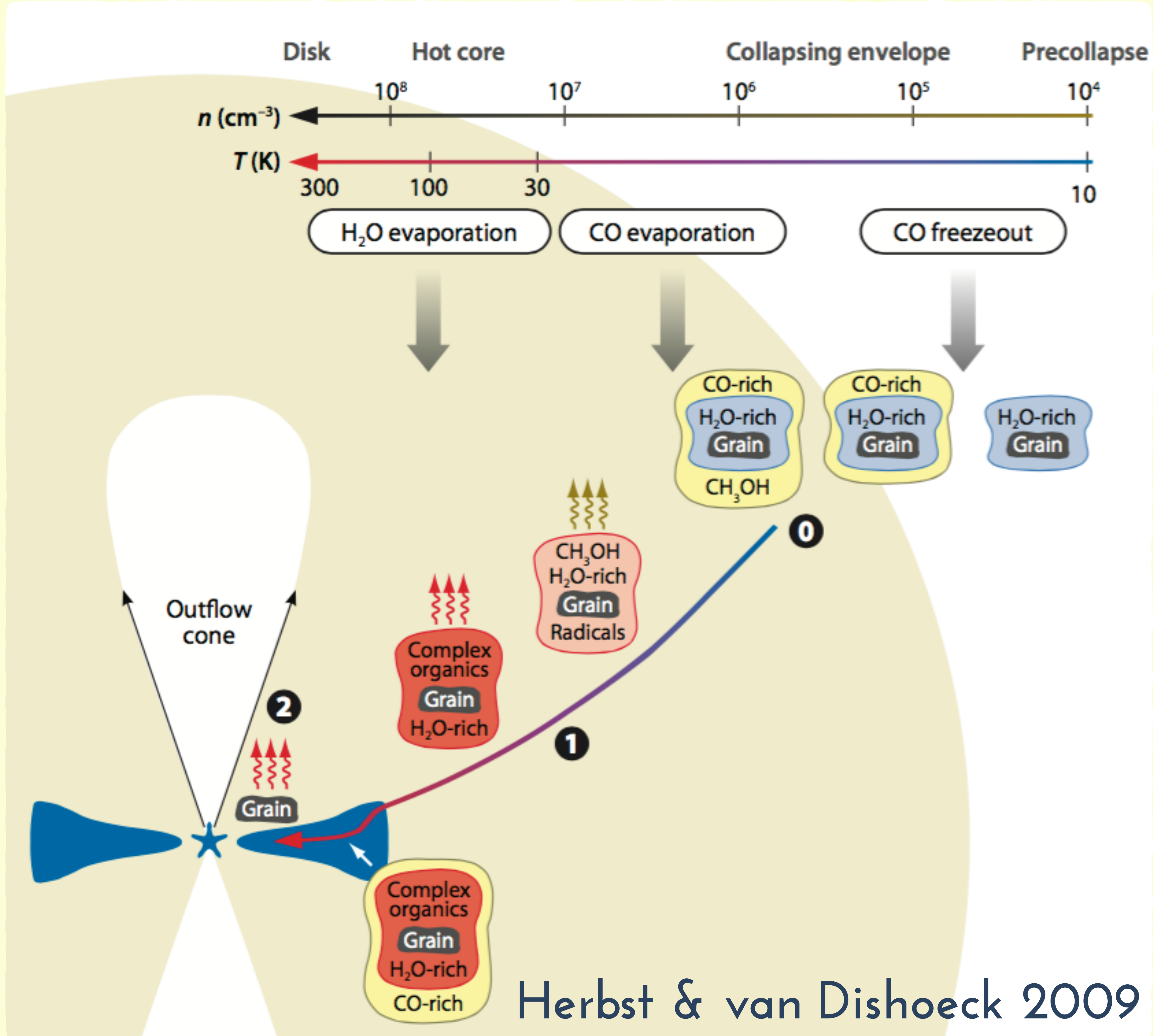



Fig. courtesy M. Hogerheijde

# Outline: Cold Water Evolution In Disks



# 1) What are the initial disk chemical conditions?




Herbst & van Dishoeck 2009

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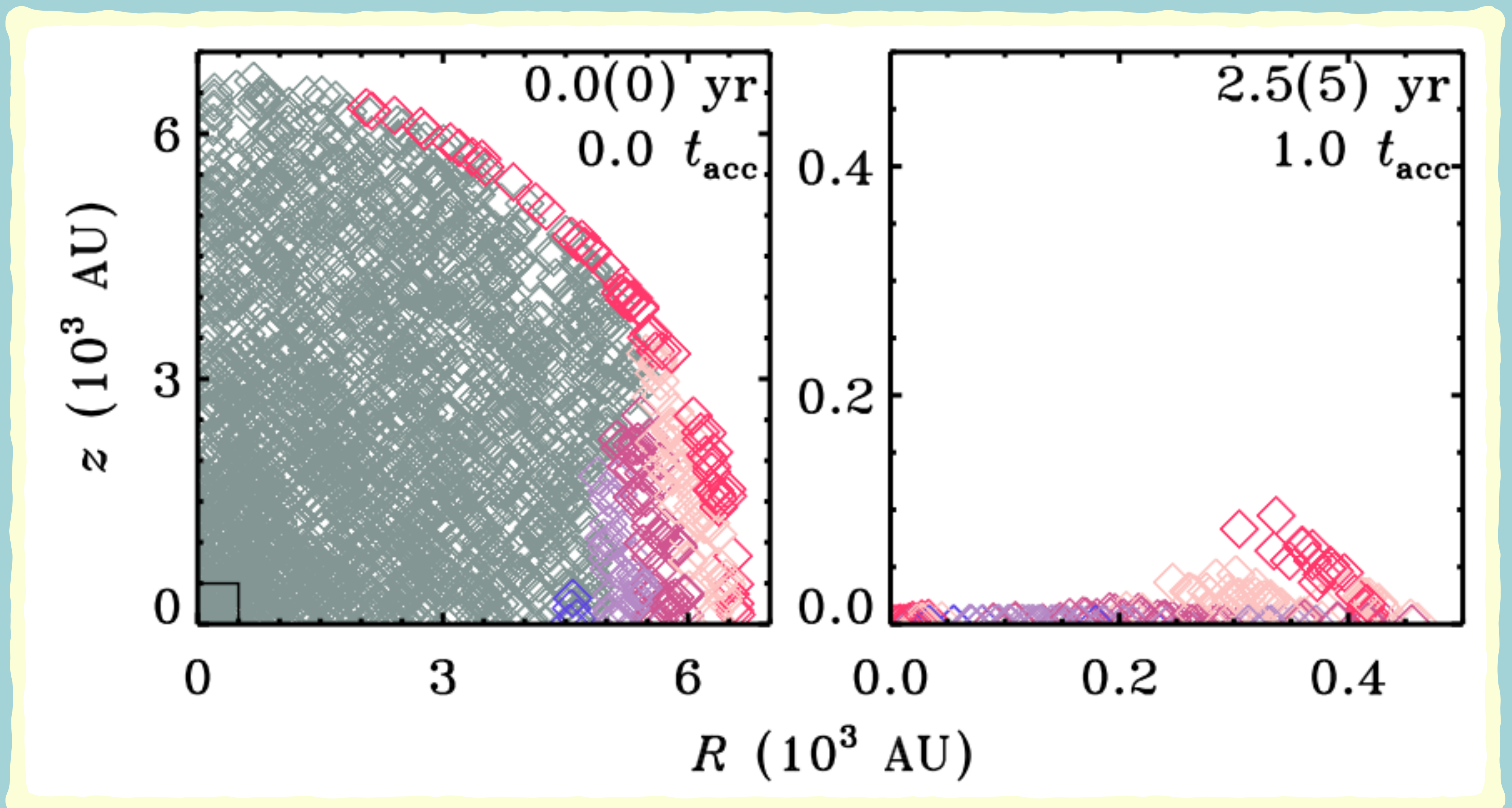
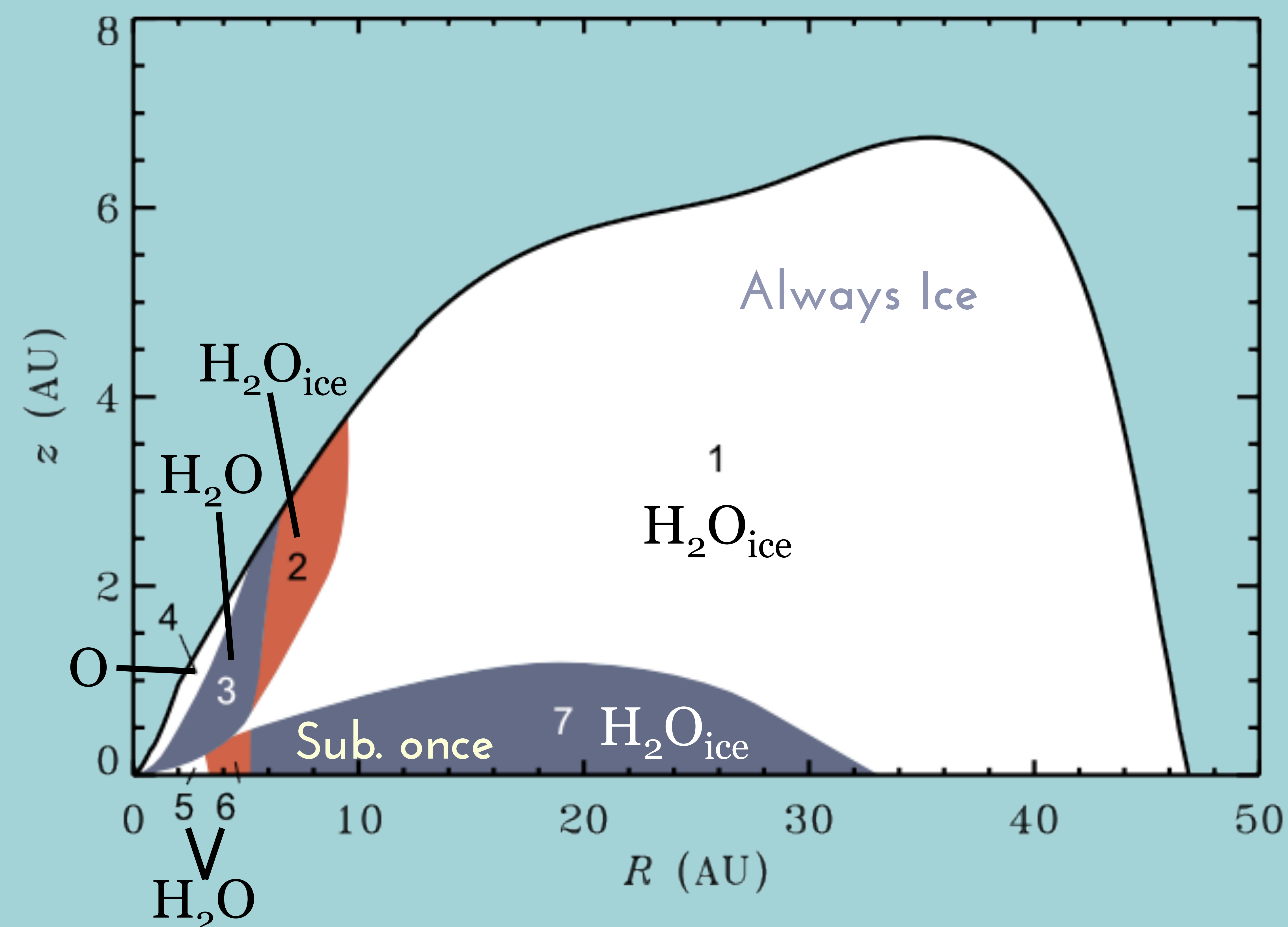
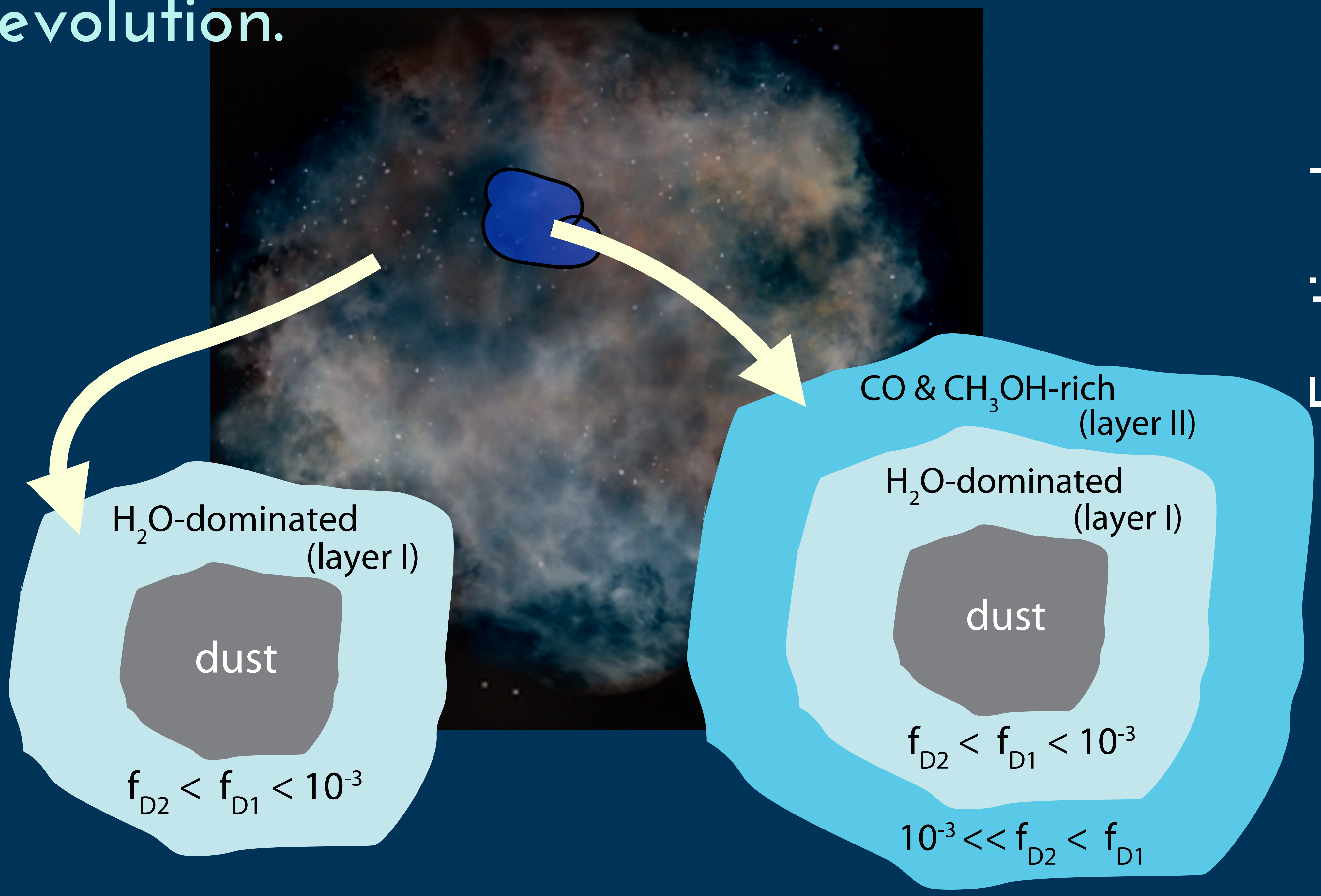


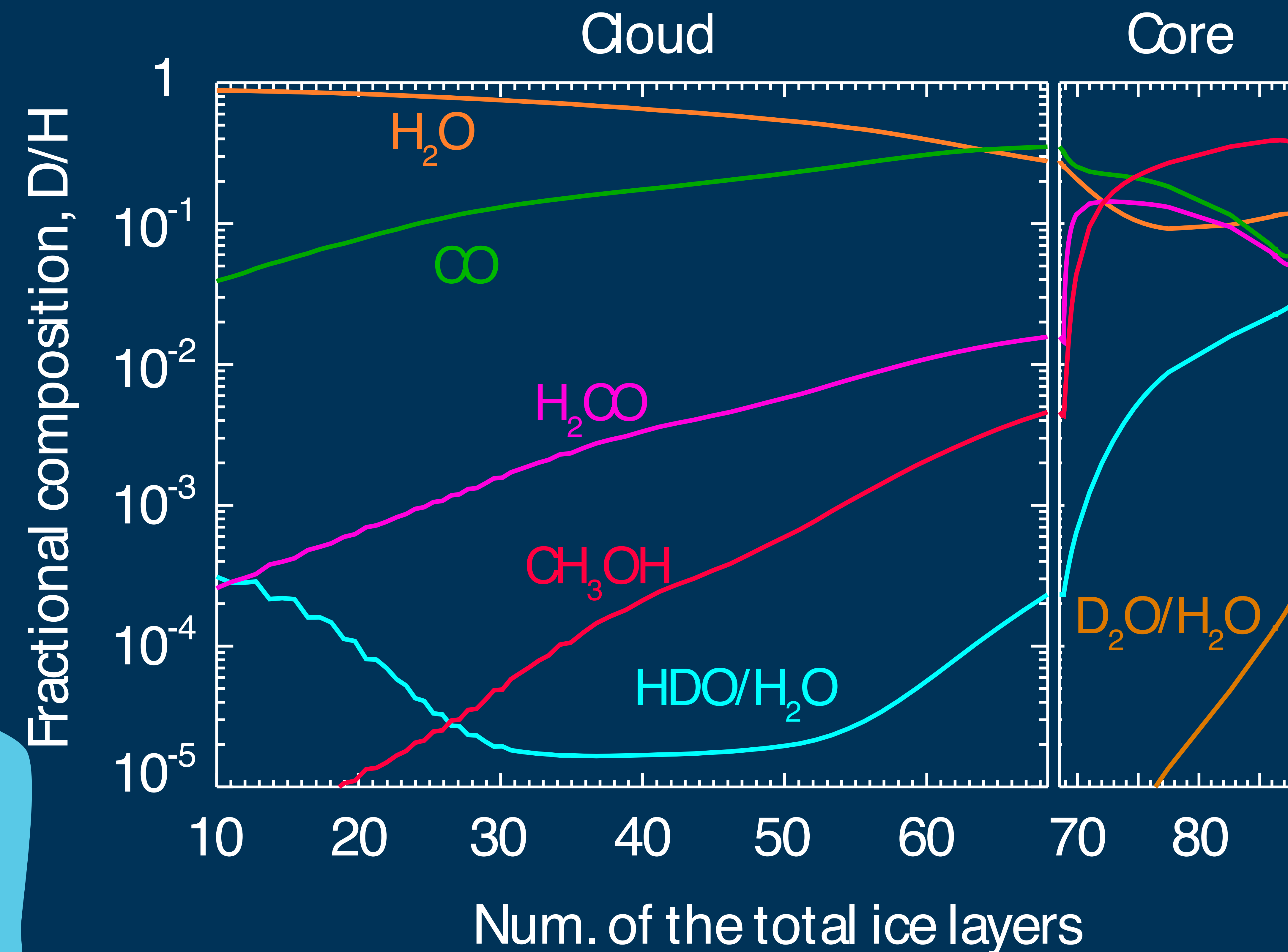

Visser, van Dishoeck, Doty & Dullemond 2009



# 1) What are the initial disk chemical conditions?

By modeling $D_2O/HDO$, $HDO/H_2O$ and using layered ice model the Furuya +2015 models can explain water's early evolution.



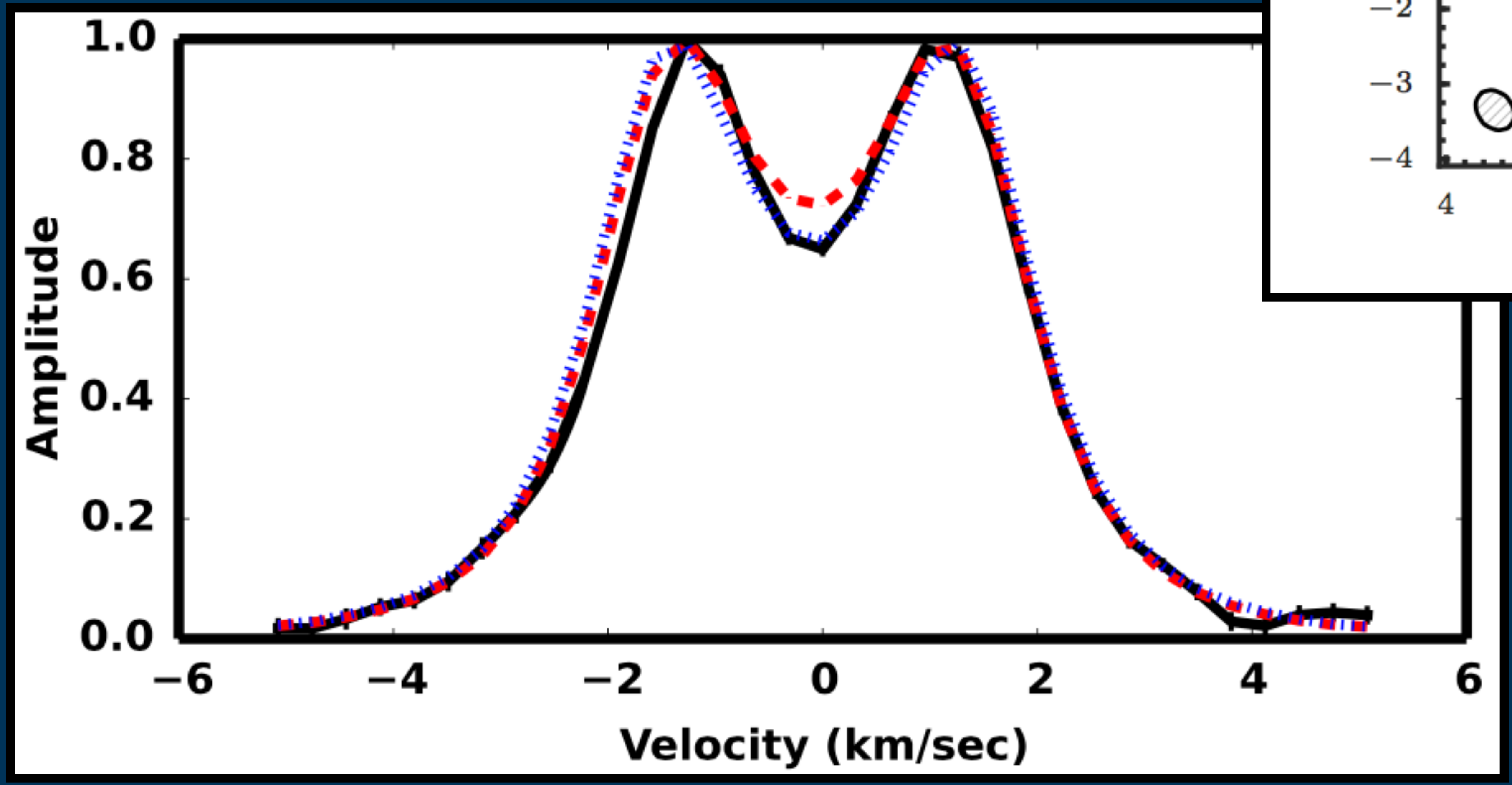




Furuya, Aikawa et al. 2015, and Furuya, van Dishoeck, & Aikawa 2015

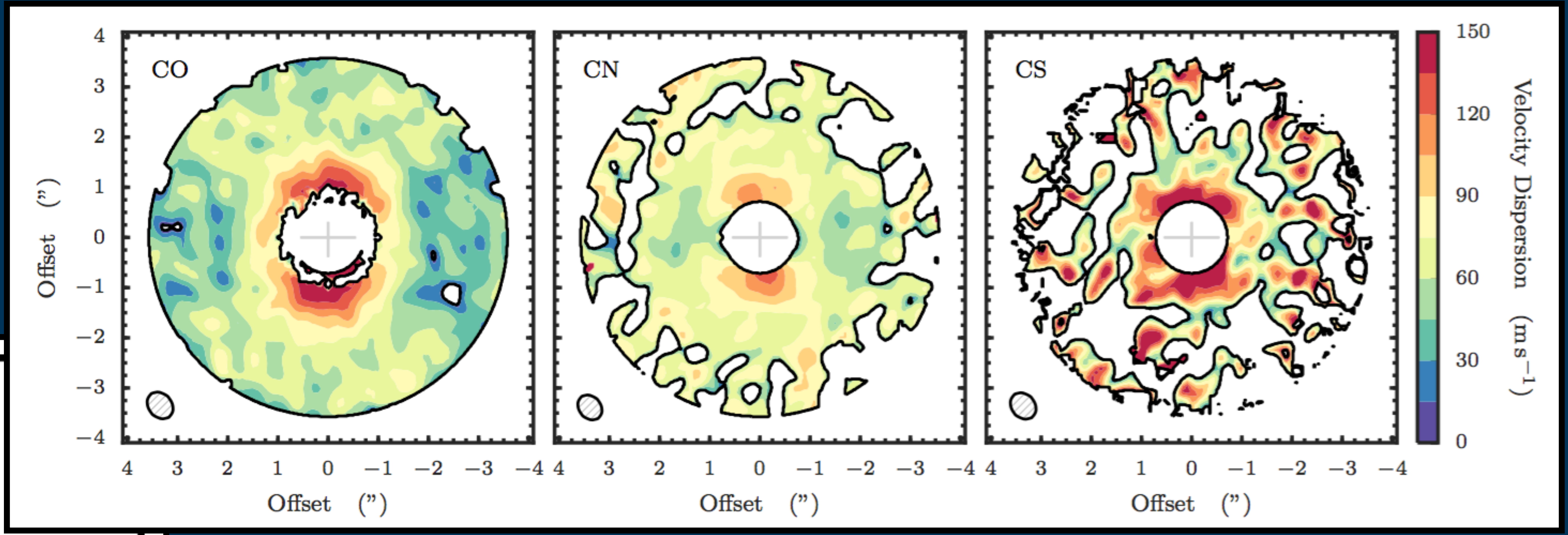
# II) The role of gas kinematics on $H_2O$?

Cold water formation via turbulent mixing? e.g., Furuya et al. 2013, Albertsson et al. 2014

Constraints on disk turbulence are low, e.g., Hughes+2011, Guilloteau+2012.




CO 2-1, Flaherty+2015

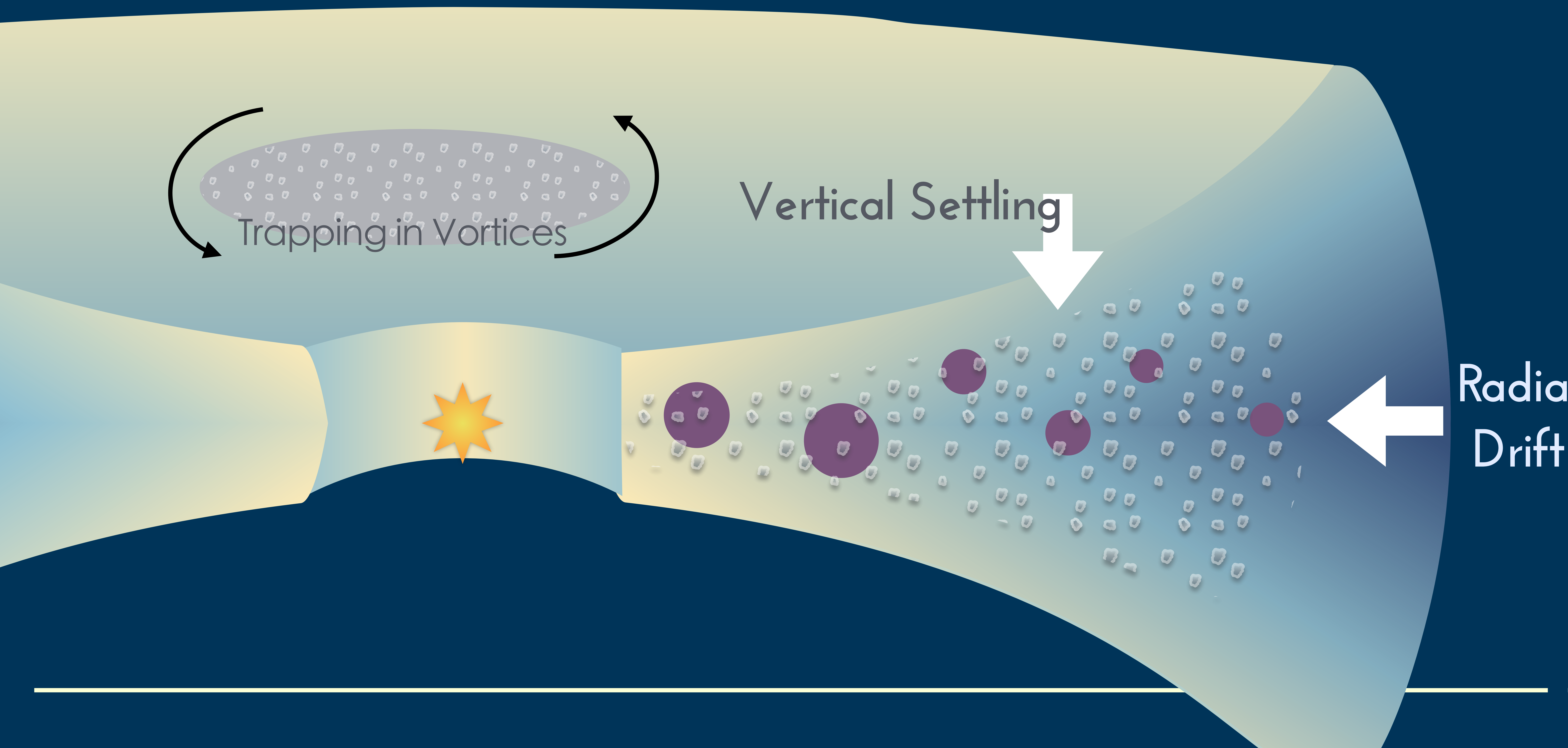



"CO and CN displayed a near constant $v_{turb}$ ~ 0.2 cs. However, the analysis of the possible sources of errors shows that these numbers should most likely be interpreted as upper limits. "

Teague+2016

# III) Aerodynamics: Differential Evolution of Solids

- Redistributes volatiles carried in the ices (Hogerheijde+2010, Bergin+2016, Du+2015, 2016, sub.). Changes the C/O ratio (e.g., Piso+2015).



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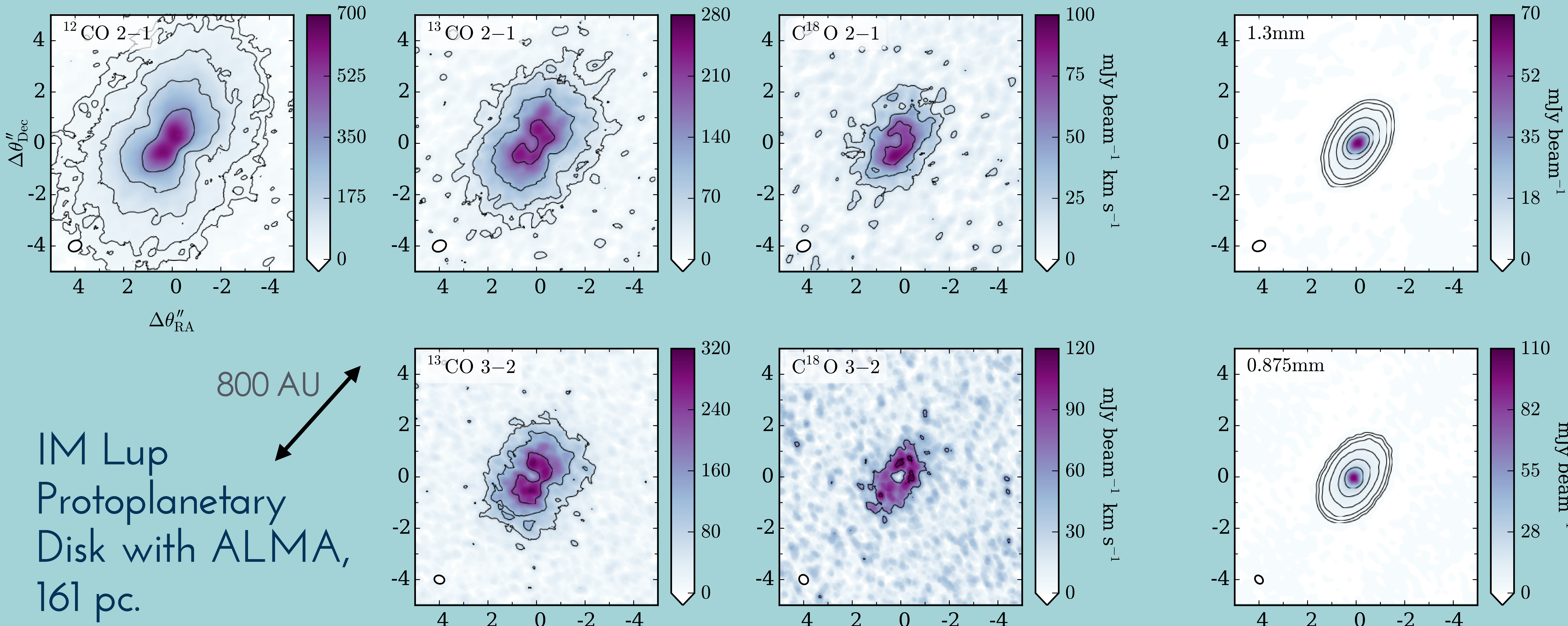
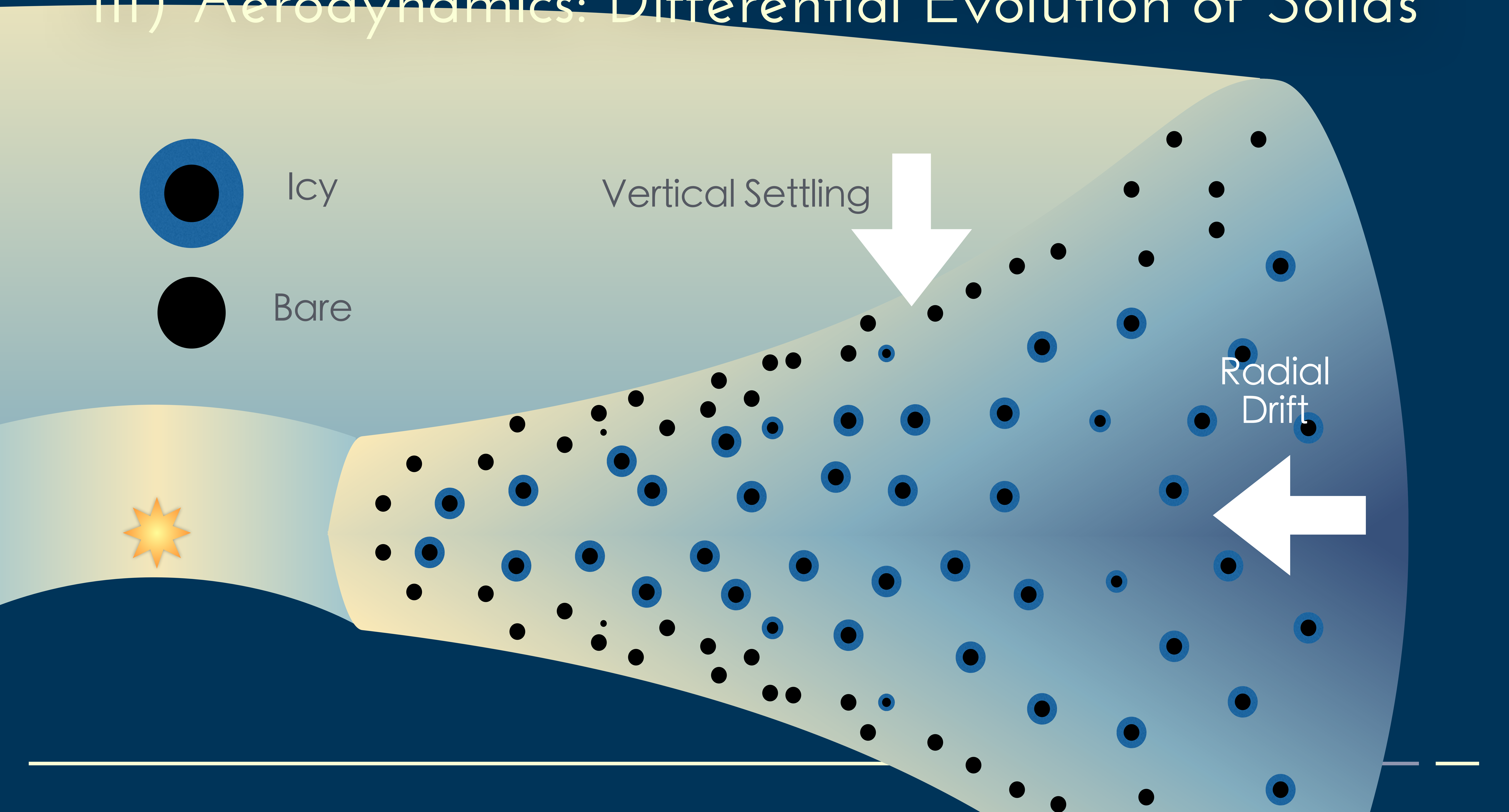



IM Lup Protoplanetary Disk with ALMA, 161 pc.

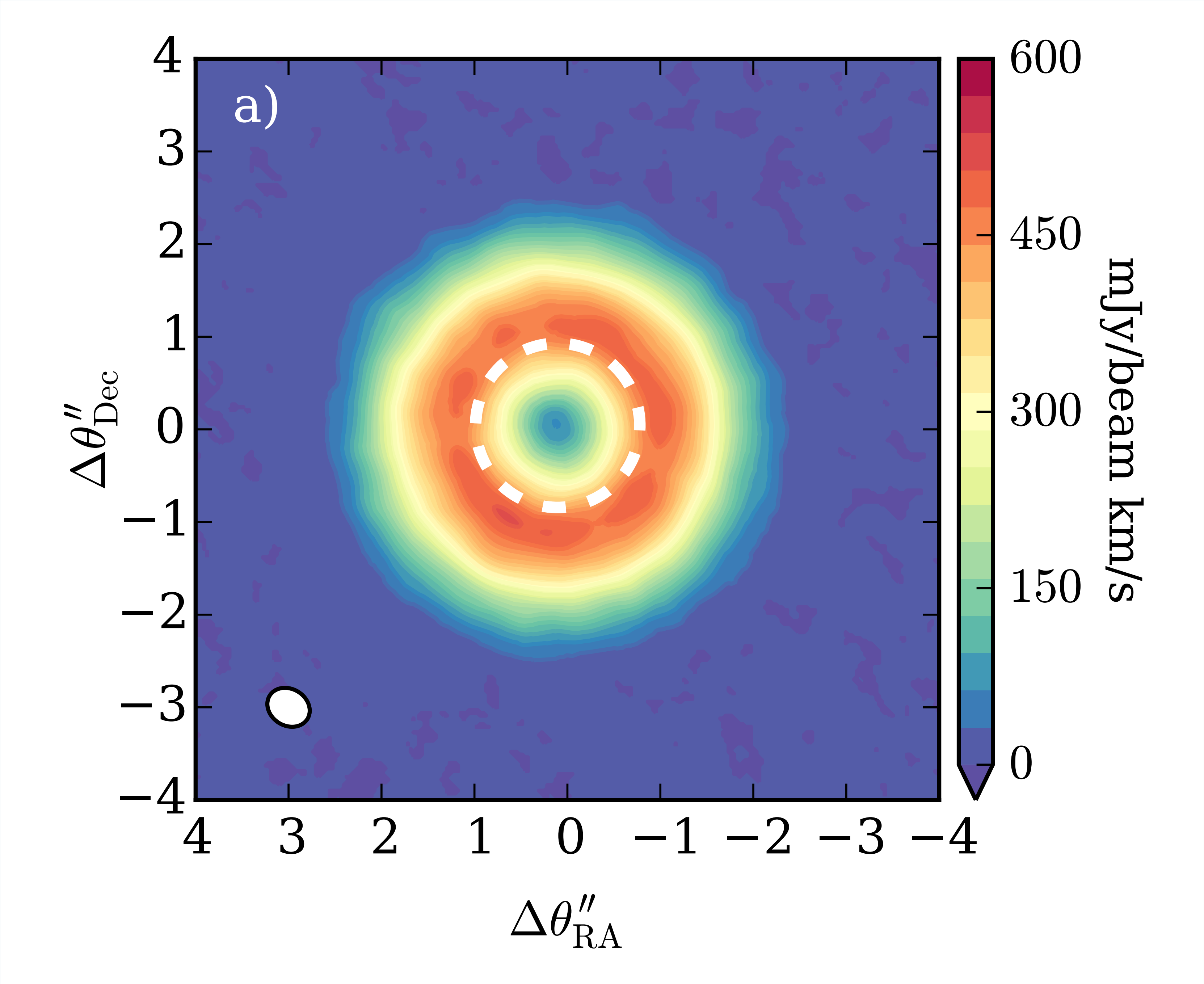
Panic et al. 2009, Cleeves et al. 2016c

# III) Aerodynamics: Differential Evolution of Solids



# III) Aerodynamics: Differential Evolution of Solids

Extremely bright $C_2H$ in two disks with ALMA! Bergin et al. 2016




Surface and outer disk is UV dominated.

C, N (little O) in $H_2$ rich gas – is a hydrocarbon factory (Du, Bergin, & Hogerheijde 2015)

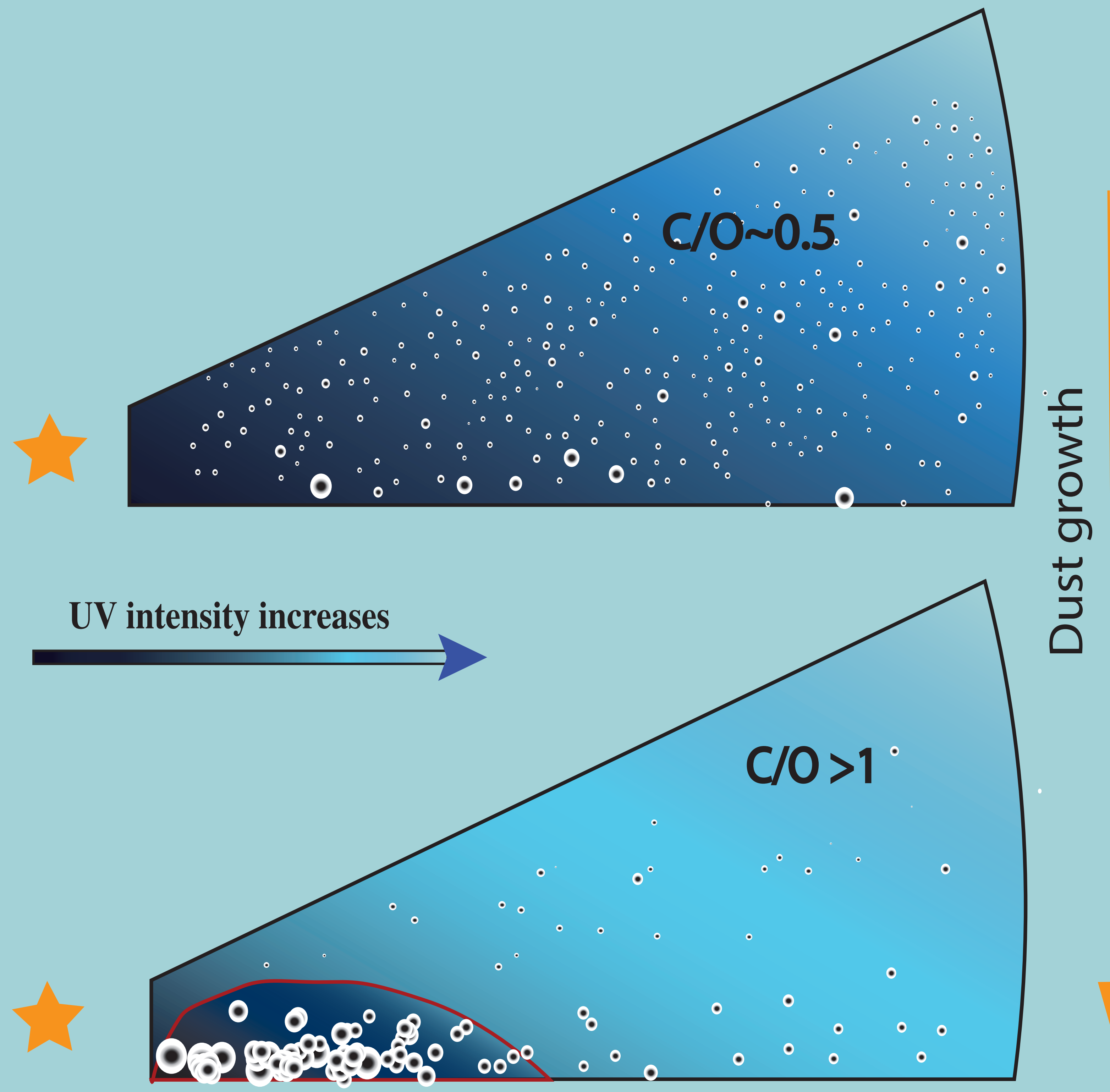
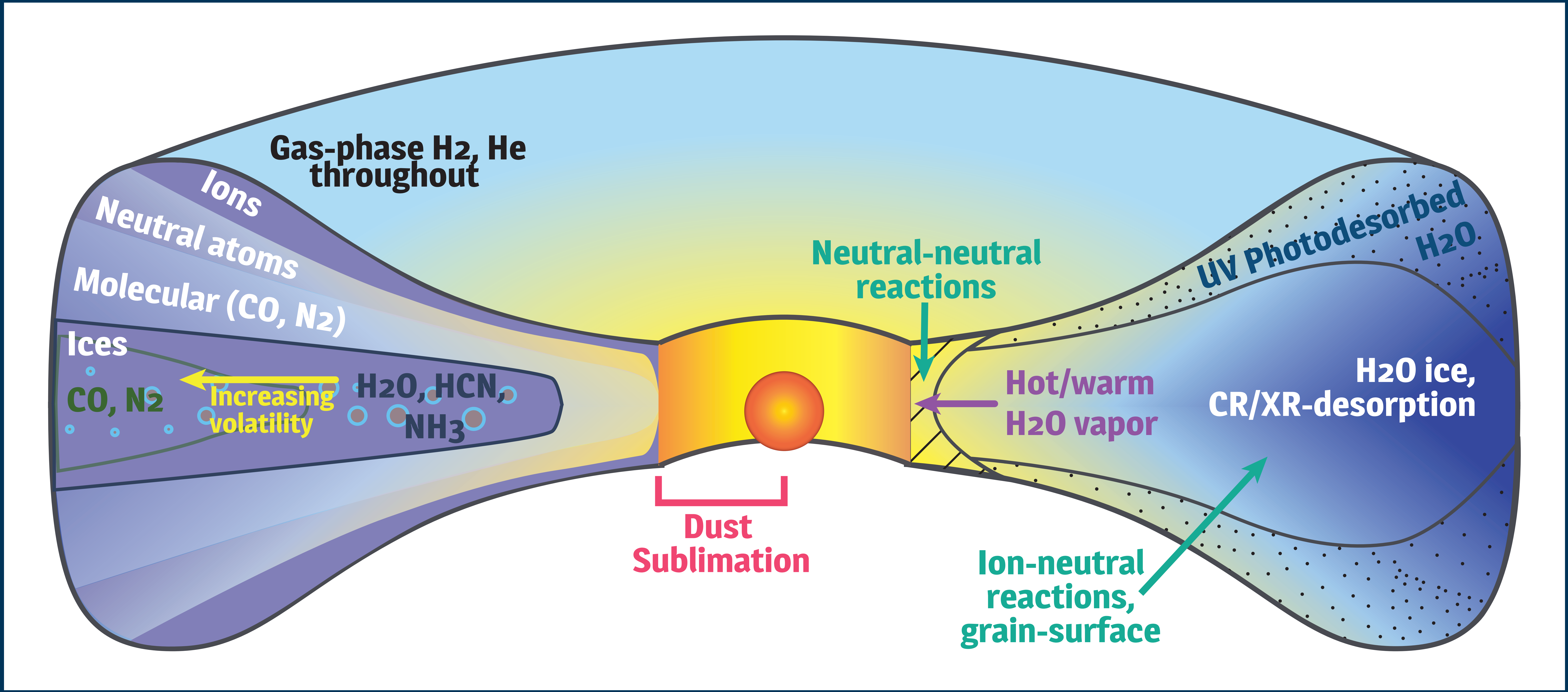



Figure courtesy of Ted Bergin

# IV. In situ disk chemistry?



# IV. In situ disk chemistry?

## I. In the Gas Phase

$H_2^+ + H_2 \rightarrow H_3^+ + H$

$H_3^+ \xrightarrow{O,OH} H_3O^+ \xrightarrow{Gr,e^-} H_2O$

Neutral-Neutral like $H_2$+OH only at high (T >200 K) temperatures.

## II. On Grain Surfaces

$H_2^+ + H_2 \rightarrow H_3^+ + H$

$H_3^+ + Gr, e^- \rightarrow$ H atoms

$O(gr) \xrightarrow{H} OH(gr) \xrightarrow{H} H_2O(gr)$

$O_2(gr) \xrightarrow{2xH} H_2O_2(gr) \xrightarrow{H,OH} H_2O(gr)$

# IV. In situ disk chemistry?

$$H_2^+ + H_2 \longrightarrow H_3^+ + H$$

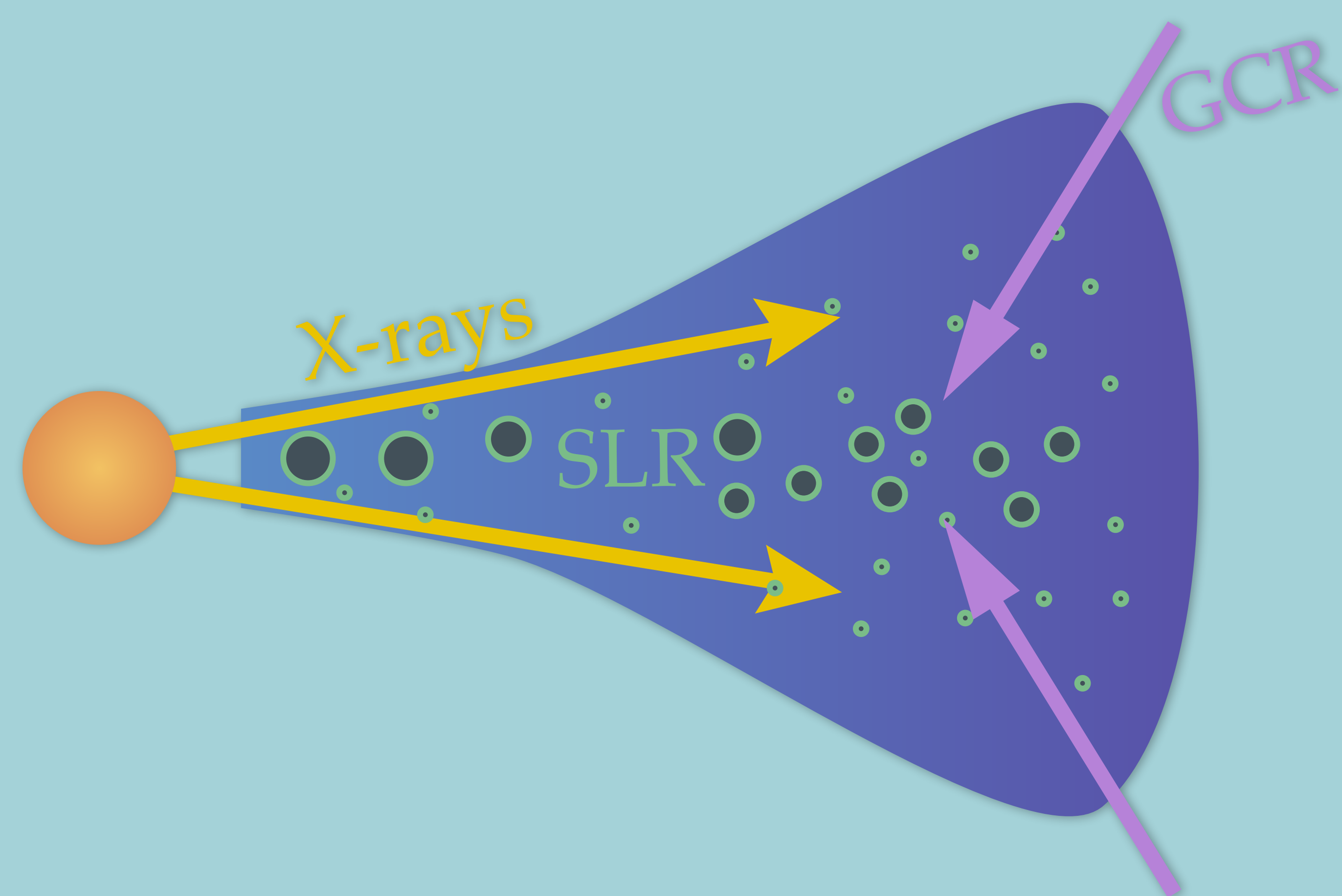
Formation of water at low temperatures requires a source of *molecular hydrogen ionization.*

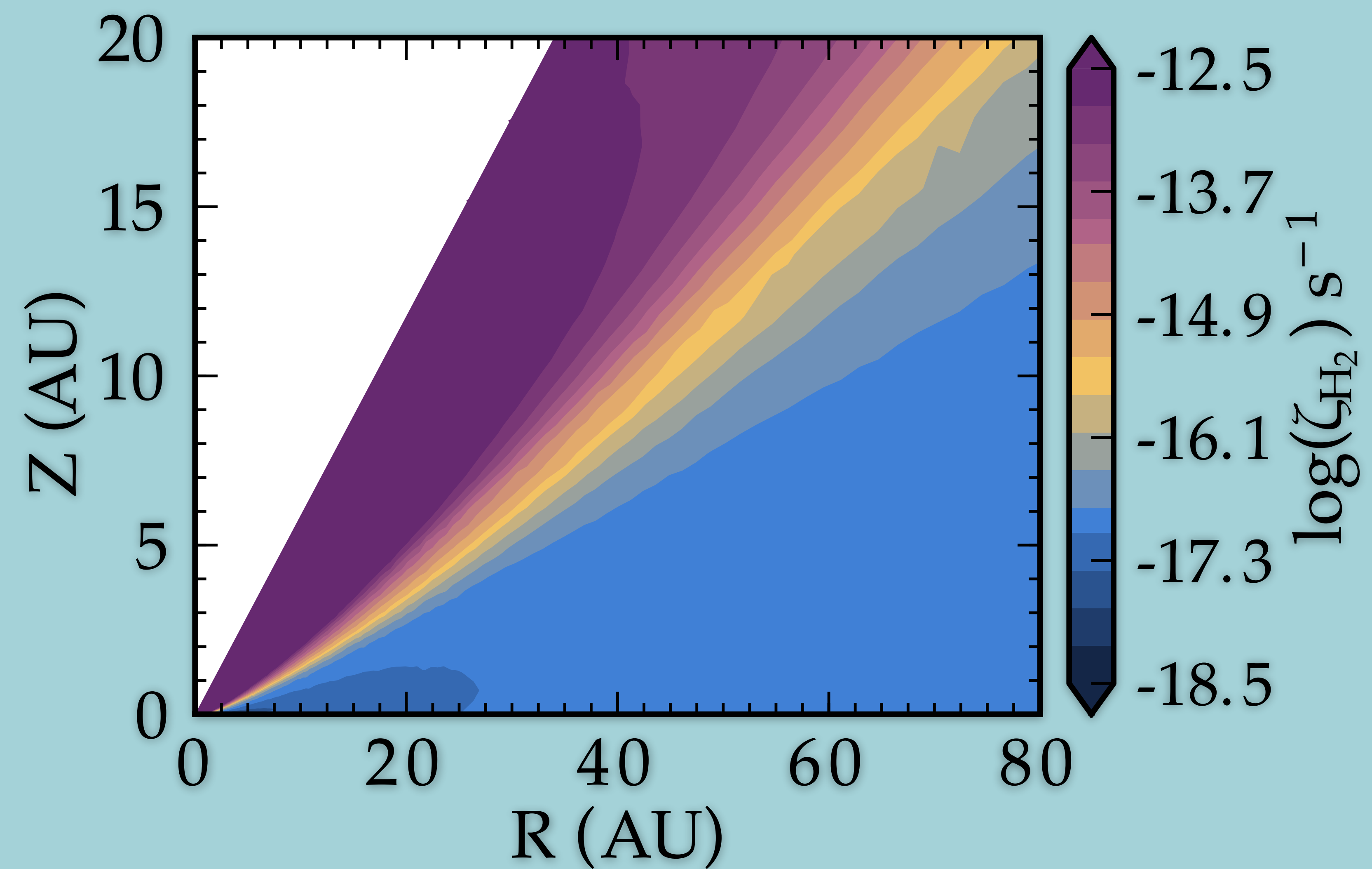
Possible sources: 1. cosmic rays, 2. X-rays, 3. radionuclide decay.

# Modeling Tools: High Energy Processes

| Ionization source: | How we treat: | How this is unique/ new: |
|---|---|---|
| X-rays (Bethell) | Monte Carlo | Treat gas and dust opacity separately |
| UV (Bethell) | MC Continuum, Line | Ly-α |
| Cosmic Rays (Cleeves) | Multiple input spectra with consistent vertical transfer. | Flexibility in CR rates beyond normalization |
| Radionuclides (Cleeves) | Infinite Slab with Loss | Loss terms with ability to include settling. |
| Interstellar External Radiation (Cleeves) | Numerically integrate outside in | 3D Treatment |

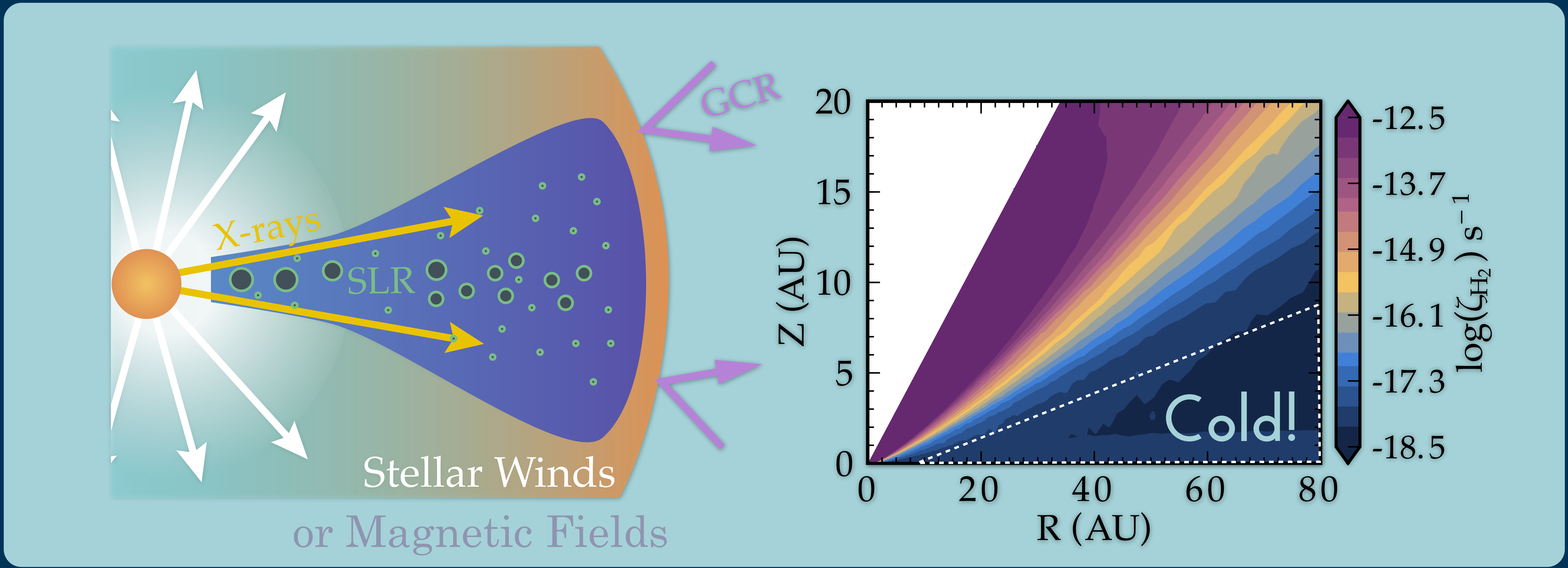
# The Classical Picture of Disk Ionization




Glassgold 1997, 2000, 2001 (and more), Igea & Glassgold 1999, Umebayashi+1989, 2009, Ilgner & Nelson 2006a/b, 2008.

# An Updated Picture of Disk Ionization

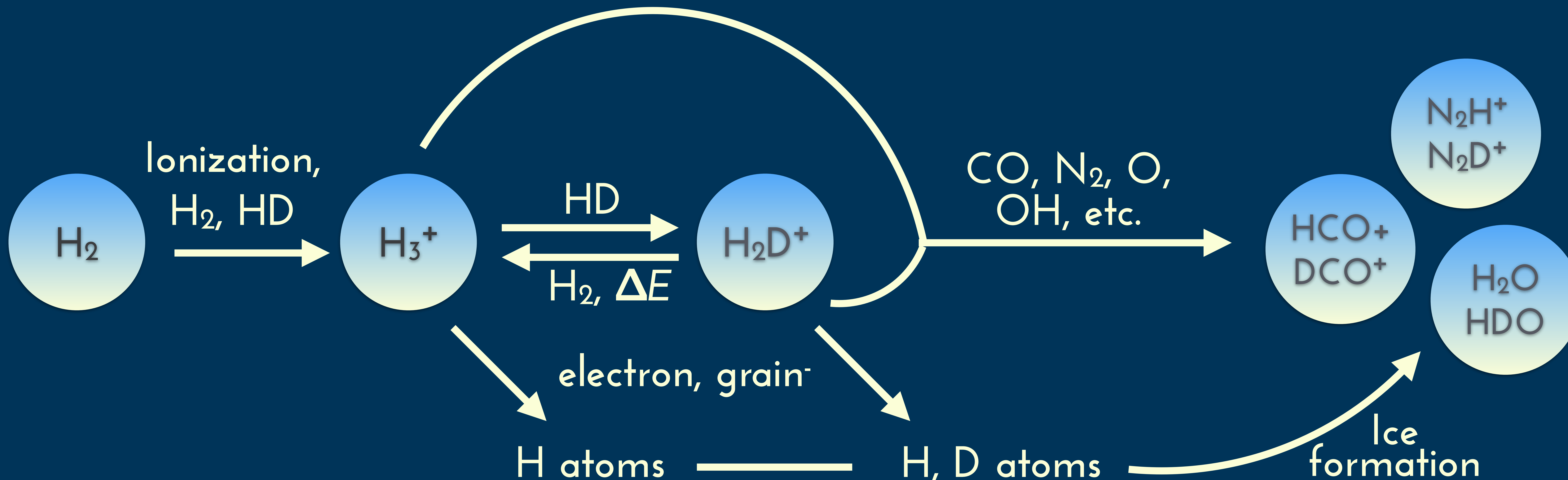



Cleeves et al. 2015 measured a significantly subinterstellar CR ionization rate in TW Hya (> 100x reduced).

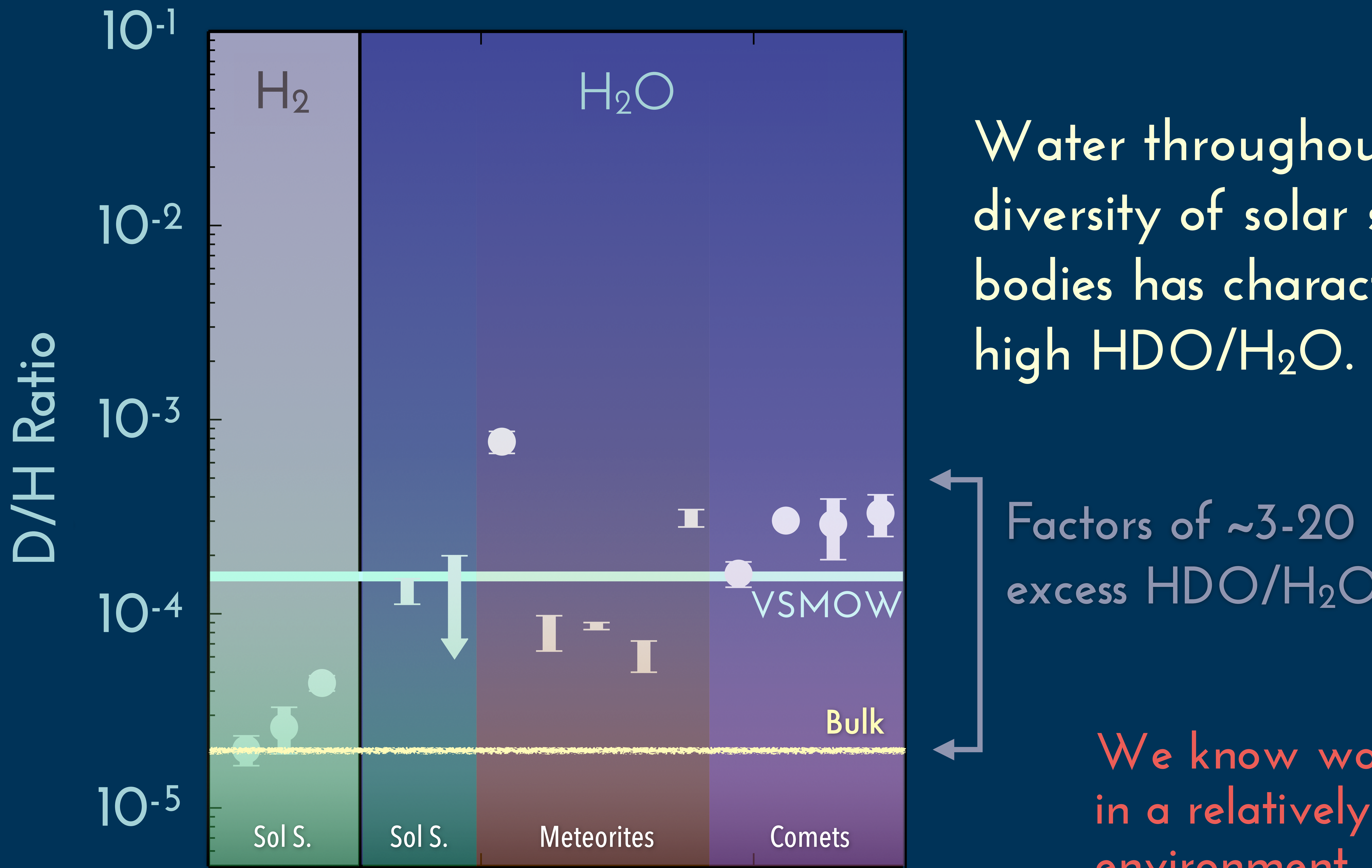
# How does the ionization environment impact disk water formation?

# Additional Clues

*Cold water "chemically tagged" with high D/H.*

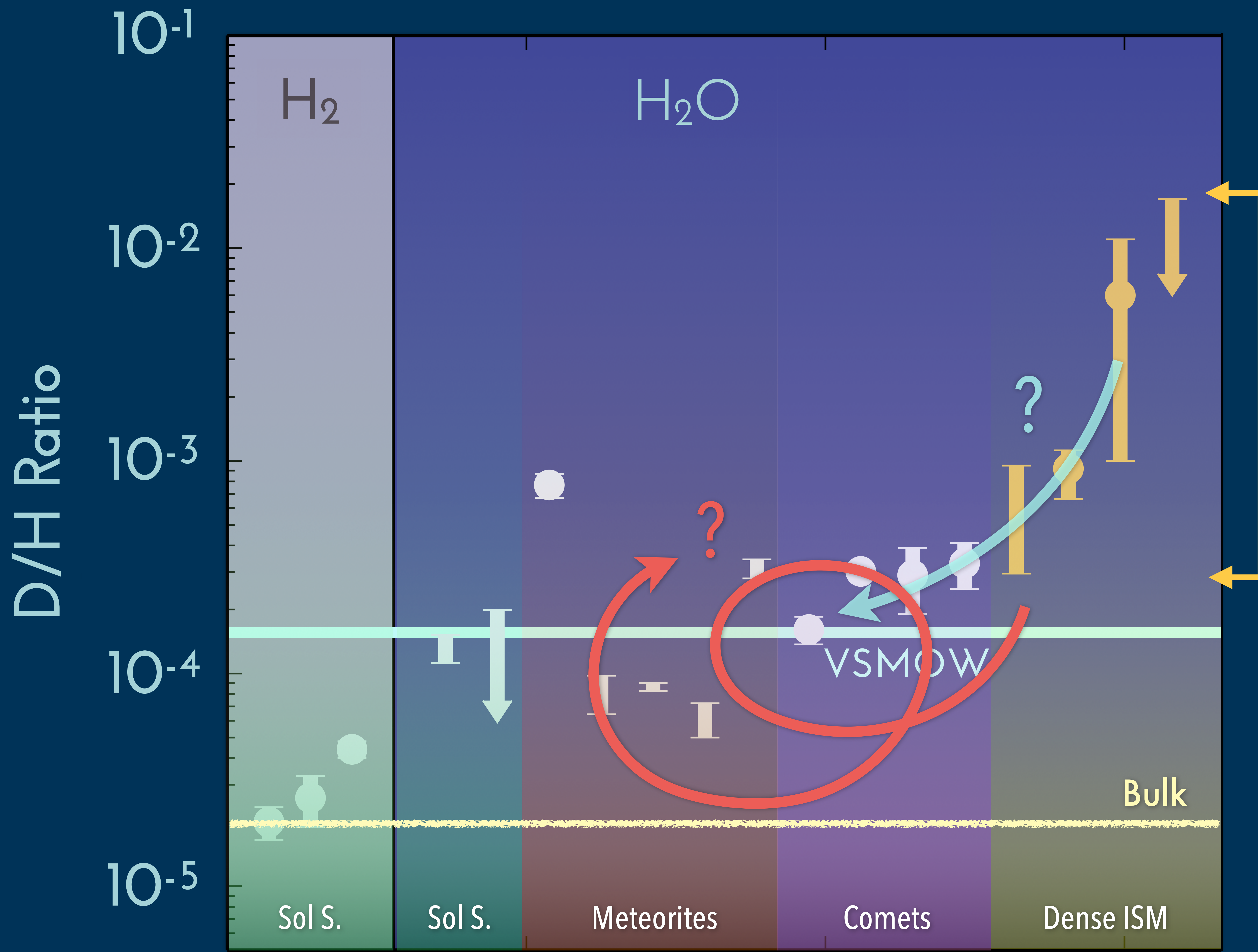



Supports fractionation
up to T < 50 K




Water throughout a diversity of solar system bodies has characteristically high $HDO/H_2O$.

We know water formed in a relatively cold environment.




Primordial ices in the envelopes of protostars exhibit a high level of D/H.

Are these early stages (the primordial ISM ices) chemically linked?

What is the role of disk chemistry?

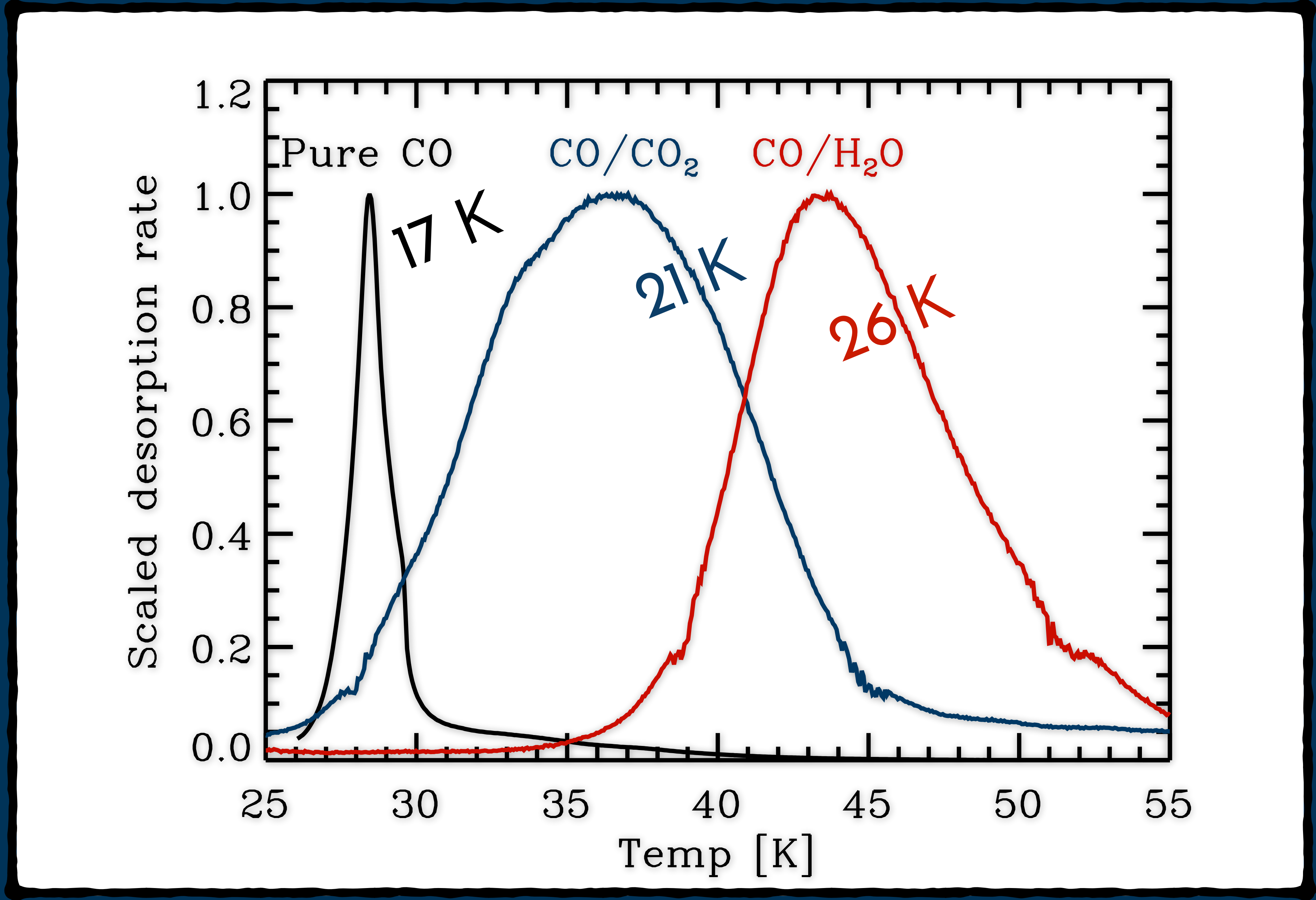
ISM: Persson+2014, 2012, Coutens+2012, Parise 2003.

## Hitting reset:

Starting out with $HDO/H_2O$ = $HD/H_2$, how much does cold water formation in the disk elevate $HDO/H_2O$?

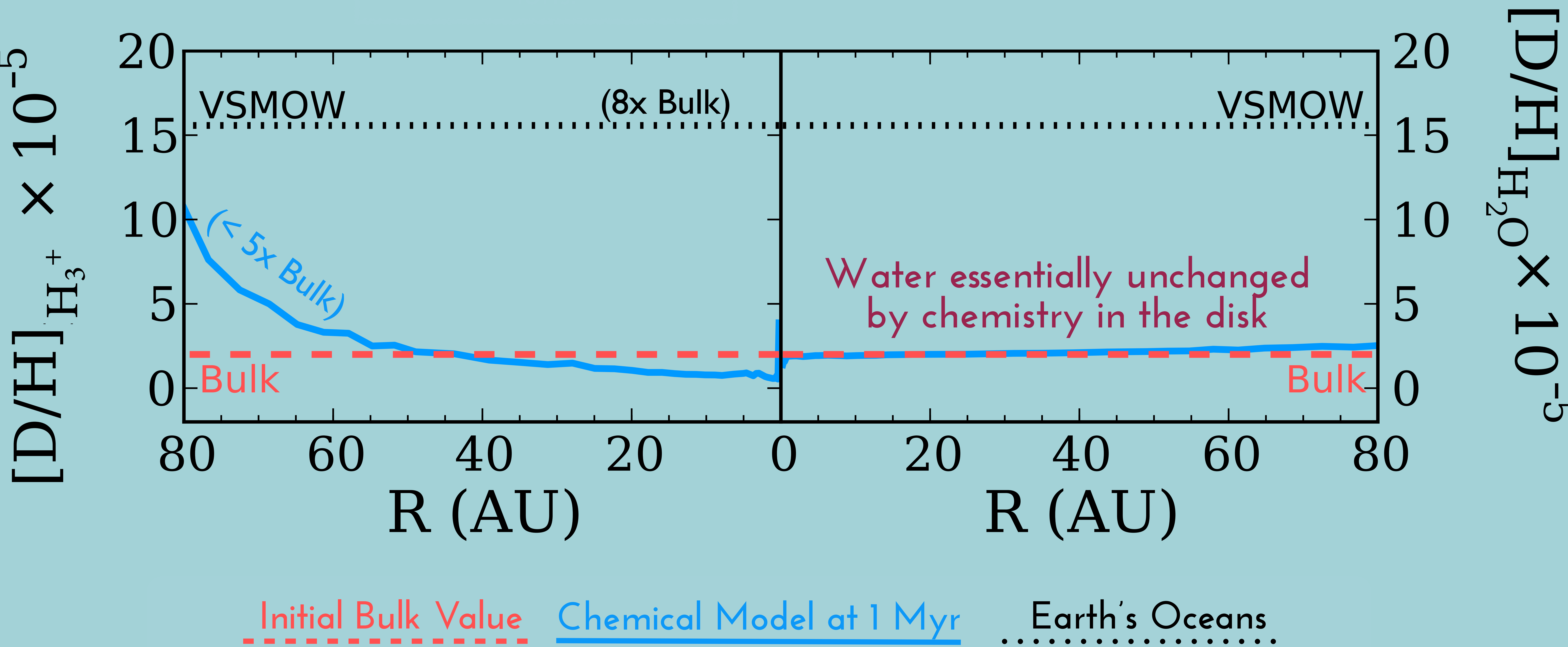
# Chemical Model

- Mini-deuterium chemical network.
  - 6268 reactions, 600 species.
- $H_2$/HD/$D_2$ self-shielding (Wolcott-Green+2011)
- Simple grain-surface chemistry (Hasegawa, Herbst, Leung 1992)
- Thermal o/p ratios for $H_2$ and $H_2D^+$ (Lee & Bergin 2015)
- Warm fractionation reactions (Thi+2010)




And updated lab data on CO binding energies for oxygen-regulation (Graninger).

# HDO/$H_2O$ Results (1 Myr)



# Disk-Sourced Cold Water: Results

- ➡ Chemistry in a laminar disk is not a viable source origin for cold (deuterated) water Solar System.
- ➡ These conditions require ISM heritage such that interstellar ices would be incorporated into comets, meteorites, and Earth's oceans, 30-40%.

Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2014, Sci, 345, 1590.

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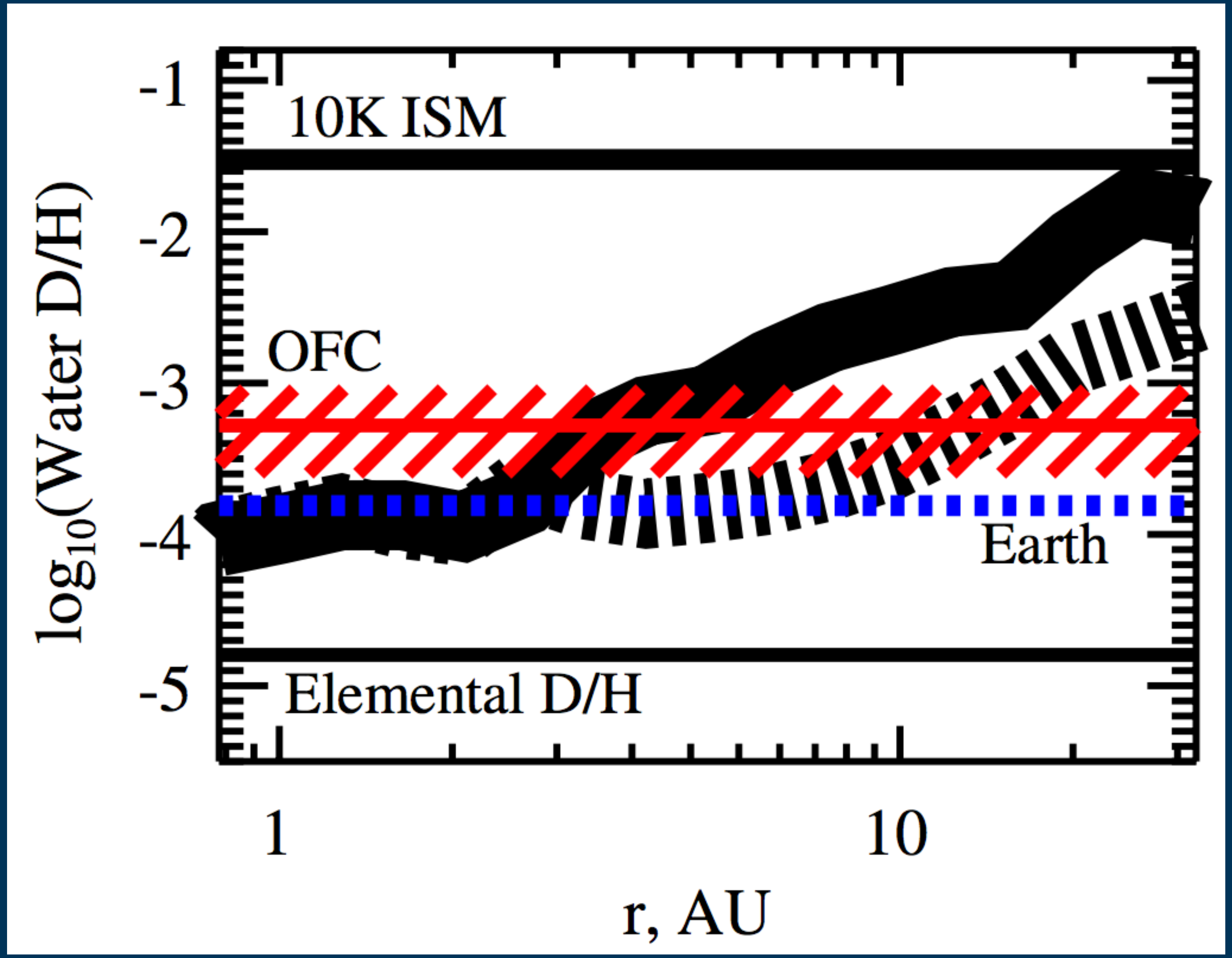
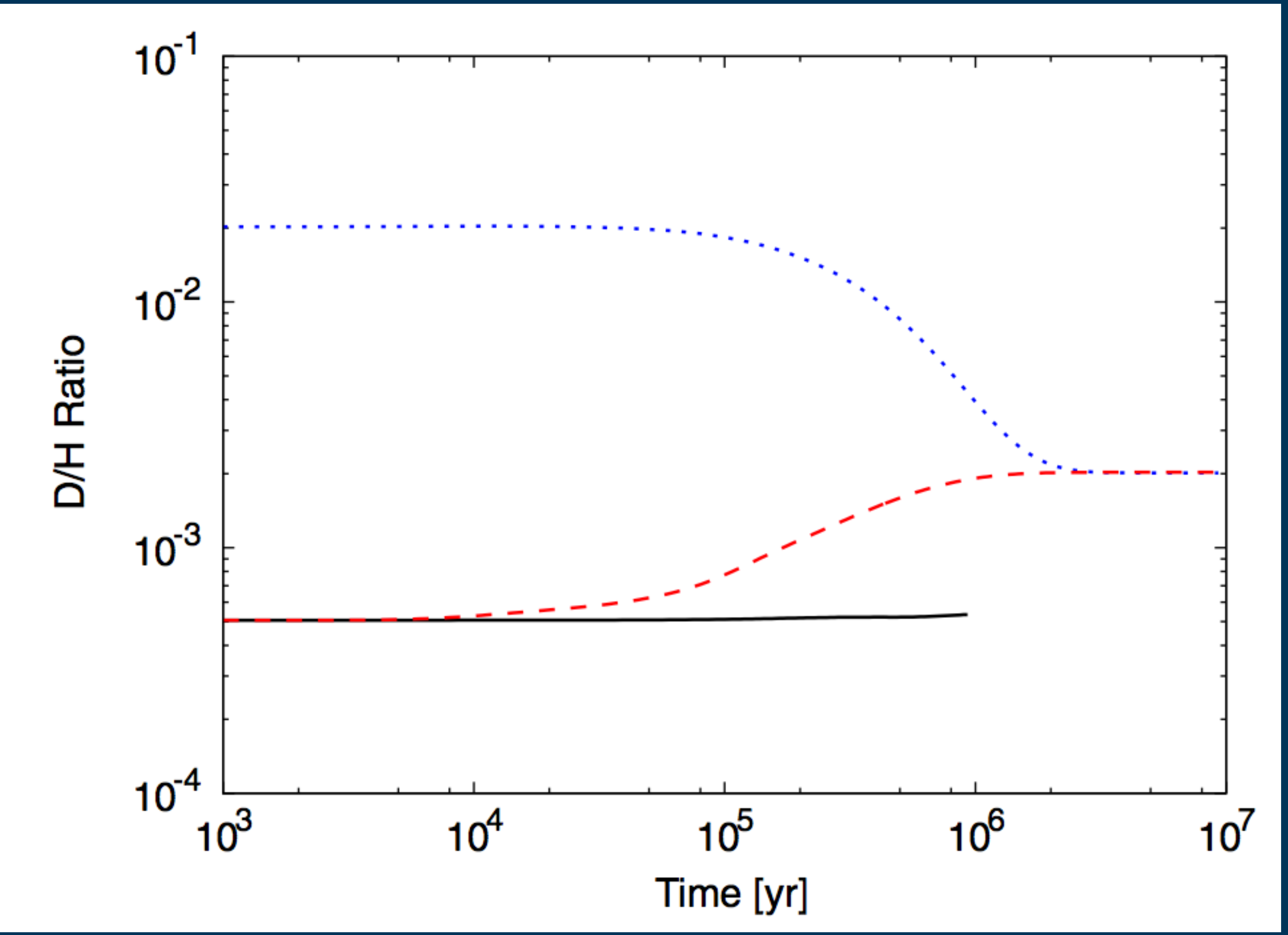
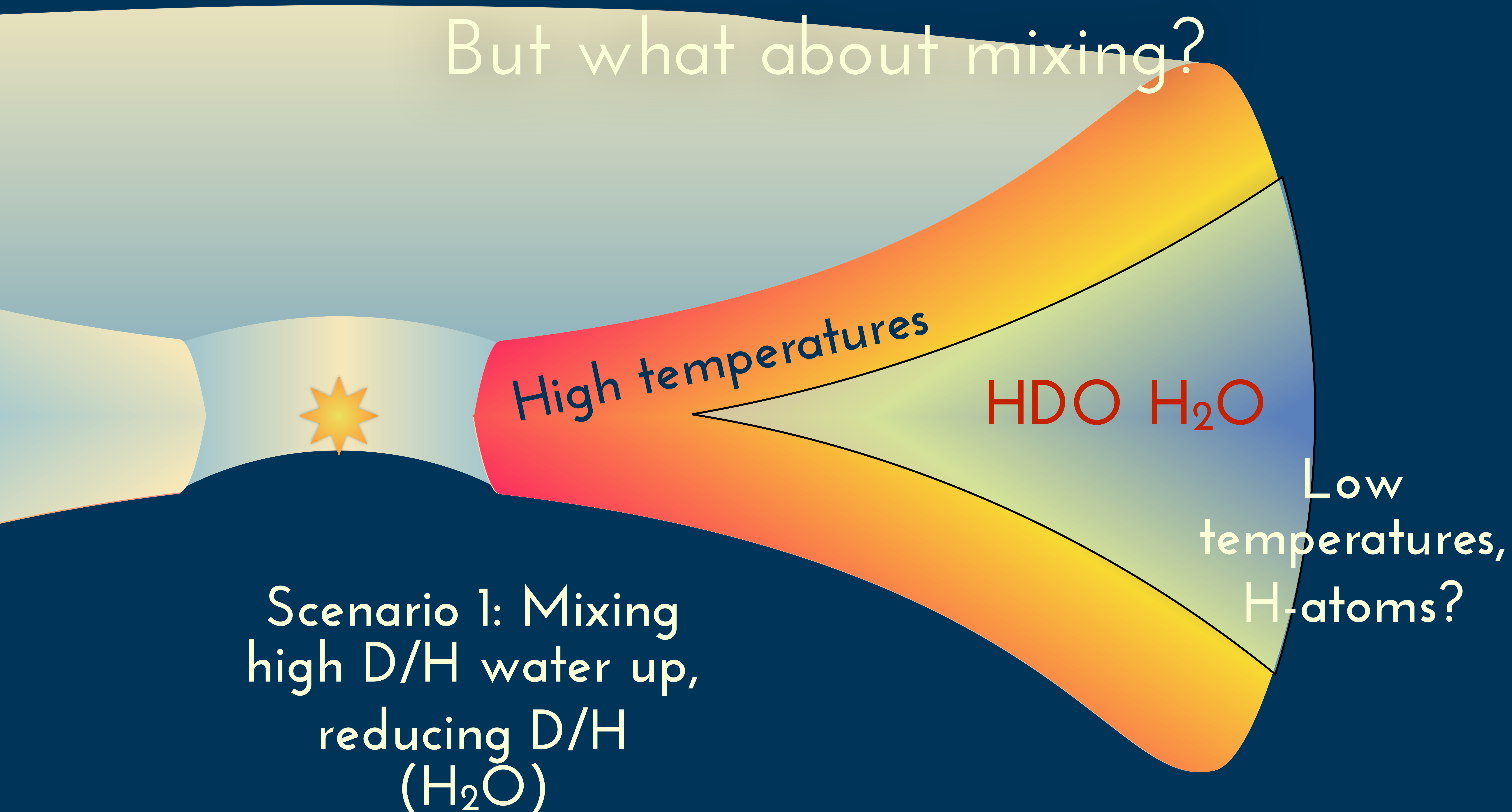
# But what about mixing?



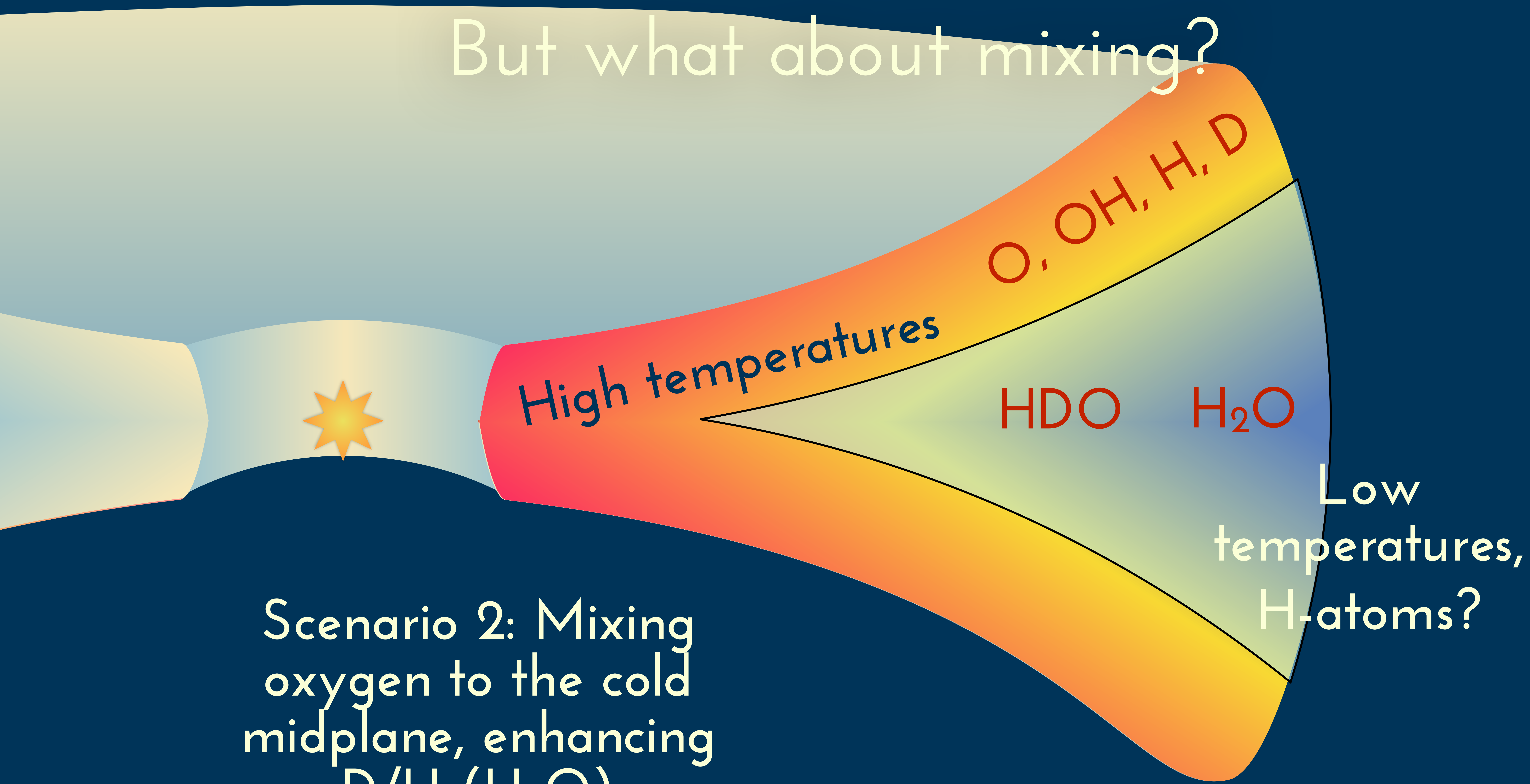

"Turbulent mixing slowly transports some of the water ice into warmer or irradiated regions where it desorbs and is quickly defractionated..." - Albertsson et al. 2014

"...atomic oxygen is transported from the surface to the deeper region and (re)forms $H_2O$ and HDO ices. " - Furuya et al 2013



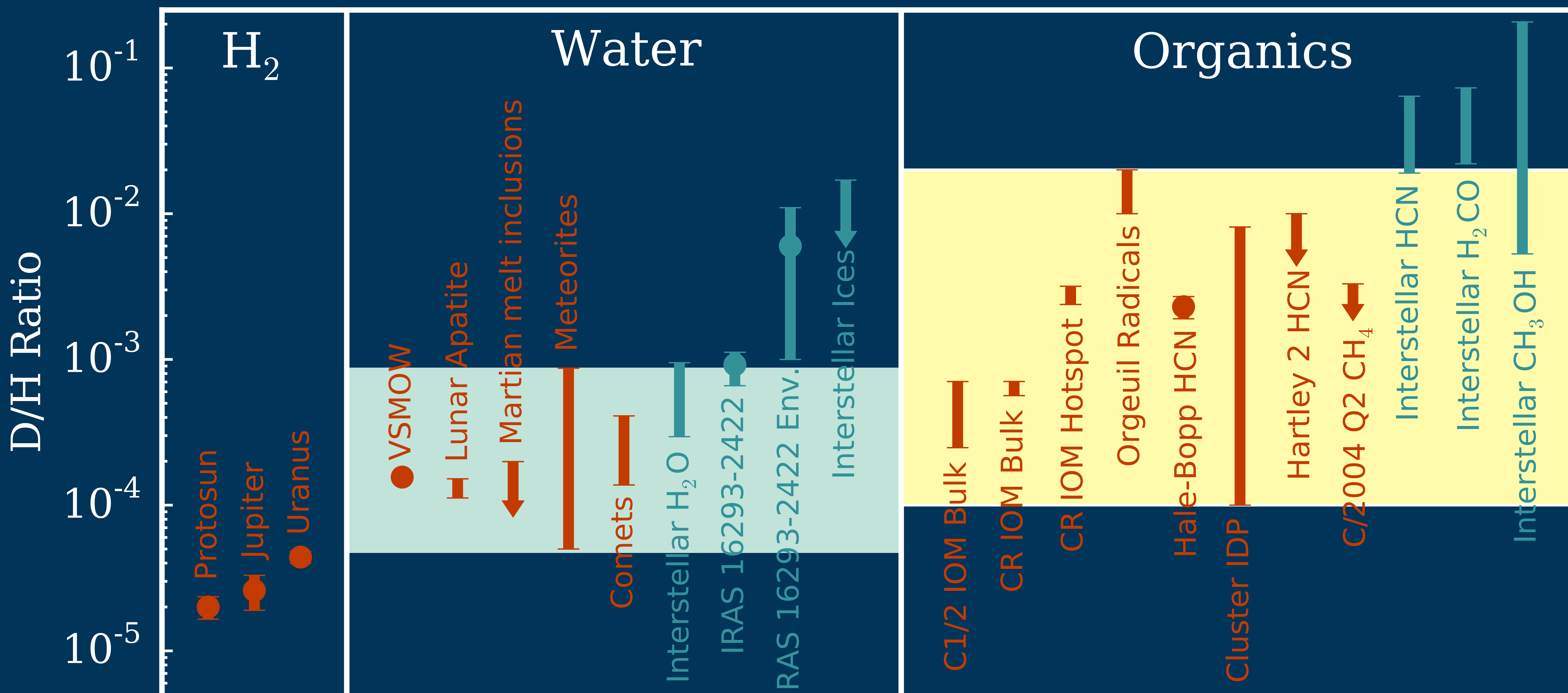
But what about mixing?
High temperatures
HDO $H_2O$
Low temperatures, H-atoms?
Scenario 1: Mixing high D/H water up, reducing D/H ($H_2O$)

# But what about mixing?




Scenario 2: Mixing oxygen to the cold midplane, enhancing D/H ($H_2O$)

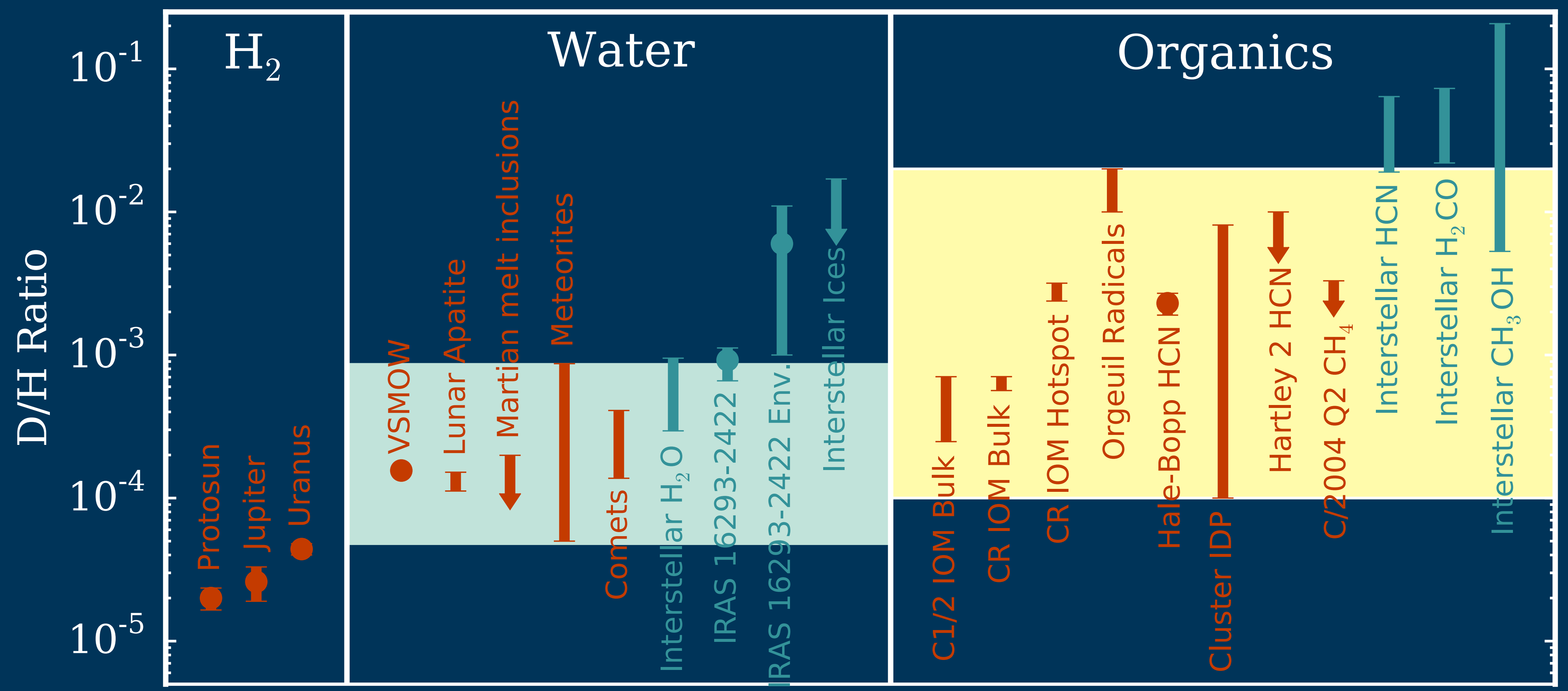
# D/H in Water vs. Organics




Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

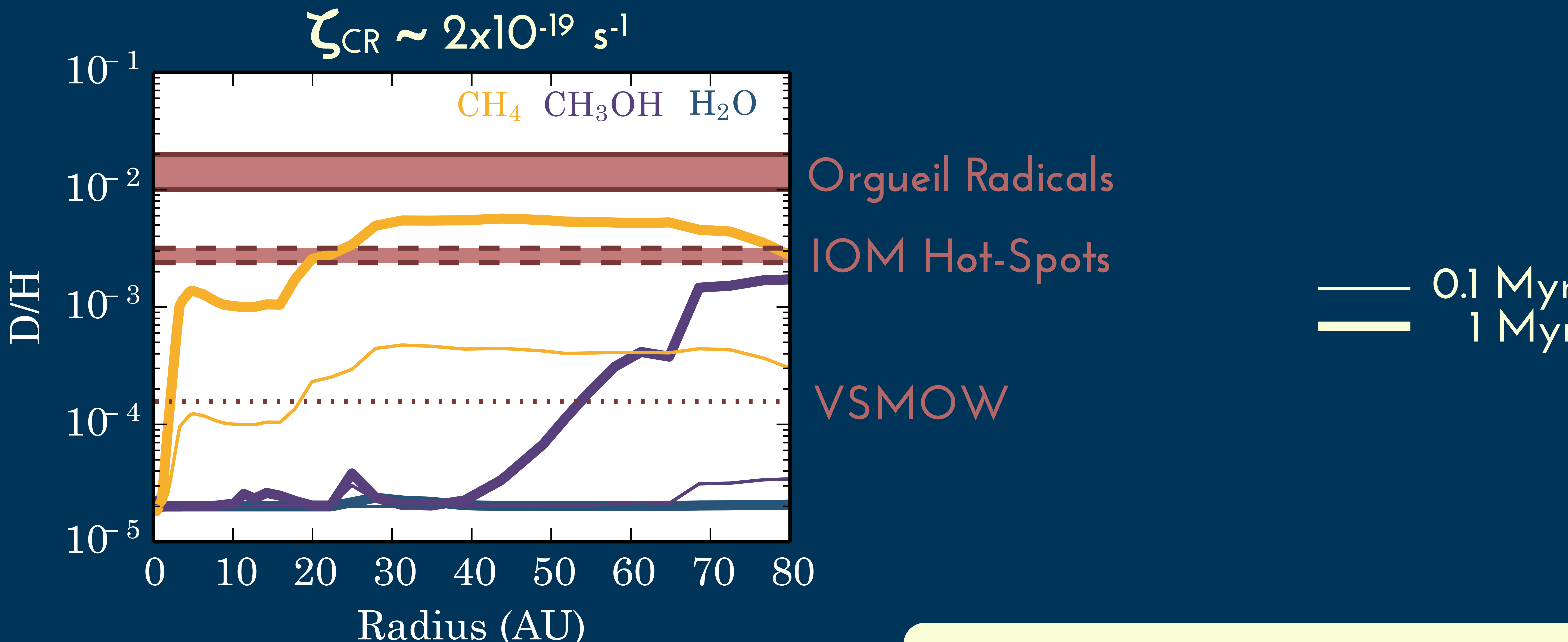
# D/H in Water vs. Organics

* Globally higher organic D/H than water. Perhaps due to:
  * $CH_3^+ + HD \rightleftarrows CH_2D^+ + H_2 + \Delta E$ (Roueff+2013).
* Larger range in organic D/H = many reaction pathways?



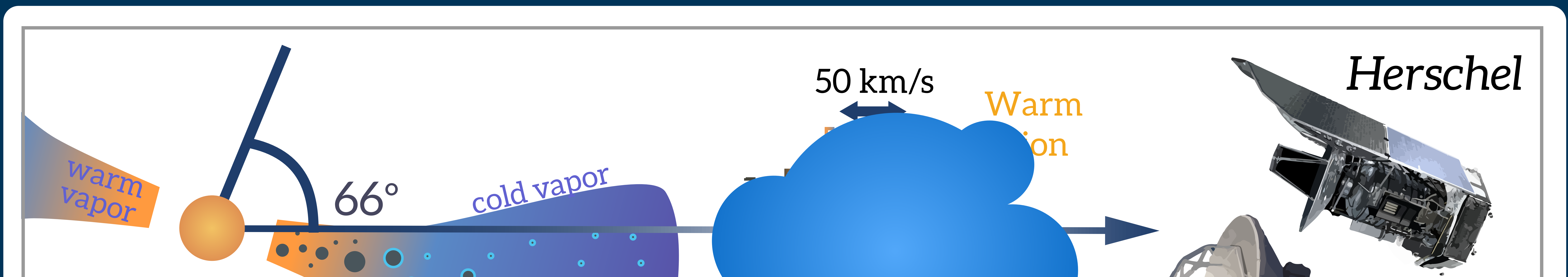

Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

# Midplane Deuterium Fractionation in Hydrides




Interesting predictions for cometary D/H in $CH_3OH$?

# *Future:* HDO/$H_2O$ in a Protoplanetary Disk

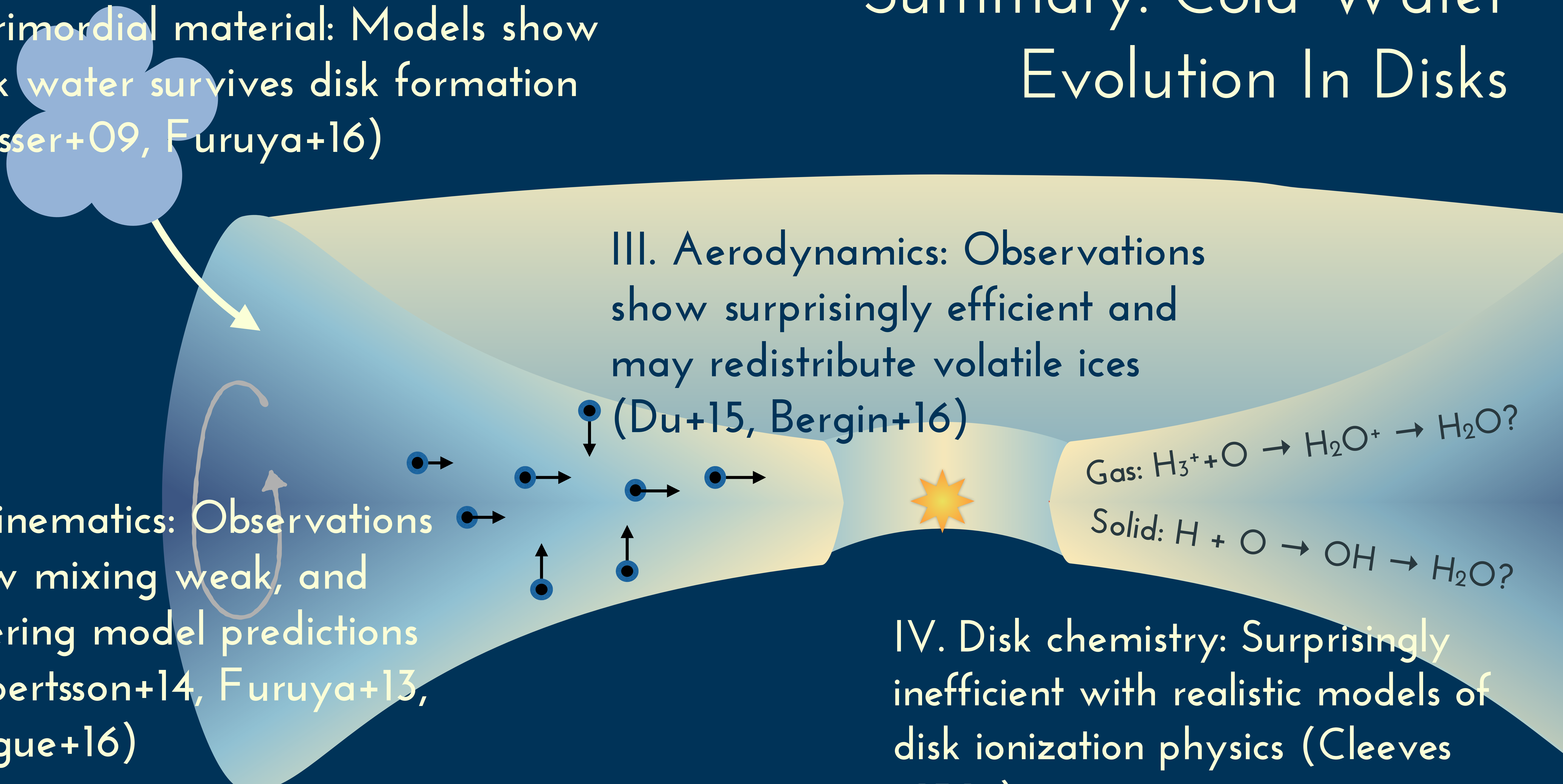



… and working towards better ionization constraints

# Summary: Cold Water Evolution In Disks

I. Primordial material: Models show bulk water survives disk formation (Visser+09, Furuya+16)

III. Aerodynamics: Observations show surprisingly efficient and may redistribute volatile ices (Du+15, Bergin+16)




II. Kinematics: Observations show mixing weak, and differing model predictions (Albertsson+14, Furuya+13, Teague+16)

IV. Disk chemistry: Surprisingly inefficient with realistic models of disk ionization physics (Cleeves +15,16)