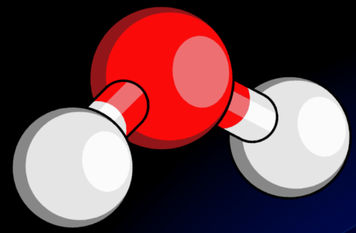
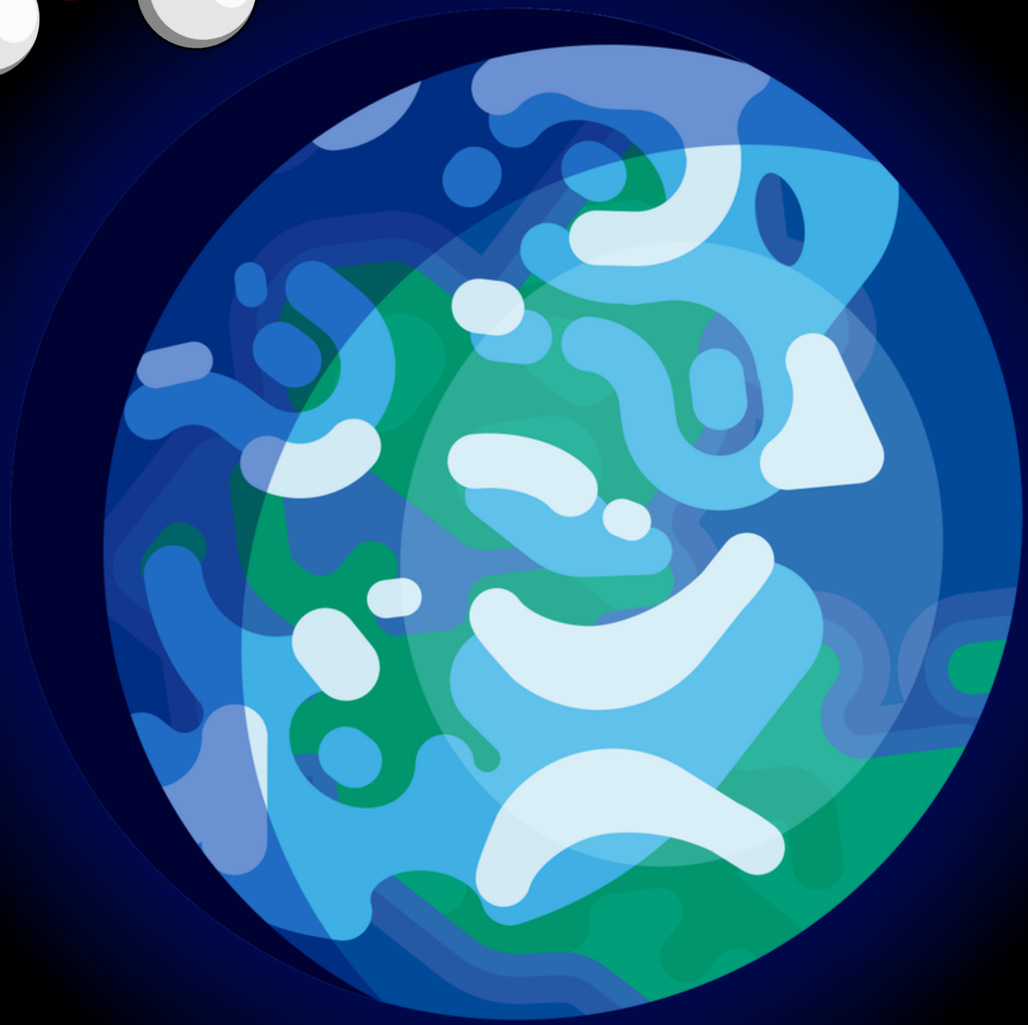
# Origin of Water on Earth (and more...)

## A Local Accretion Scenario from Computational Chemistry

Lise Boitard-Crépeau,
*2nd year PhD student, IPAG, Grenoble*

*with Cecilia Ceccarelli, Piero Ugliengo, Stefano Pantaleone, Pierre Beck and Lydie Bonal*





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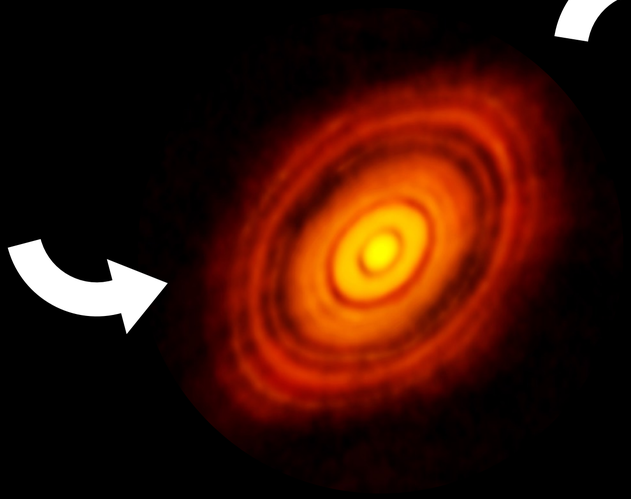
# When was Water formed ?

*Formation in the pre-stellar phase*

Molecular Cloud

Protostar



Protoplanetary Disk

Planets Formation

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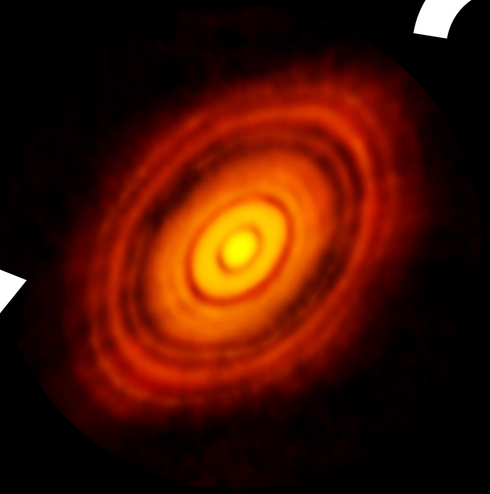

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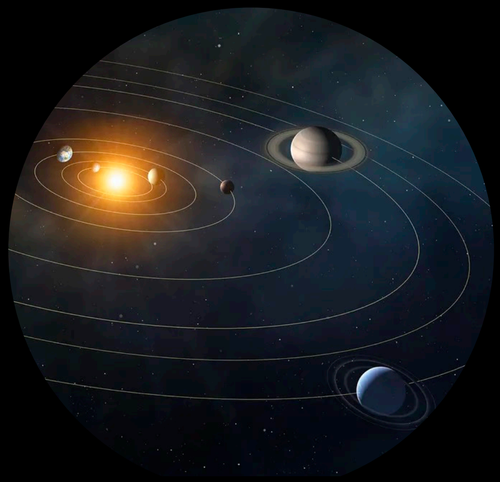
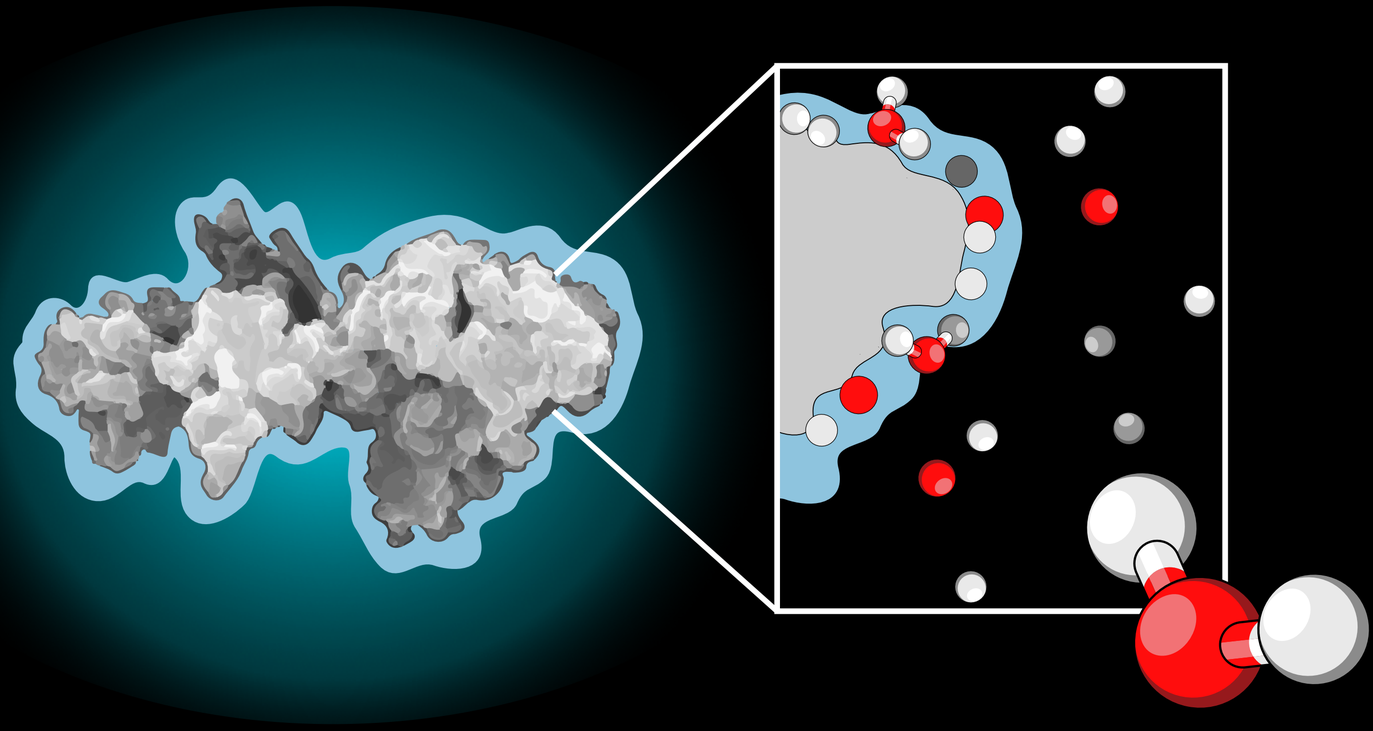


# How was Water formed ?

*Icy Water on dust grains*

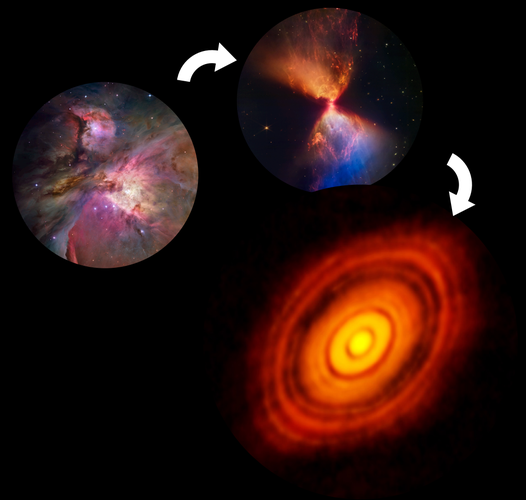
Molecular Cloud



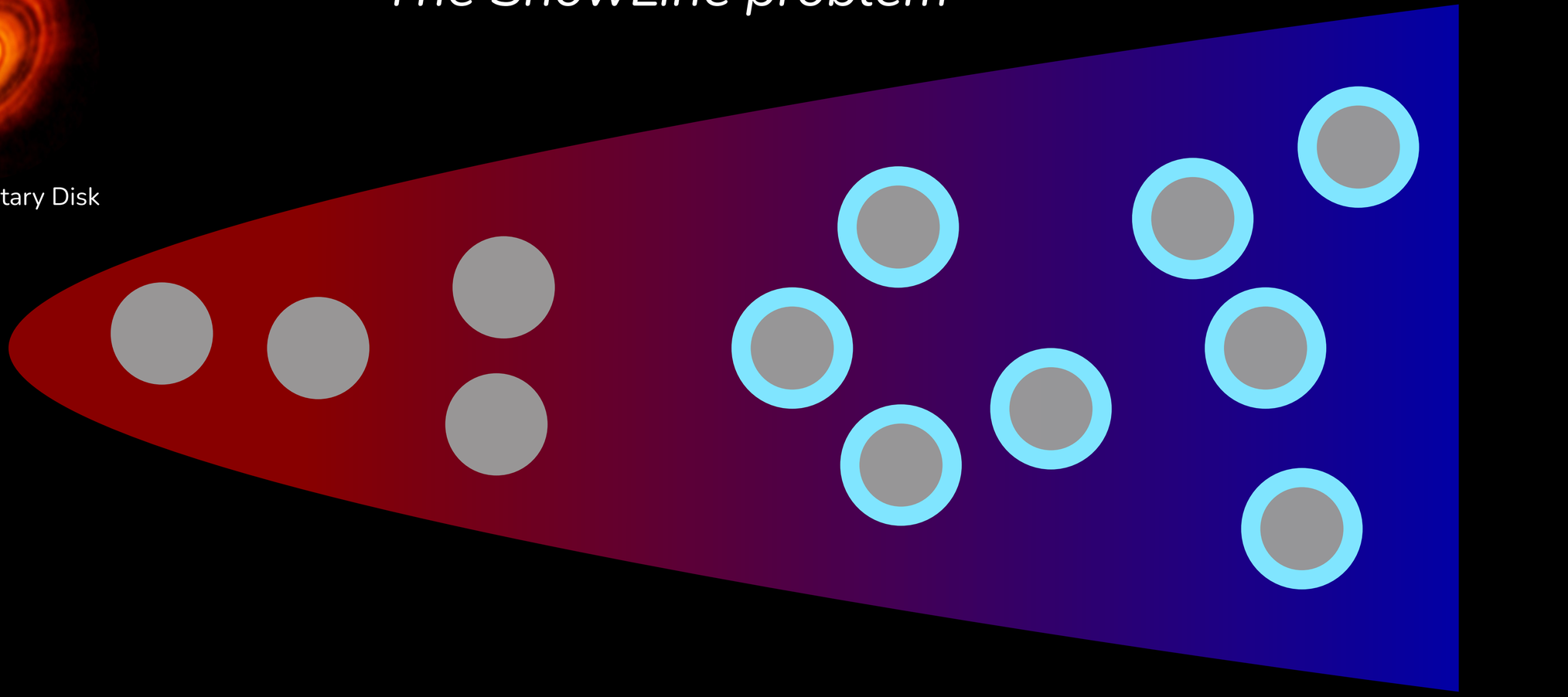
< 20 K

# Where does Water go ?

*The SnowLine problem*



Protoplanetary Disk



*Temperature*

# Where does Water go ?

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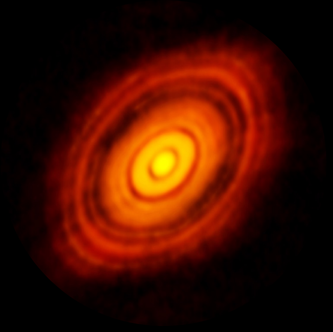
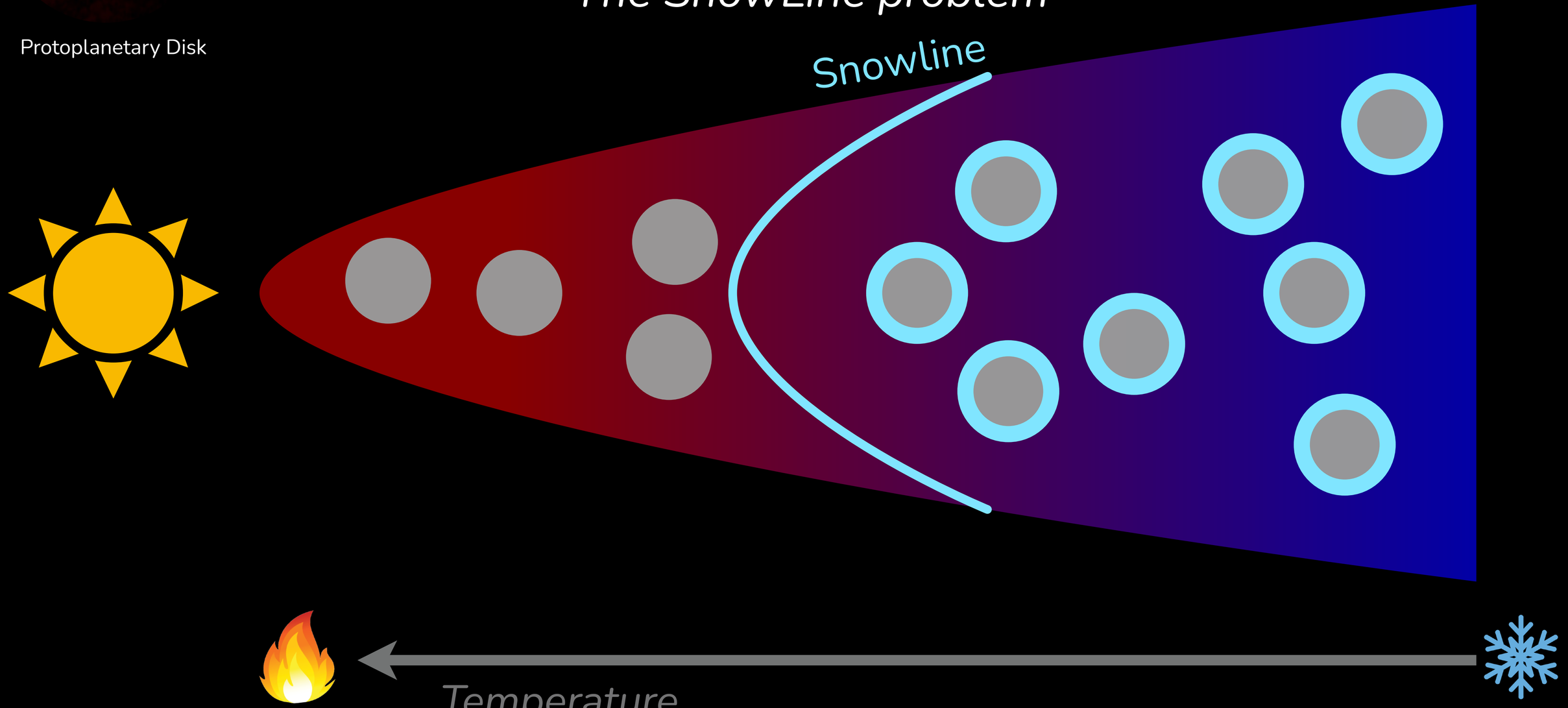
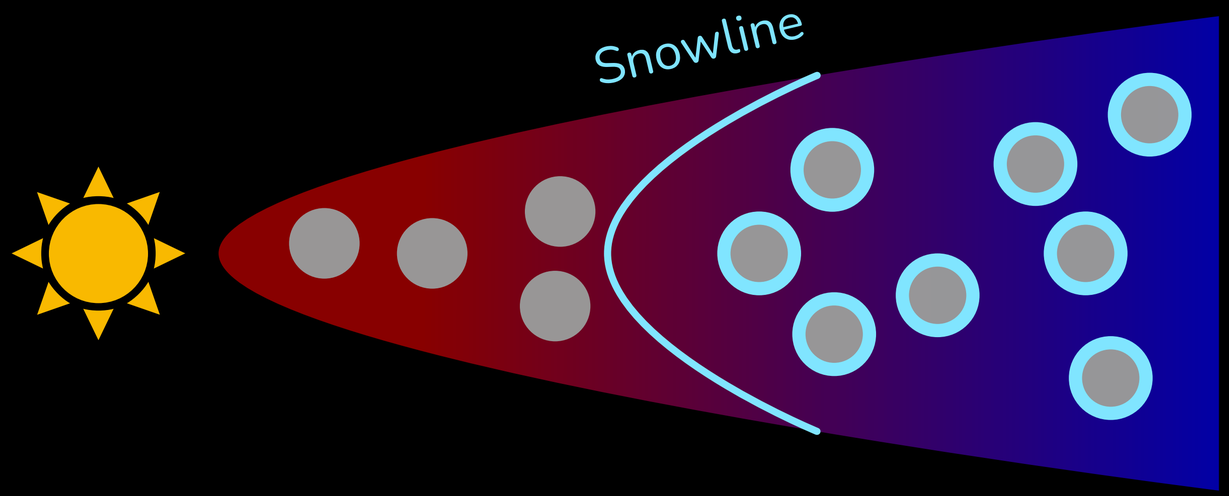


Protoplanetary Disk



# Defining the **Snowline**

*from icy to dry grains*



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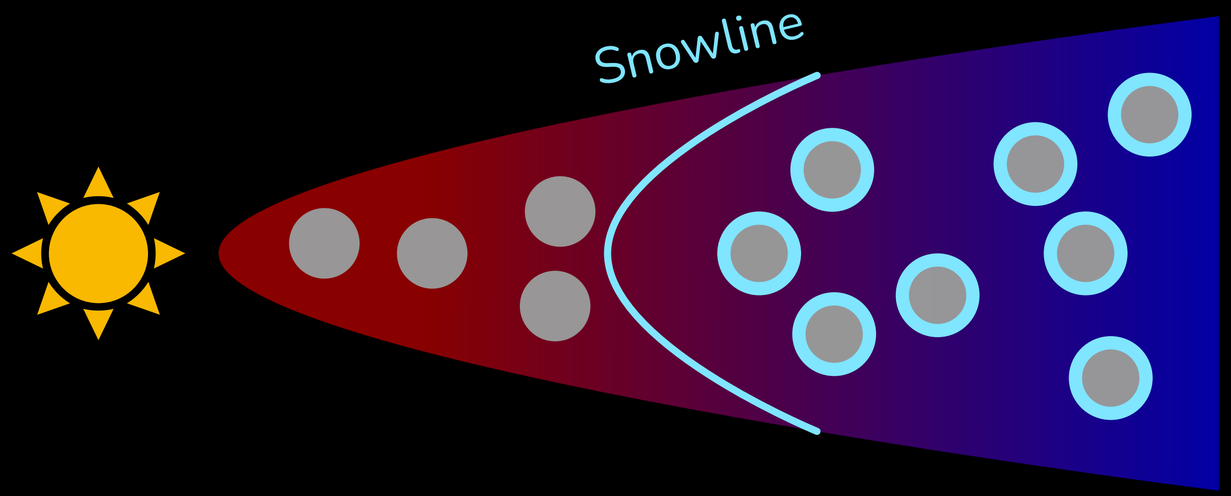


**Partial Pressure**

$P(H_2O) = P_{sat}(T)$

➜ Snowline @~170-180K

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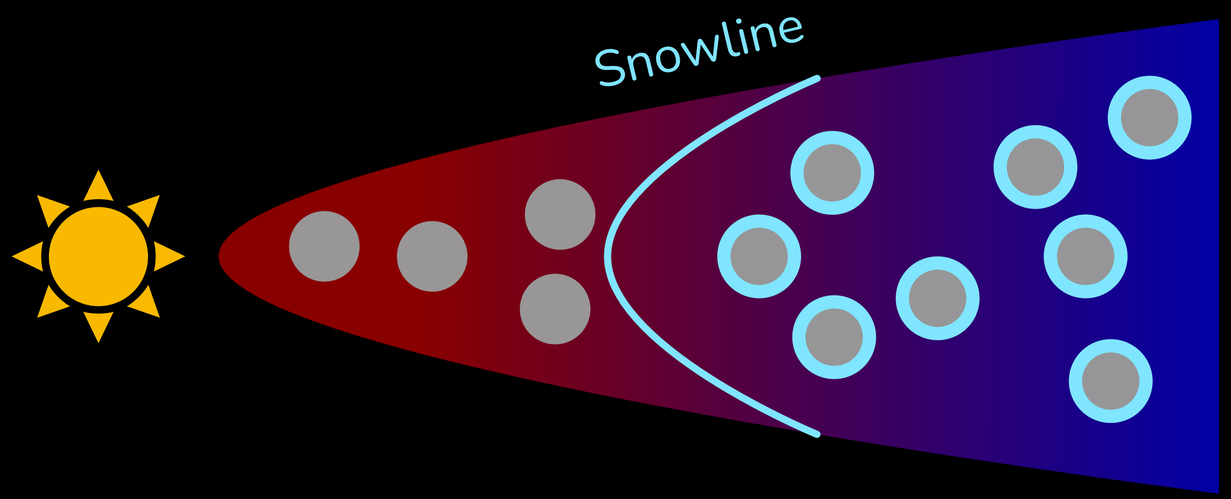



## Partial Pressure

$P(H_2O) = P_{sat}(T)$

➜ Snowline @~170-180K

## Kinetic desorption

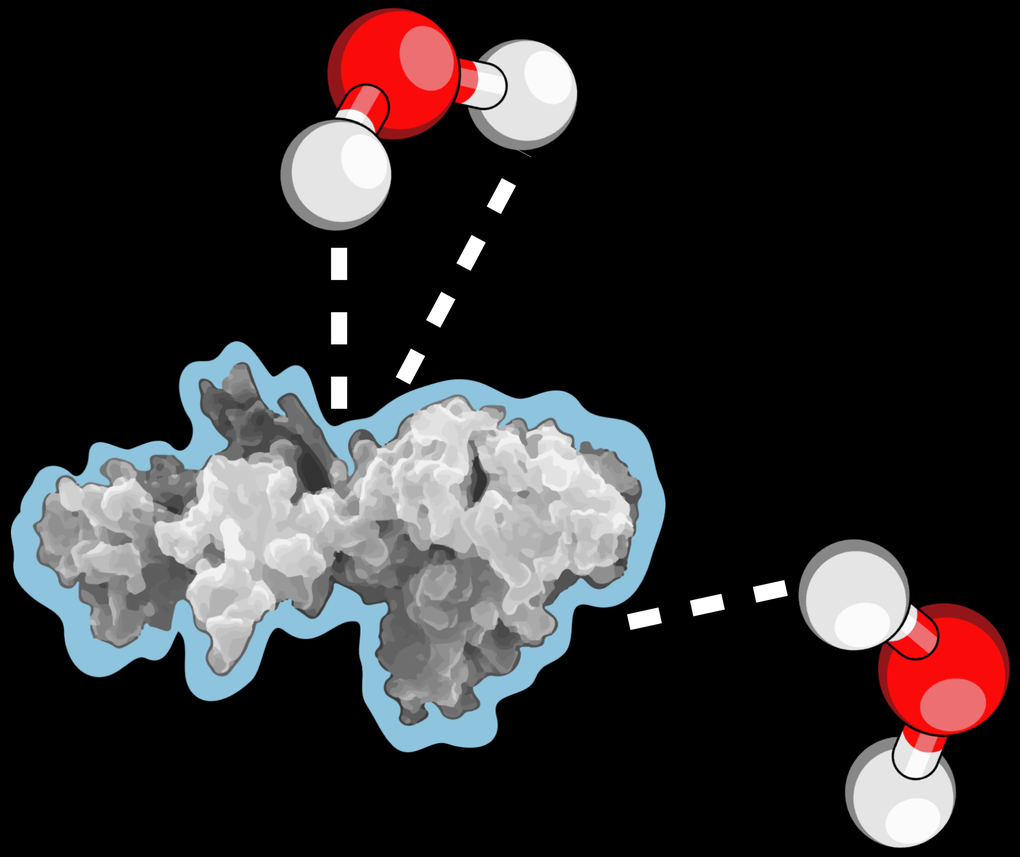
$R_{adsorption}(T) = R_{desorption}(T)$

$$R_{des} = \nu \exp\left(-\frac{BE}{T}\right)$$

BE = *Binding Energy (K)*
*= adsorption strength*
*of the molecule on the surface*

# Redefining the **Snowline**

*with the Binding Energy of Water onto the dust grains*



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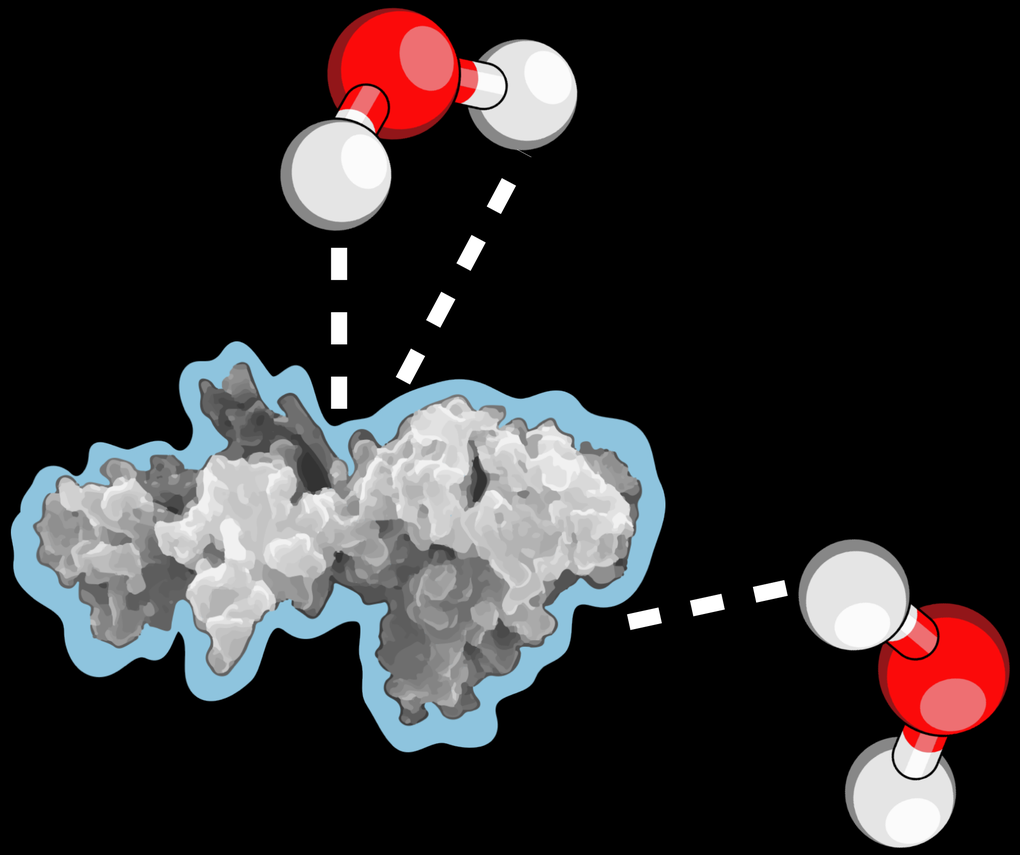

**Binding Energy :** A Unique Value ?

Multiple binding sites with different geometries

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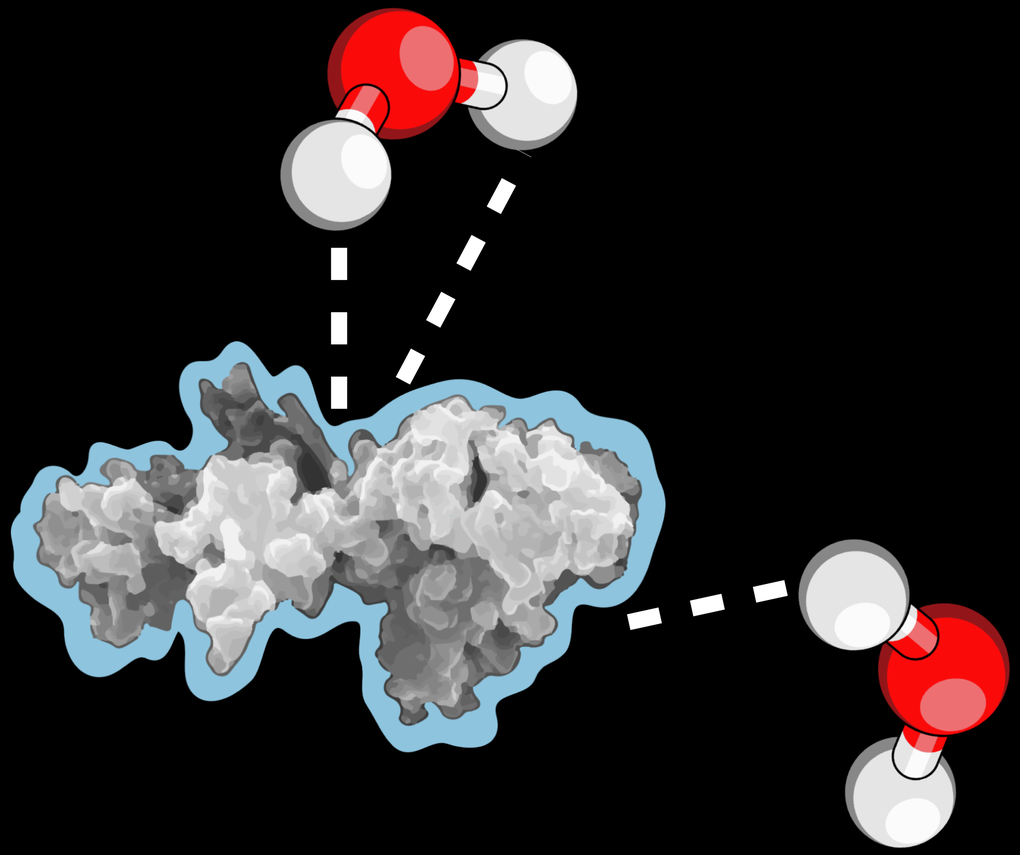

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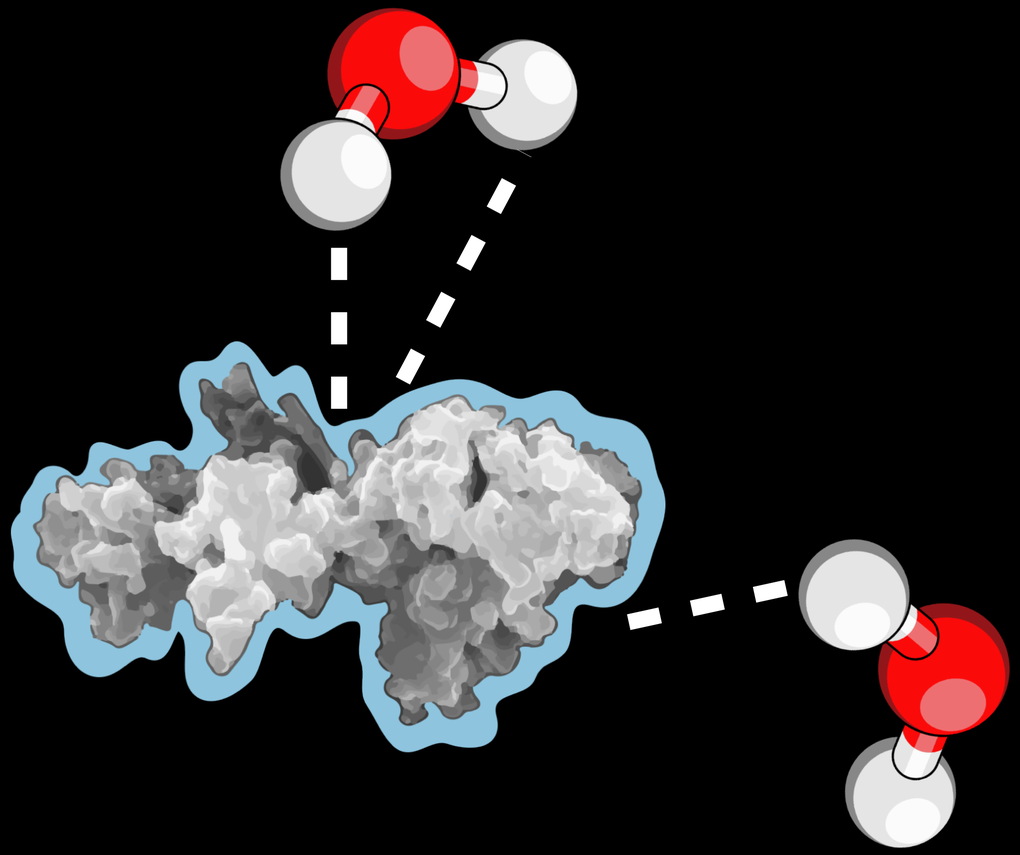


**Binding Energy :** A Unique Value ?

Multiple binding sites with different geometries

➳ need some help from **computational chemistry**

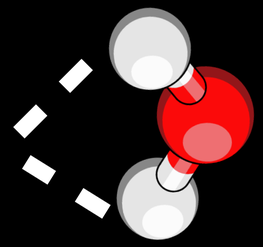
**Computational Chemistry ?**

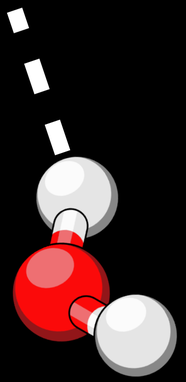
Solving the Schrödinger equation for molecules to predict their optimal structure and properties

Requires some approximation for complex systems, but still very accurate results

# Binding Energy of Water on interstellar grains

*From a single experimental value to a computationally determined distribution*





$$BE = E_{grain} + E_{H_2O} - E_{grain+H_2O}$$

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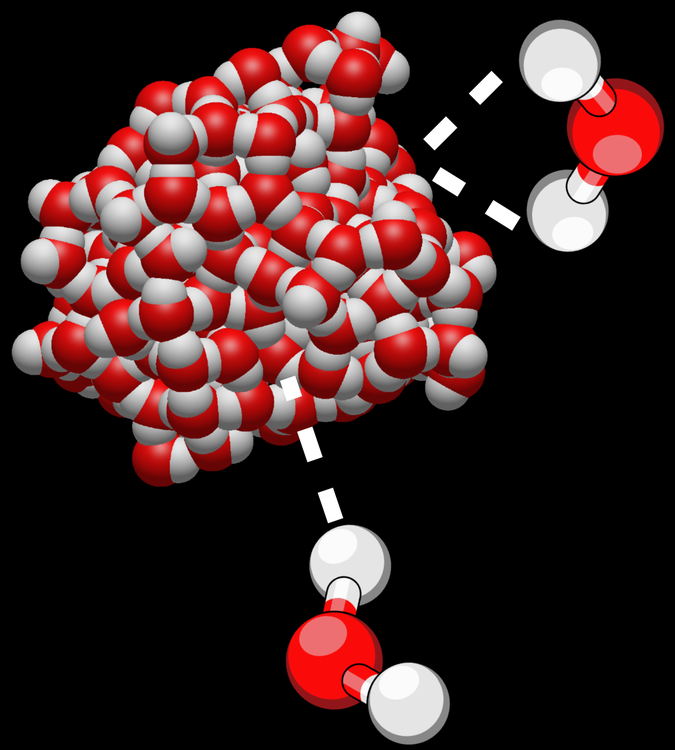

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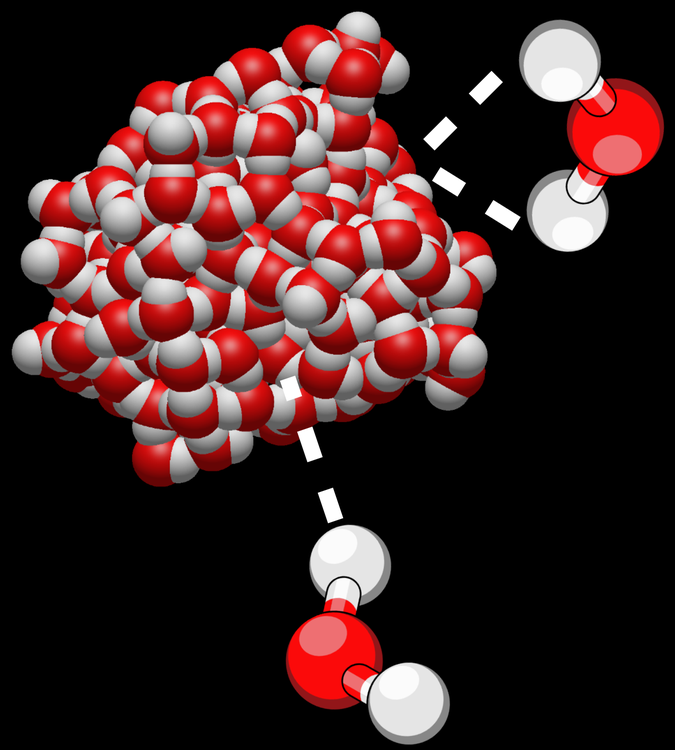
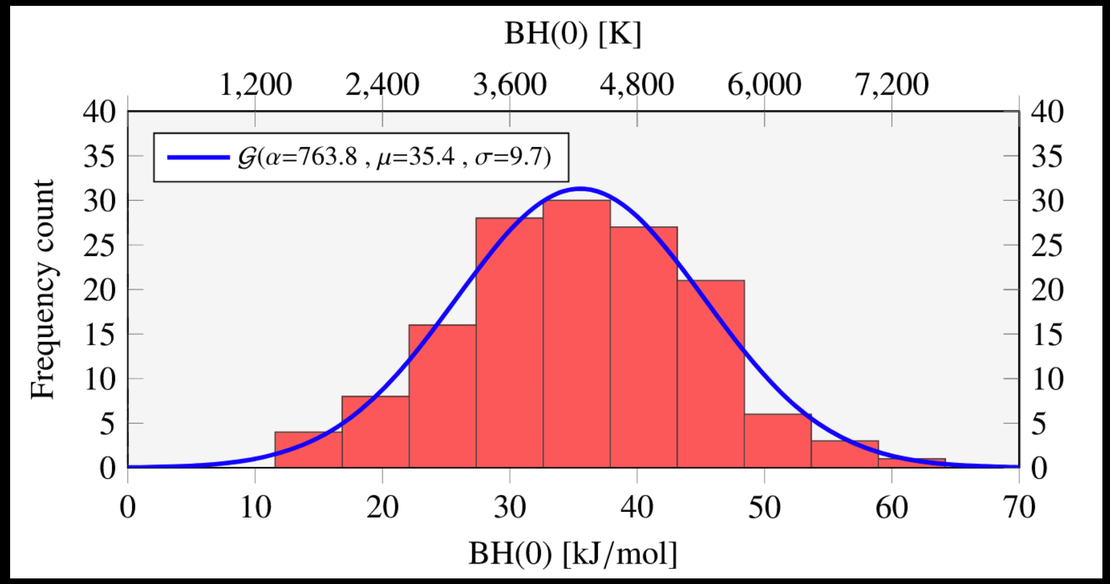


## Results



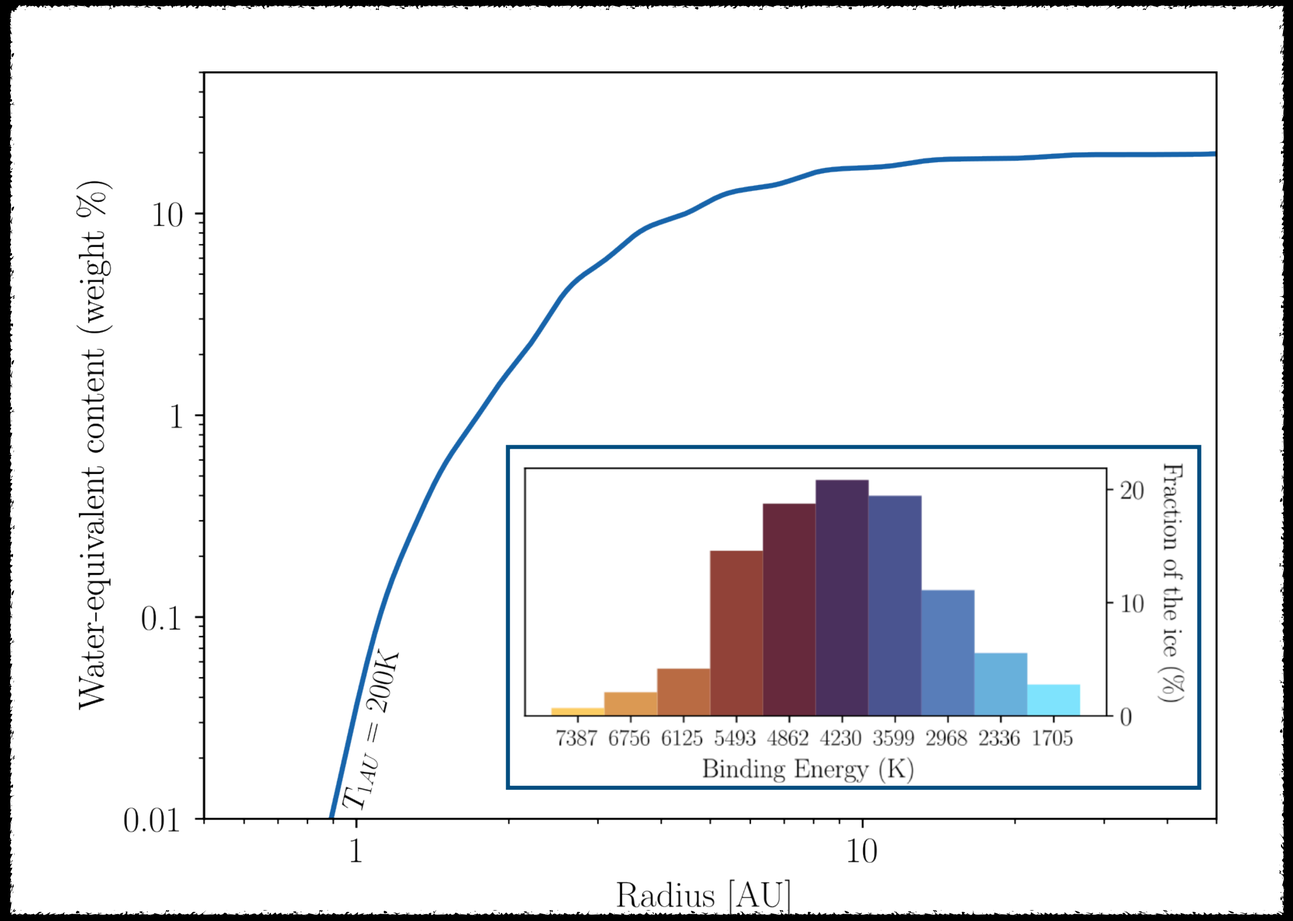

*Tinacci et al. 2023*

$$BE = E_{grain} + E_{H_2O} - E_{grain+H_2O}$$

# Were the grains actually dry ?

*Gradual desorption of water ice*

$$\frac{m_{ice}}{m_{grains} + m_{ice}}$$

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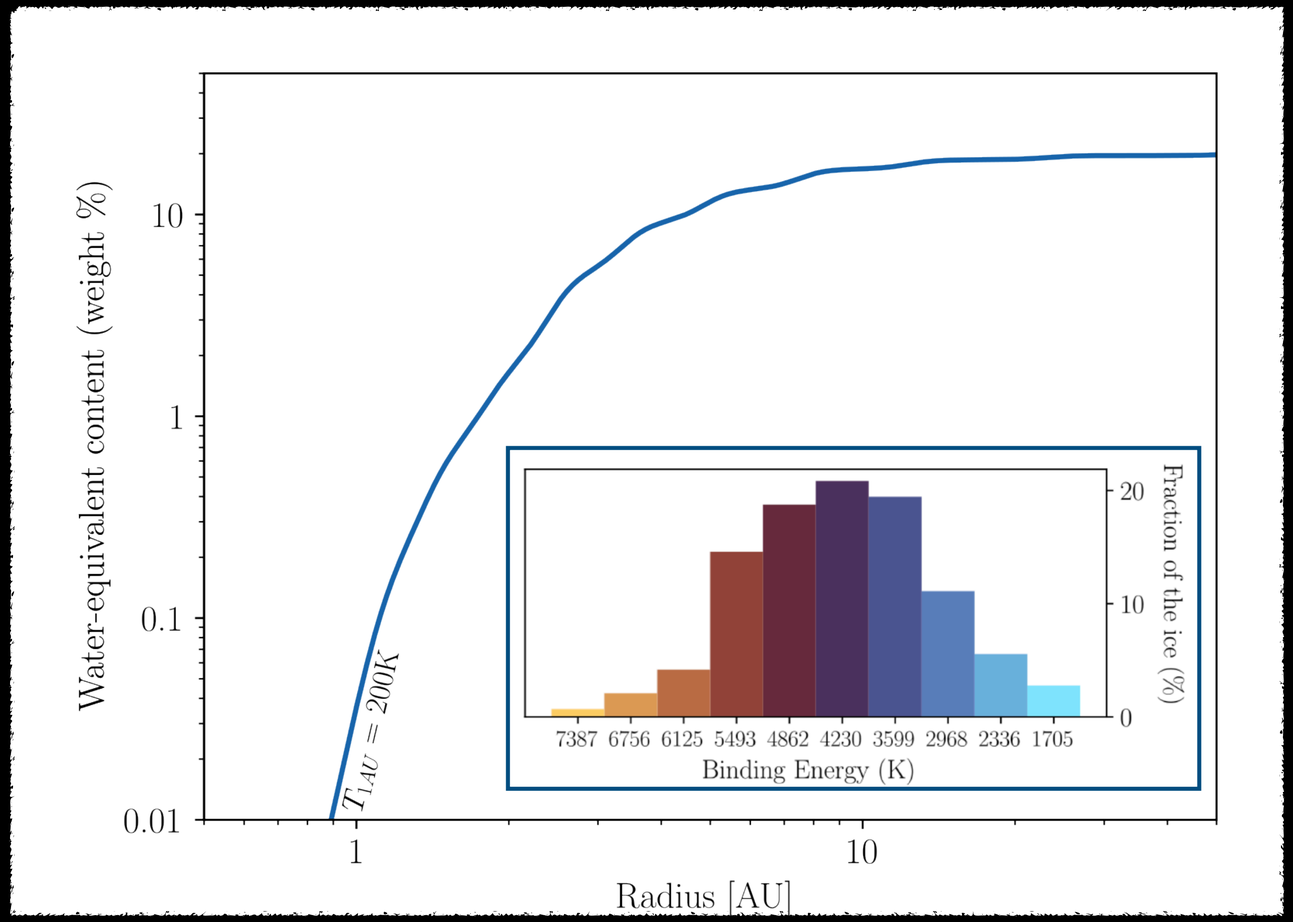


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📚Boitard-Crépeau et al, ApJL 2026

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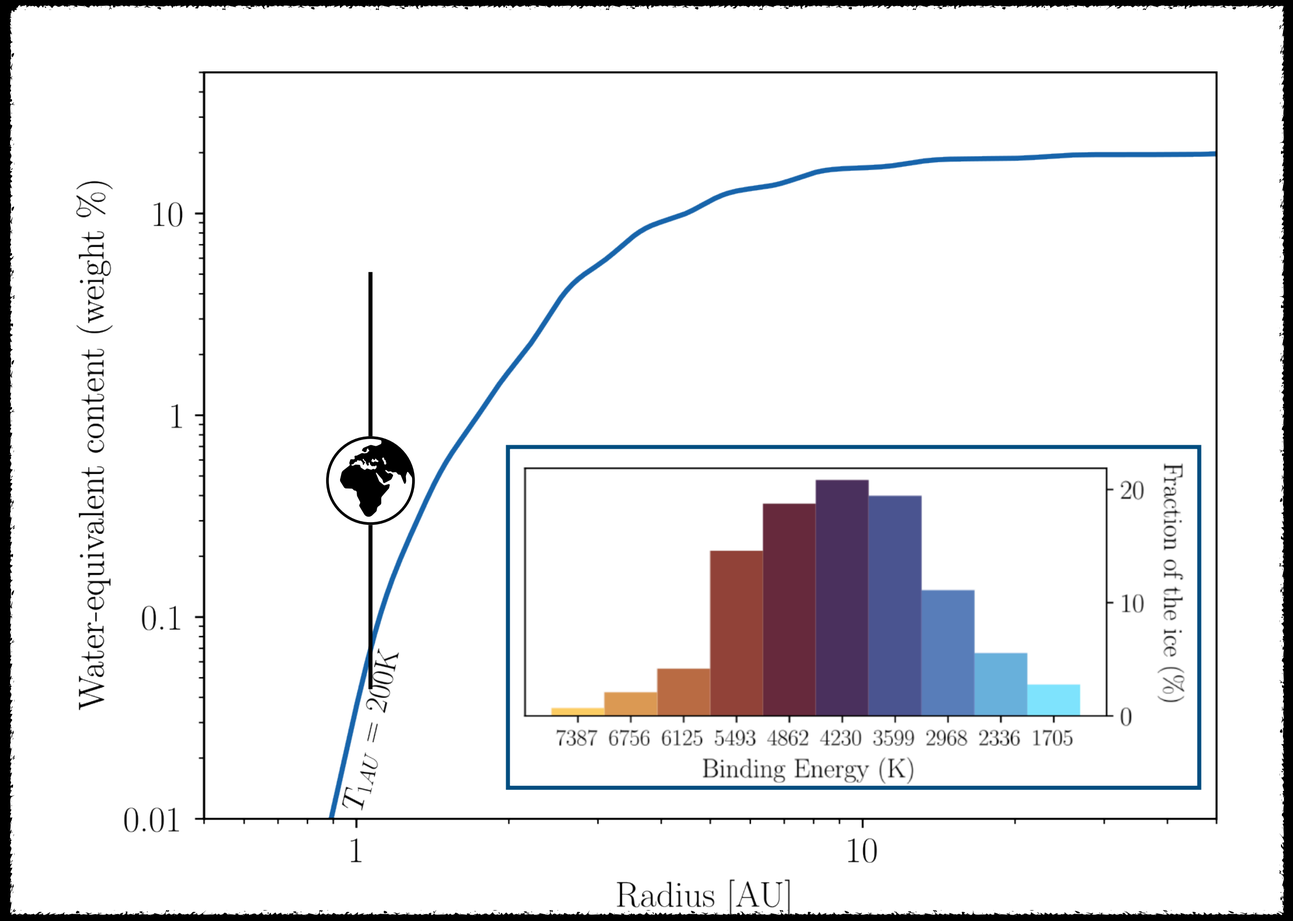


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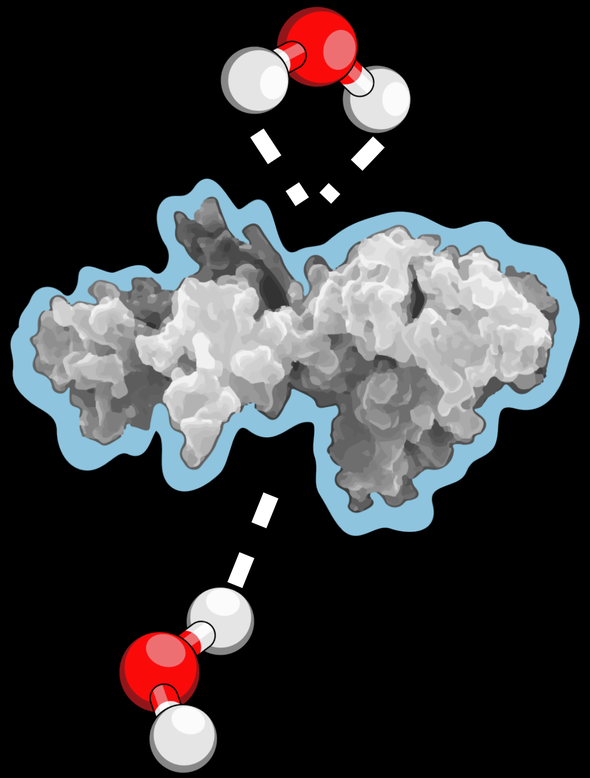
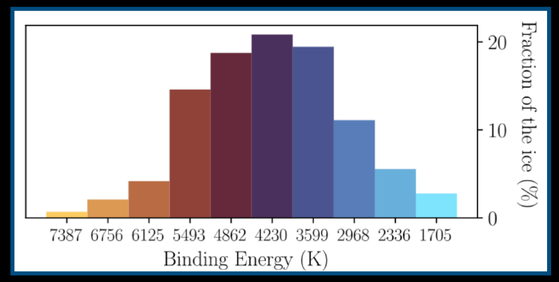


BE of water on icy mantle



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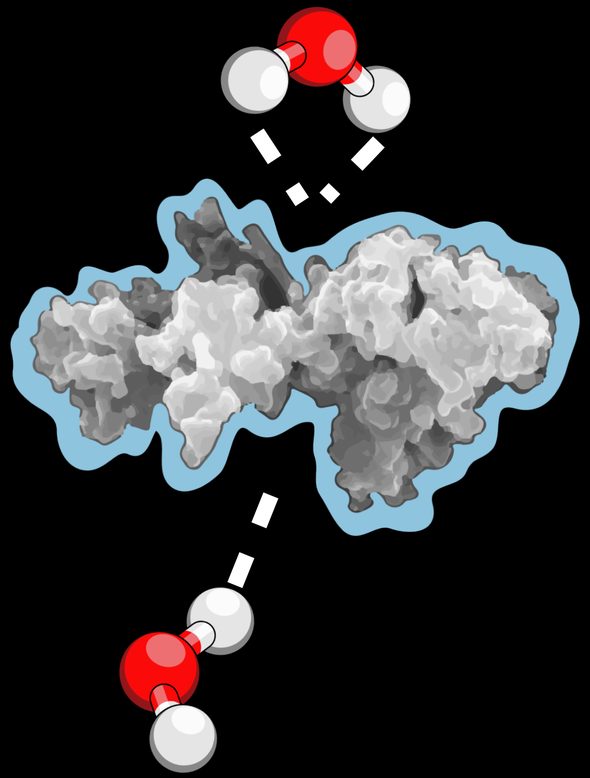

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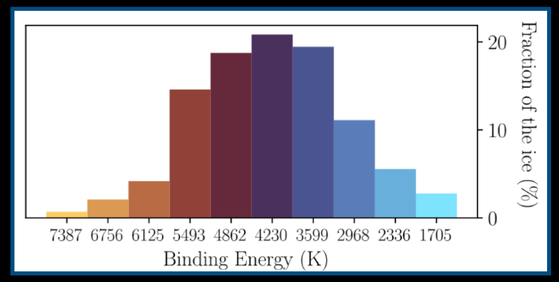
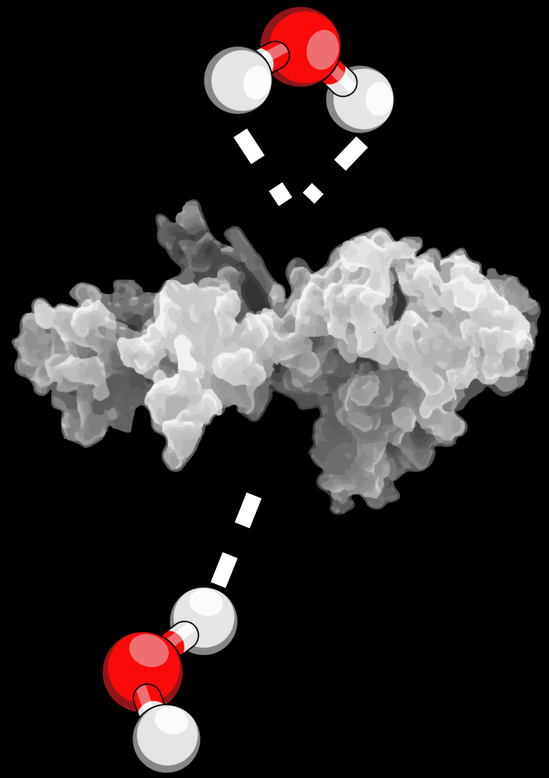


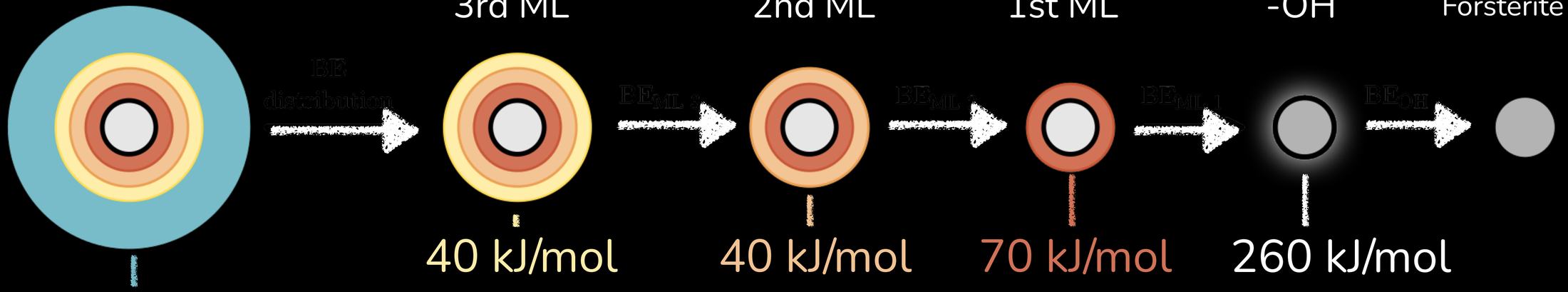



BE of water on silicate surface

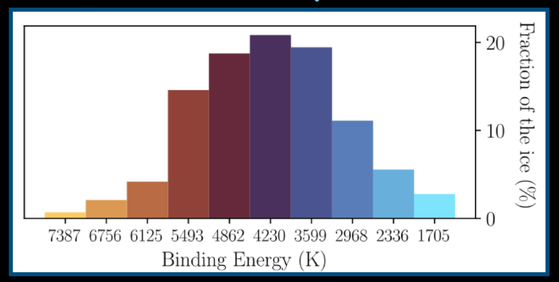
?

# Building Monolayers of water around a forsterite grain

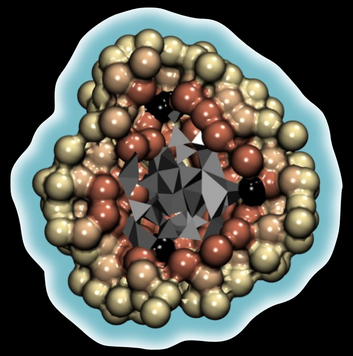
Icy mantle
(ML ≥3)




10-60 kJ/mol




10 30 40 60 kJ/mol



**Monolayer = ML*

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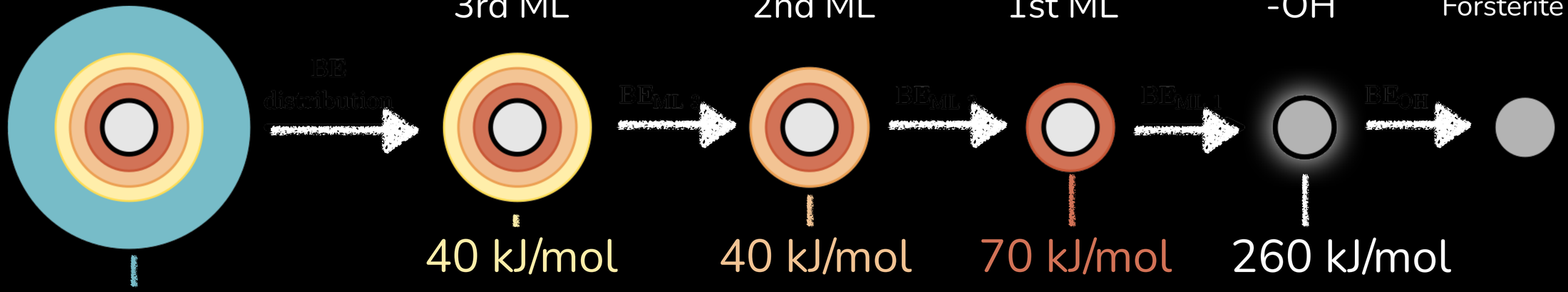


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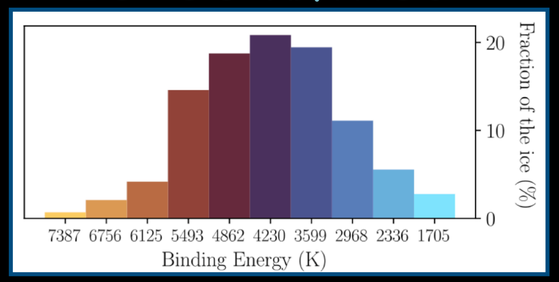


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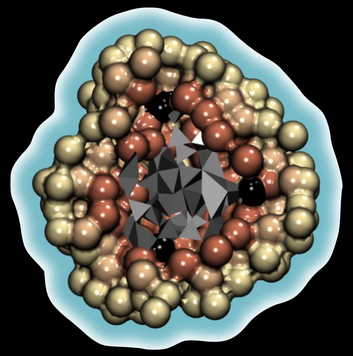

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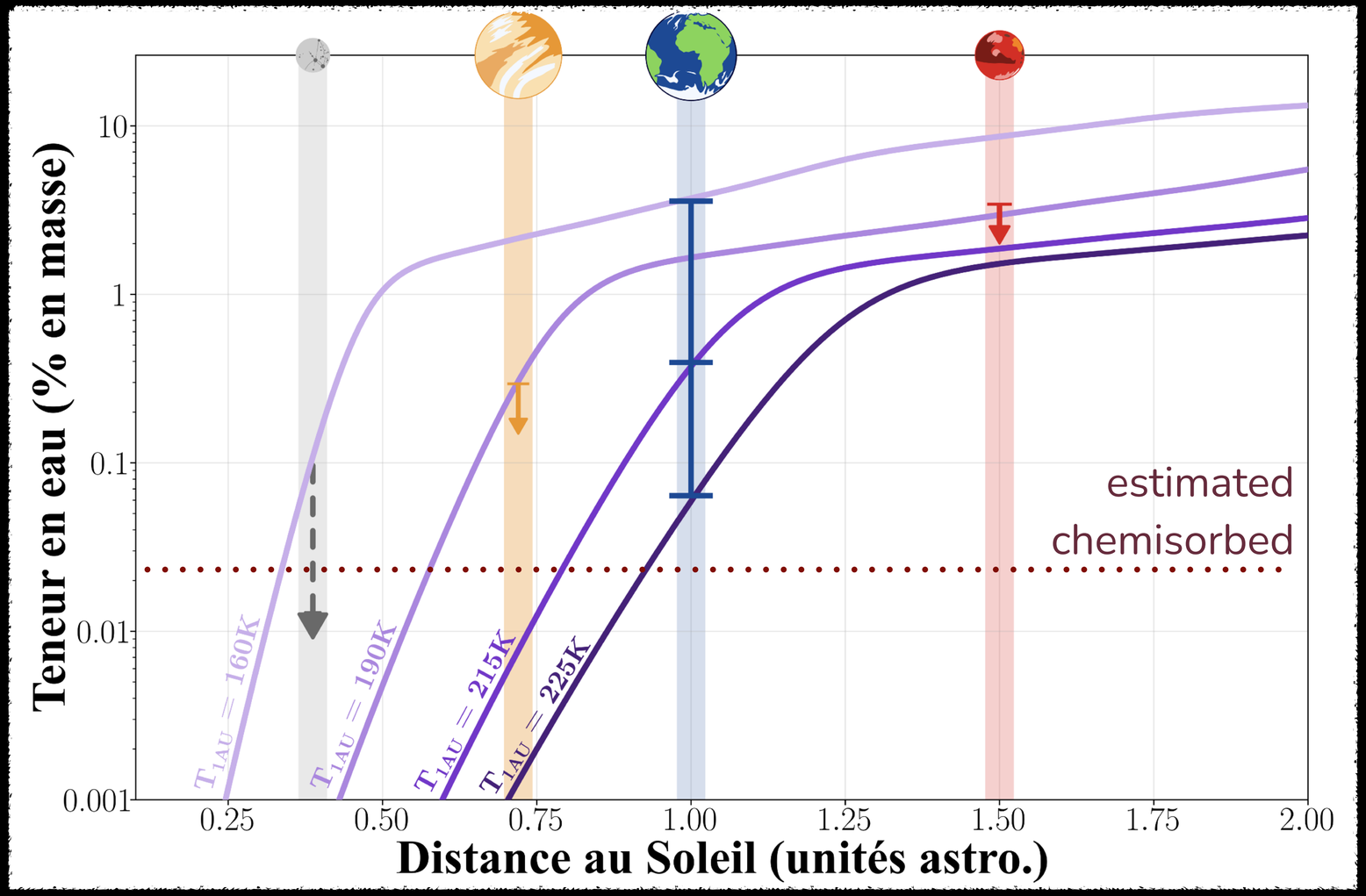
# How close to the Sun can water be retained ?



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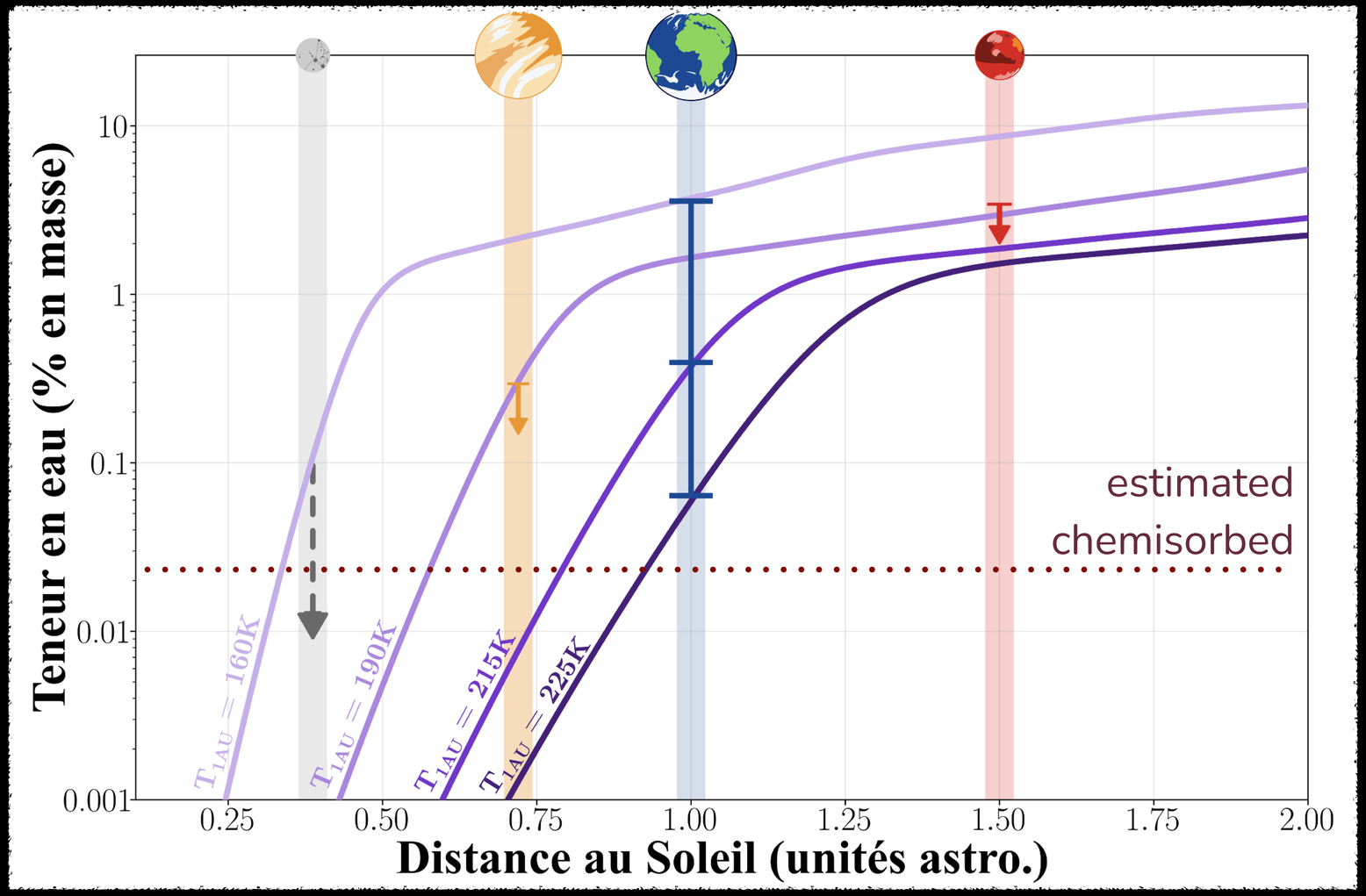


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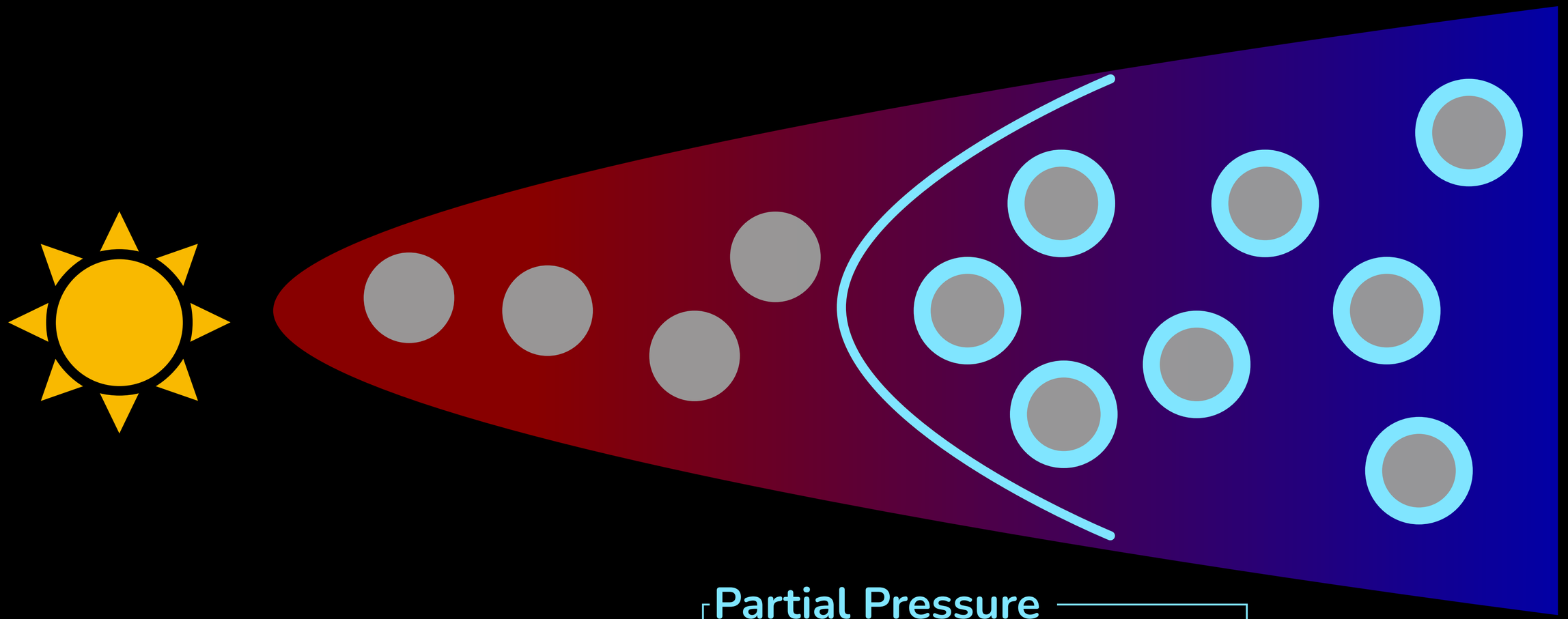


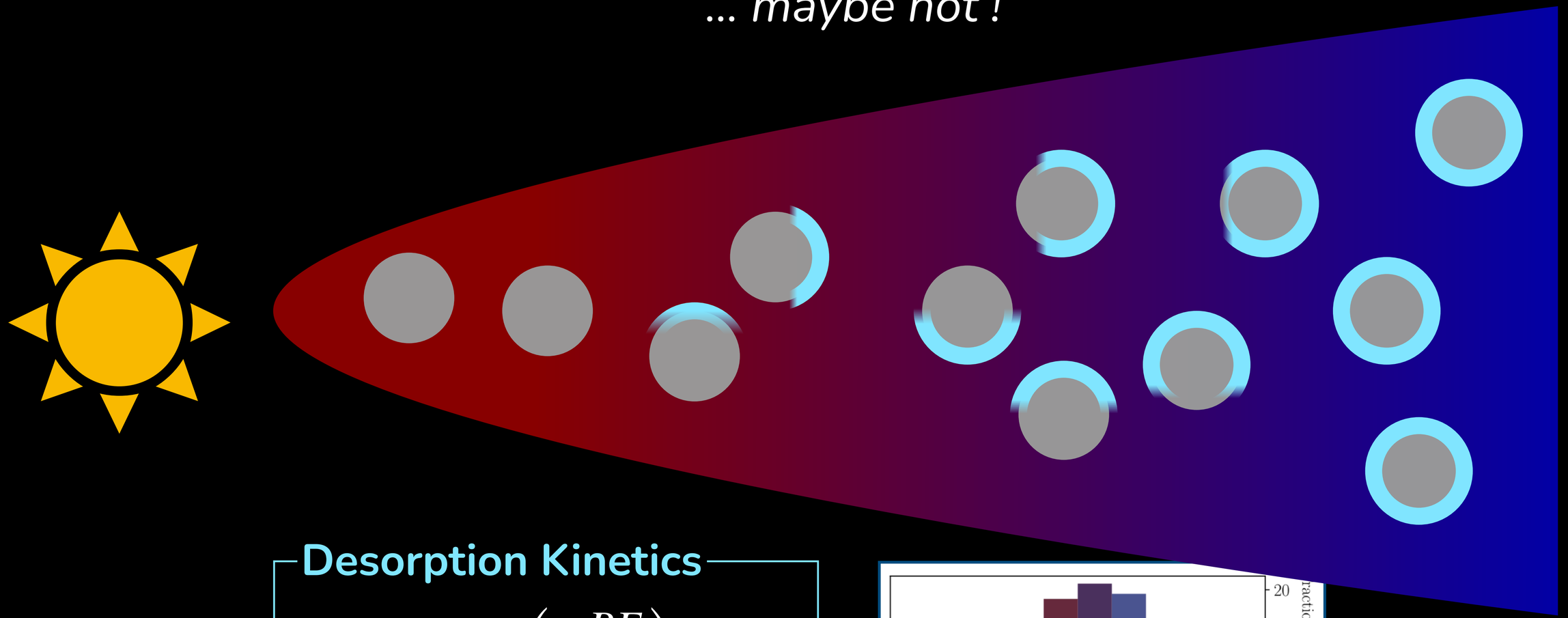
**Partial Pressure**

$P(H_2O) = P_{sat}(T)$

➜ Snowline @~170-180K

# Were the grains actually dry ?

*... maybe not !*

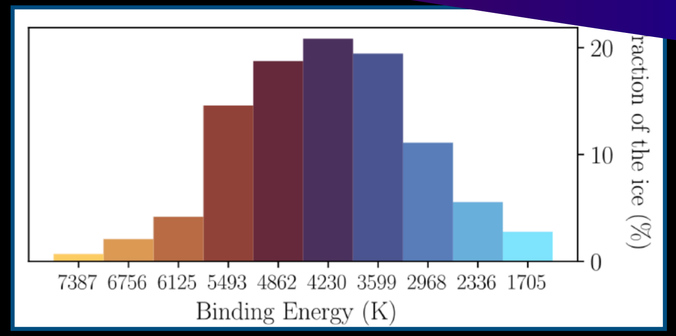


## Desorption Kinetics

$$R_{des} = \nu \exp\left(-\frac{BE}{T}\right)$$

BE = *Binding Energy (K)*

+



Terrestrial water could have been acquired **locally**, inherited from the early stages of the Solar System

➜ **Boitard-Crépeau et al, ApJL 2025**

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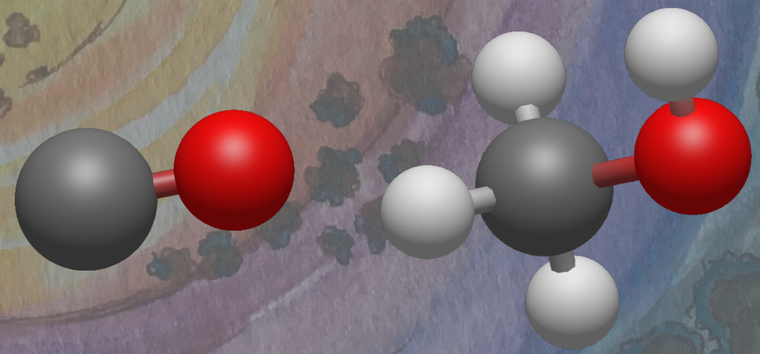
➜ **apply this method to more key interstellar molecules**



🚧 **Work in progress, stay tuned :)**

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➜ **Boitard-Crépeau et al, ApJL 2025**

If the Earth inherited its water from the ISM, Mars and the other terrestrial planets should also have accreted some water

➜ **Boitard-Crépeau & Pantaleone et al, MNRAS 2026**

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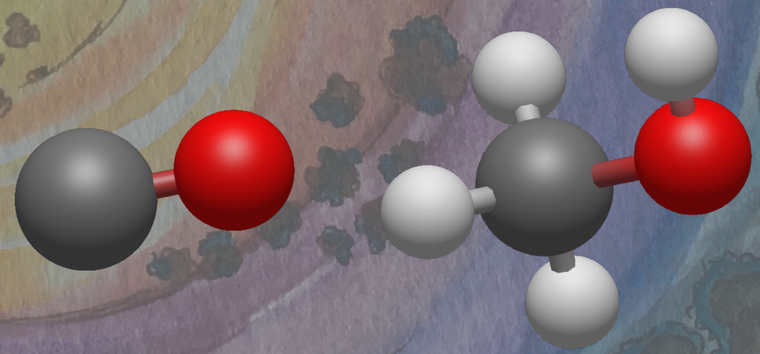

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L.Boitard-Crépeau