Salt particle hydration

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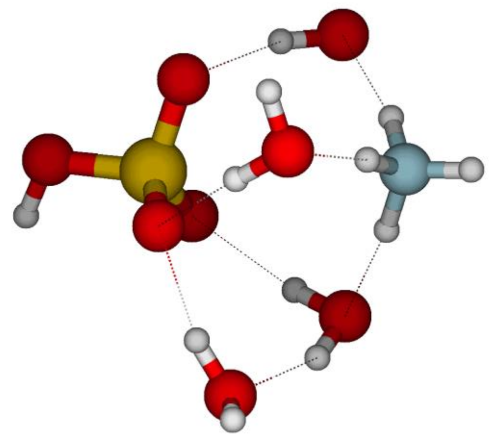
What?

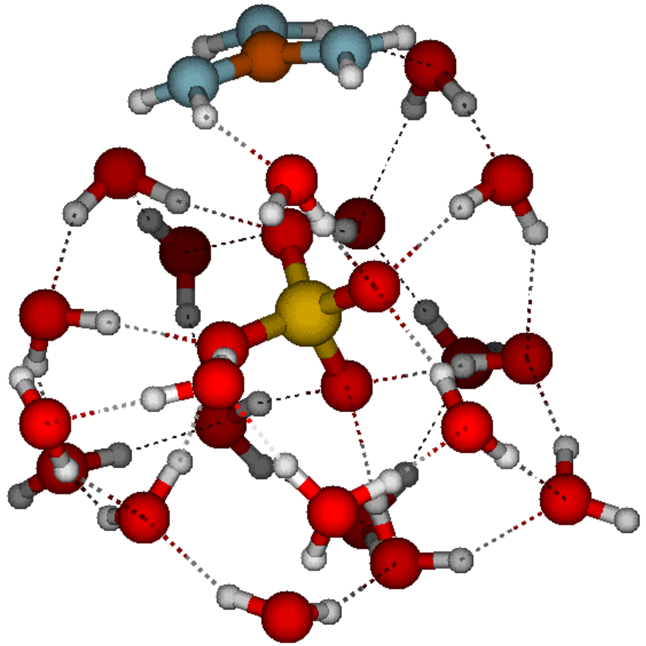
- NPF from condensable acid and base molecules is a ubiquitous phenomenon in the atmosphere
- Water can stabilize or destabilize cluster structures

➢ DIFFICULT

  ➢ affect non-linear effects on the cluster formation dynamics

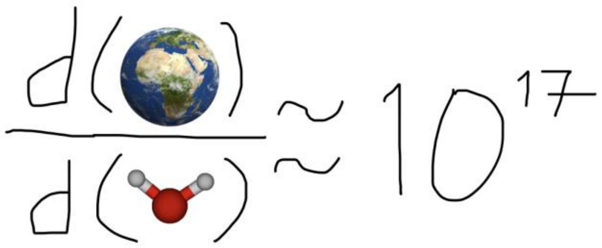
  ➢ role of water in NPF is not well-understood

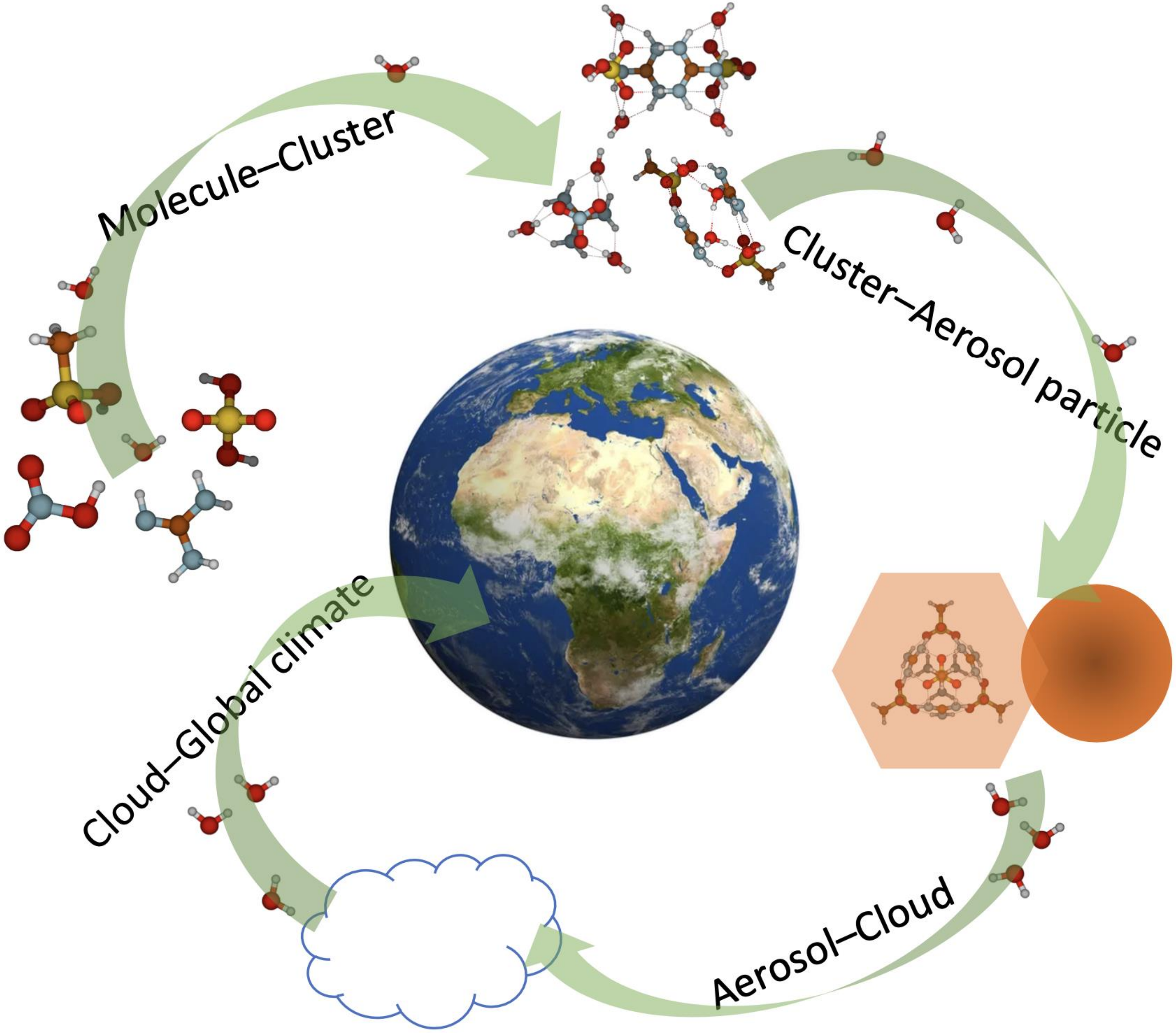




Why?

Water molecules (d=0.00000000027 m) impact the radiation balance of Earth (d=12 700 000 m)

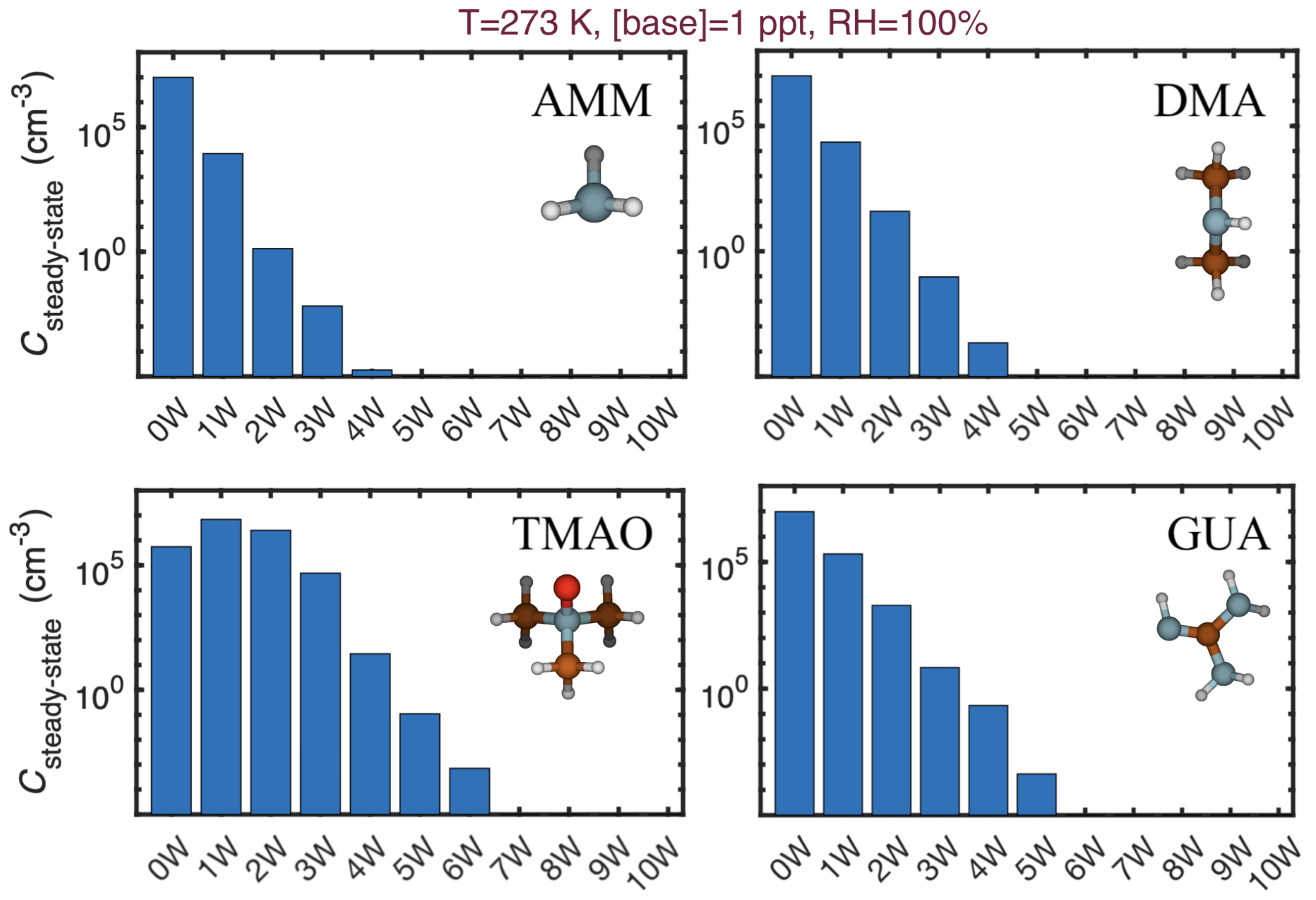




Monomer hydration

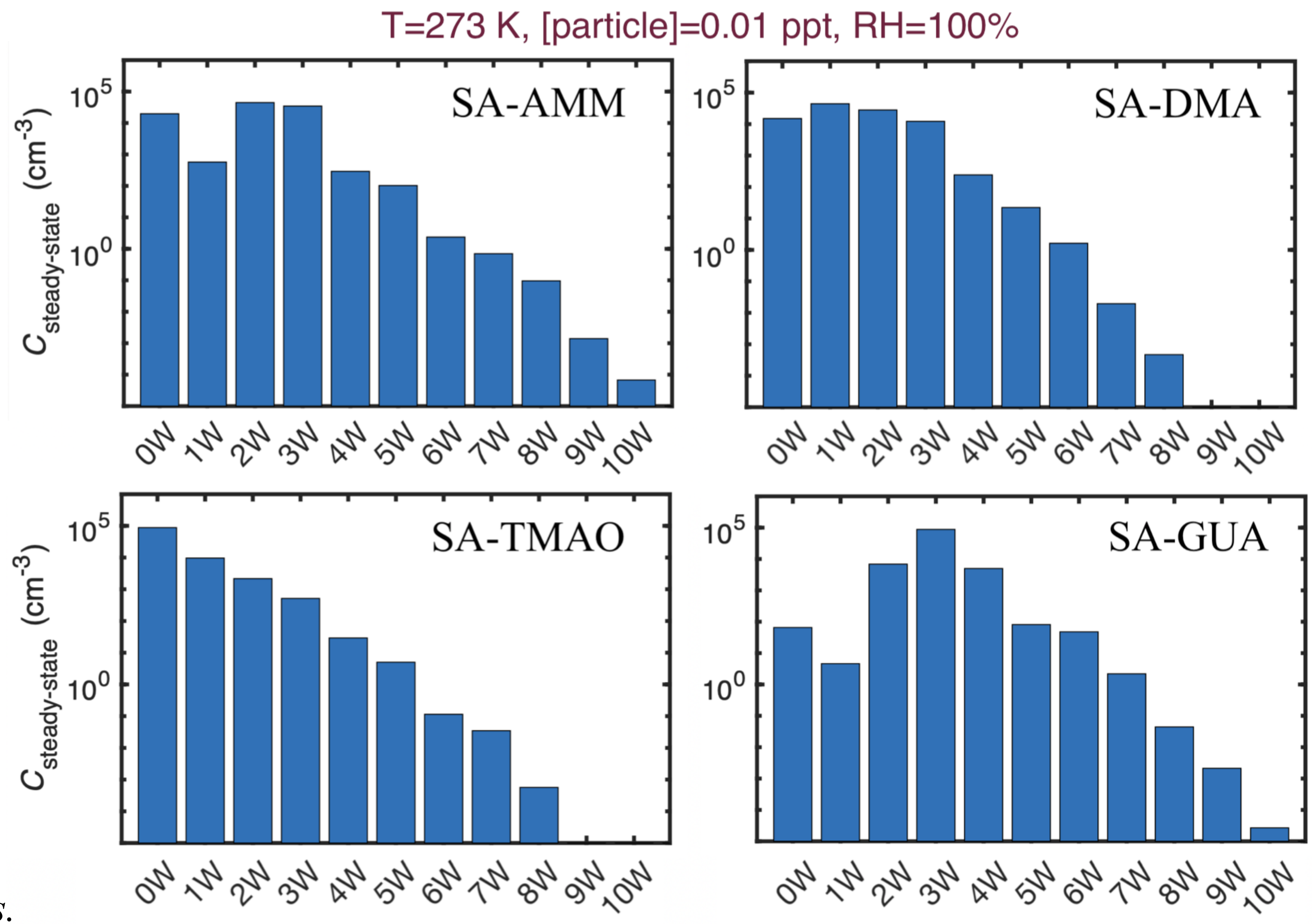
- Base monomers mainly exist as a dry form in the atmosphere
- TMAO is a special case due to its zwitter ionic structure
- Base monomer hydration seems to increase as gas-phase basicity increases

TMAO > GUA > DMA > AMM



Particle hydration

- Sulfuric acid–base particles exist as hydrated in the atmosphere
- SA–AMM and SA–DMA are present more in their hydrated forms
- Only 0.1% of the SA–GUA particles exist as a dry form



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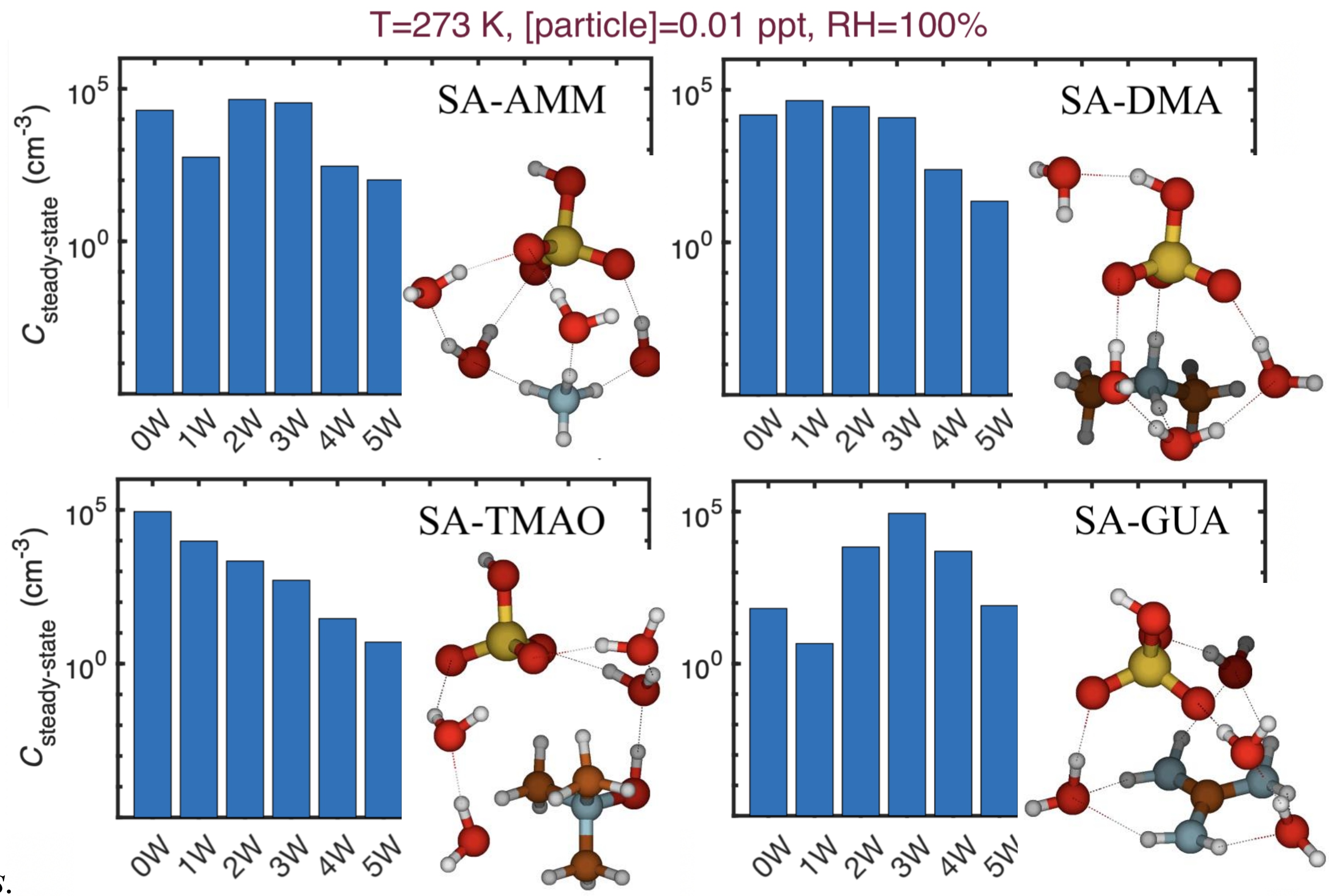
- **Particles seem to be more hydrated when #H-bonds increase**



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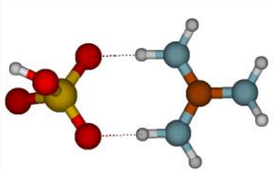
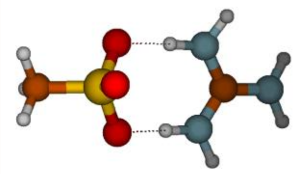
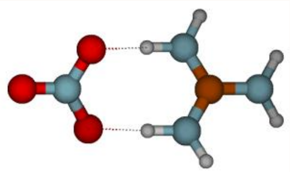
Cluster (de)stabilation

RH=100%, T=273 K	SA	MSA	NA
1acid1GUA	$2 * 10^{-2}$	$5 * 10^{-5}$	$2 * 10^{-2}$
1acid2GUA	4.0	62.5	0.3
2acid1GUA	114	200	3.8
2acid2GUA	10^{4}	$3 * 10^{5}$	3.3

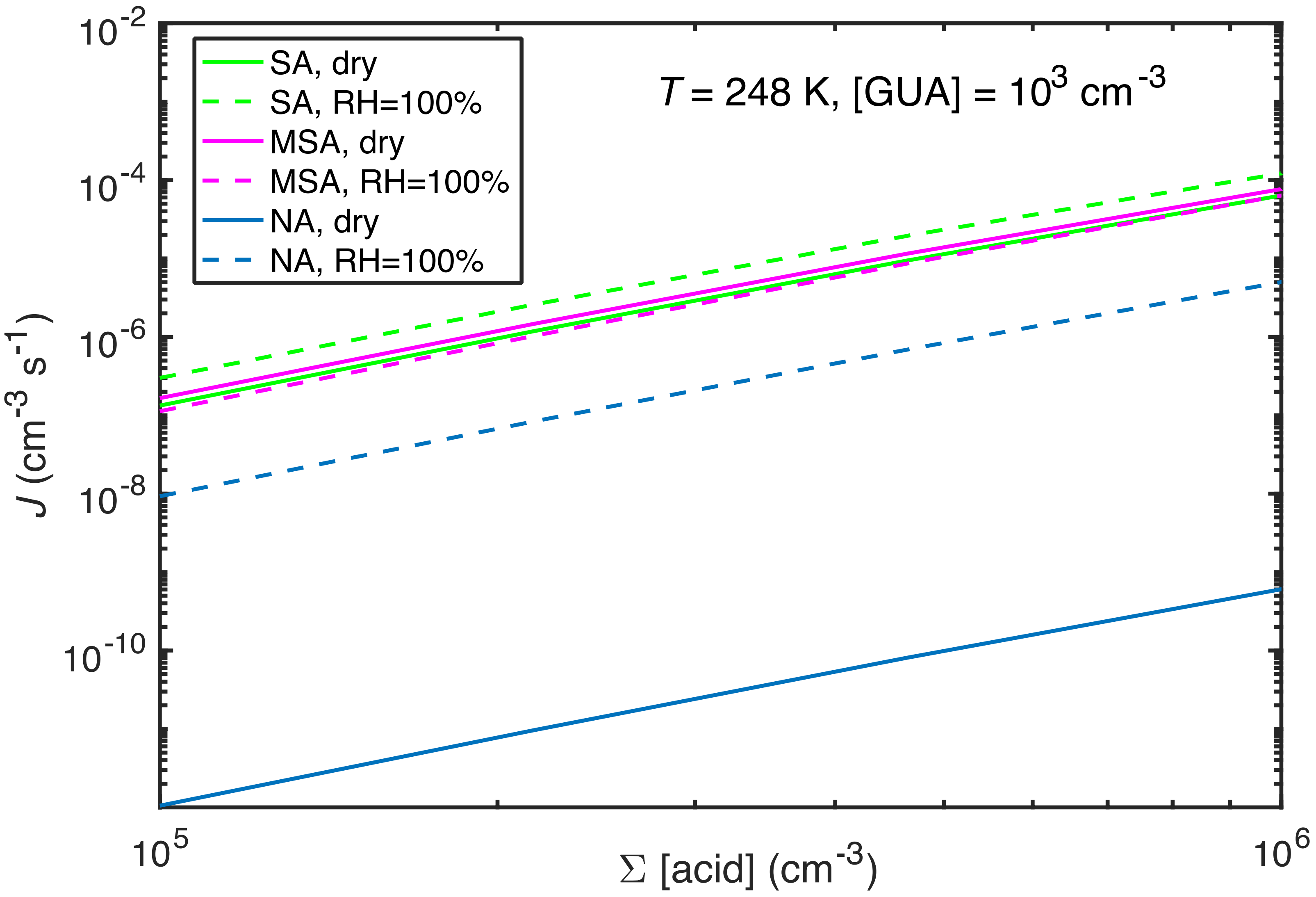
$$\text{Effect of } RH \text{ on the evaporation rate} = \frac{\sum \gamma(RH = 100\%)}{\sum \gamma(RH = 0\%)}$$

- Depending on the size and composition of the cluster, water may stabilize (green) or destabilize (red) the cluster
- This is the reason for the non-linear effects of hydration on cluster formation dynamics

Effect of *RH* in particle formation

- Water slightly increases SA–GUA NPF
  - *HF*≈1.9
- Water slightly decreases MSA–GUA NPF
  - *HF*≈0.8
- Water significantly increases NA–GUA NPF
  - *HF*≈10000
- **Water may intensify or inhibit NPF**

$$HF = \frac{J_{\mathrm{humid}}}{J_{\mathrm{dry}}}$$



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Note: *HF* is condition dependent

[Acid] cm^{-3}	T = 248 K and [GUA] = 10^3 cm^{-3}				T = 273 K and [GUA] = 10^4 cm^{-3}				T = 298 K and [GUA] = 10^5 cm^{-3}			
	J_{dry}	HF_{10}	HF_{50}	HF_{100}	J_{dry}	HF_{10}	HF_{50}	HF_{100}	J_{dry}	HF_{10}	HF_{50}	HF_{100}
[SA]												
10^6	6×10^{-5}	1.5	1.8	1.9	7×10^{-4}	1.3	1.5	1.3	4×10^{-1}	1.1	0.9	0.9
10^7	7×10^{-4}	1.2	1.5	1.6	7×10^{-1}	1.2	1.4	1.5	5×10^1	1.1	1	1
10^8	6×10^{-1}	1.2	1.4	1.5	4×10^1	1.1	1.3	1.3	10^3	1	1.1	1.1
10^9	4×10^1	1.1	1.3	1.3	10^3	1	1.1	1.2	2×10^4	1	1.1	1.1
10^{10}	10^3	1	1.1	1.1	10^4	1	1.1	1.1	2×10^5	1	1	1.1
[MSA]												
10^6	8×10^{-5}	1.4	1	0.8	3×10^{-4}	1.2	1.1	1.1	10^{-4}	22	272	297
10^7	8×10^{-4}	1.3	1.3	1.2	6×10^{-1}	1.2	1.1	1.1	2×10^{-1}	20	164	174
10^8	7×10^{-1}	1.2	1.3	1.3	5×10^1	1.1	1.1	1.1	4×10^1	10	29	30
10^9	4×10^1	1.1	1.2	1.2	10^3	1	1.1	1.1	9×10^3	1.5	1.8	1.9
10^{10}	10^3	1	1.1	1.1	2×10^4	1	1	1	2×10^5	1	1	1
[NA]												
10^6	6×10^{-10}	1.2	219	8284	4×10^{-11}	1.1	31	1910	9×10^{-12}	1	6.6	239
10^7	10^{-7}	1.2	207	7752	7×10^{-9}	1.1	30	1790	2×10^{-9}	1	6.3	224
10^8	10^{-5}	1.2	205	7568	8×10^{-7}	1.1	29	1767	2×10^{-7}	1	6.2	222
10^9	10^{-4}	1.2	204	6840	8×10^{-5}	1.1	29	1764	2×10^{-5}	1	6.2	221
10^{10}	10^{-1}	1.2	197	3723	8×10^{-4}	1.1	29	1760	2×10^{-4}	1	6.2	221

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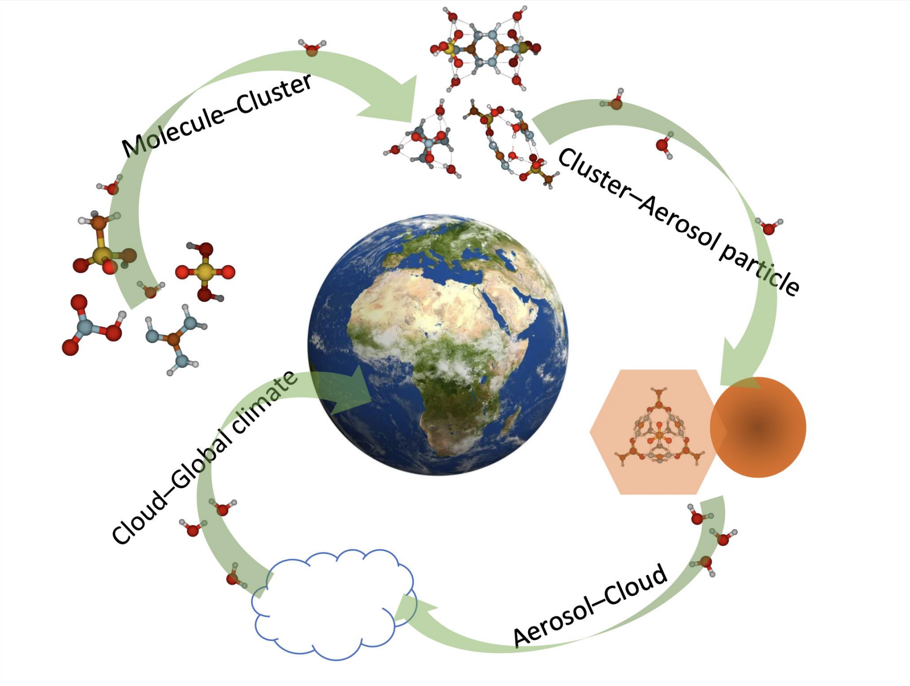
Conclusions



- Monomers mainly exist in the atmosphere as dry
  - Hydration depends on the gas-phase basicity
- Particles mainly exist in the atmosphere as hydrated
  - Hydration depends on the number of hydrogen binding sites
- Effect of RH in NPF varies many orders of magnitude depending on the system and conditions
  - This depends on the (de)stabilization effect on clusters
- Neglecting effect of hydration in NPF may introduce remarkable inaccuracies in large-scale models
  - ➢ Computationally cheap but accurate molecular-level parametrization to compute HF is needed

Thanks for your attention!

Molecular Level Atmospheric Science group

CSC

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