Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Accelerating water evaporation from salty droplets on polar substrate: A molecular dynamics study

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1. Evaporation from sodium chloride (NaCl) solution droplet

We consider the evaporation of salty droplet for different concentrations of $MgCl_2$-solution as shown below.

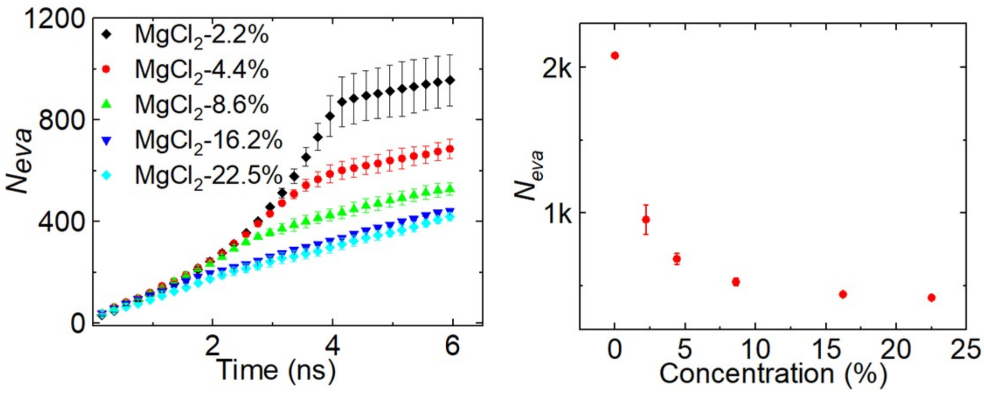

Figure S1. Evaporation changes as the concentration of $MgCl_2$ and the concentration in water droplet is considered as 0.

Besides the $MgCl_2$-solution, we study the water evaporation from NaCl-solution droplet as shown in the following figure. The NaCl suppresses the water evaporation as the $MgCl_2$. The evaporation is further decreased with elevated concentration of NaCl. The results show that ions in the droplet suppress the water evaporation compared to the pure water droplet, which is not dependent on the ion type.

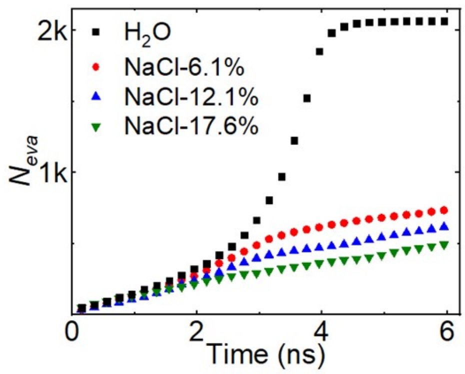

Figure S2. Evaporation of water molecules as time for NaCl droplets with different concentrations.

2. Effects of water models and temperatures

The different water models and temperatures affect the evaporation rate, but show no effects on the fact that ions in the salty droplet suppress the water evaporation compared to the pure water droplet.

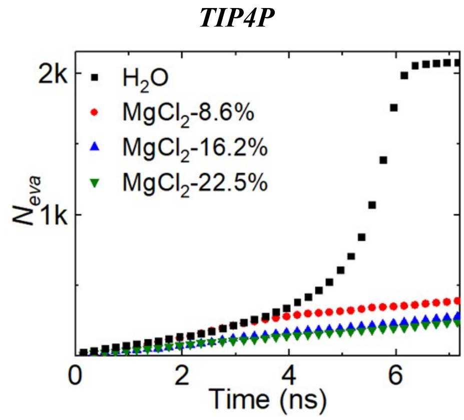

Figure S3. Evaporation of water molecules as time for water and $MgCl_2$ droplets by using the TIP4P water model.

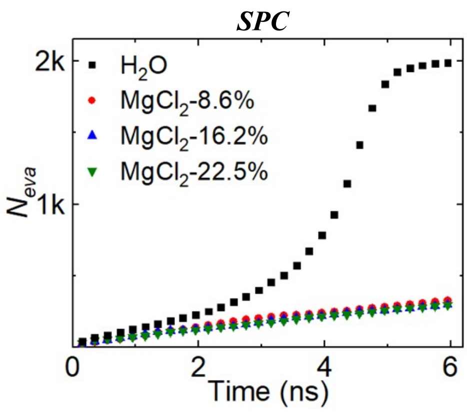

Figure S4. Evaporation of water molecules as time for water and $MgCl_2$ droplets by using the SPC water model.

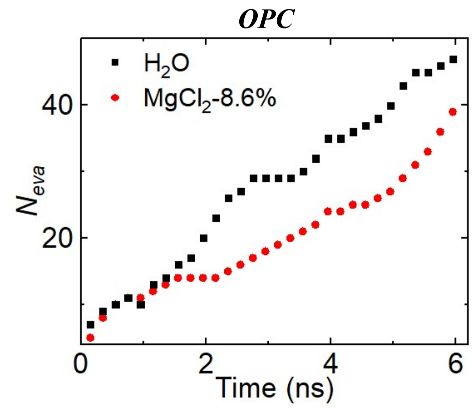

Figure S5. Evaporation of water molecules as time for water and $MgCl_2$ droplets by using the OPC water model.

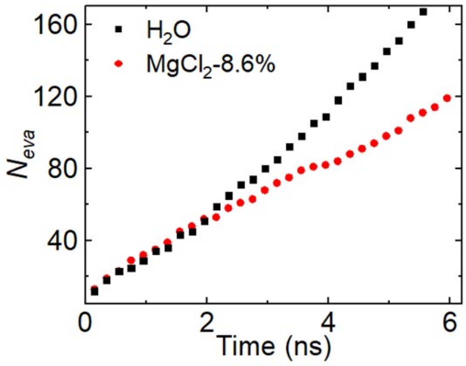

Figure S6. Evaporation of water molecules as time for water and $MgCl_2$ droplets at 300 K.

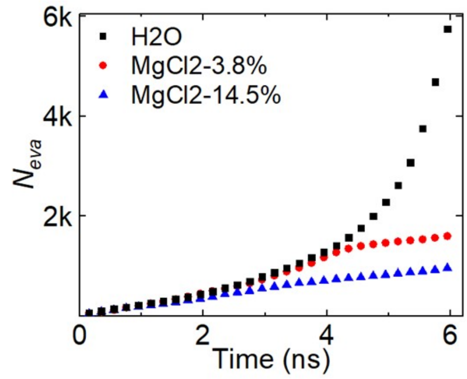

Figure S7. Evaporation of water molecules from droplet containing ~ 6500 molecules with different concentrations.

3. Cohesive energy calculation

The cohesive energy is derived from the following equation S1:

$$E_c = \frac{3}{N}\sum_{i}^{N}\left\{\sum_{j\neq i}^{M}4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12}-\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]+\sum_{j\neq i}^{M}\frac{1}{4\pi\varepsilon_{water}}\cdot\frac{q_iq_j}{r_{ij}}-\sum_{j'\neq i}^{P}4\varepsilon_{ij'}\left[\left(\frac{\sigma_{ij'}}{r_{ij'}}\right)^{12}-\left(\frac{\sigma_{ij'}}{r_{ij'}}\right)^{6}\right]+\sum_{j''\neq i}^{Q}\frac{1}{4\pi\varepsilon_{water}}\cdot\frac{q_iq_{j''}}{r_{ij''}}\right\} \quad (S1)$$

where N is the number of atoms in each region, M and P are the number of atoms in the droplet and the solid surface in the cutoff range, Q is the ions number within the cutoff; ε and σ are the well depth and zero-potential distance in L–J equation

(SI); r is the distance between two atoms; ε_{water} is the permittivity of water; and q is the value of charge. Secondly, we calculate the average value for each region from the 100 snapshots of our simulation results to give the value of cohesive energy.

4. Cohesive energy for droplets with different concentrations

We show the profile of the cohesive energy for $MgCl_2$-solution droplets with the concentration of 16.2% and 22.5%. The widths of the green part are further decreased as the elevated mass concentration, suppressing the water evaporation rate from the droplet.

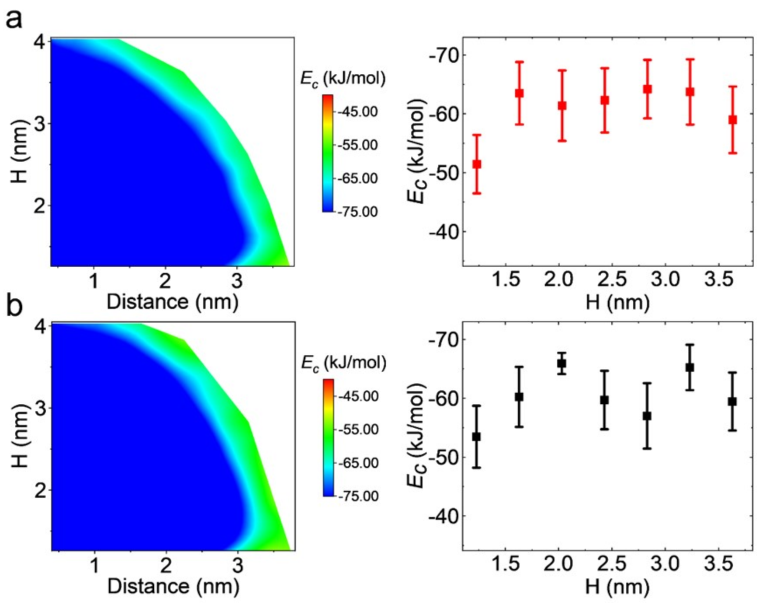

Figure S8. Profile of the cohesive energy of droplets of $MgCl_2$-solution at the mass concentration of 16.2% (a) and 22.5% (b).

5. Width of the green part by another definition

We show the width of the evaporating region by another definition. The region is defined as the part with $\Delta E_c <$ 15 kJ/mol to the outmost part. As the height (H) increases, the width in water droplet is larger than that in the solution droplet until the top part of the droplet (H=3.63 nm).

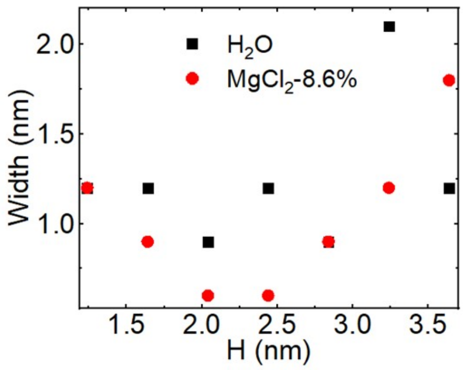

Figure S9. The width of the evaporating region if the region is defined as the region with the difference of cohesive energy to the outmost part less than 15 kJ/mol.

6. Evaporation changes linearly with the concentration

We fit the relationship of the evaporation rate as the mass concentration and conclude that the evaporation rate is almost linearly related with the mass concentration.

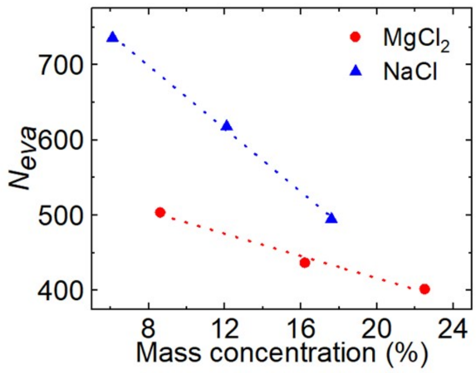

Figure S10. The relationship of the evaporation in 6-ns evaporation process of water molecules as a function of the mass concentration from NaCl-solution and $MgCl_2$-solution droplets.

7. Evaporation on copper substrate

We study the evaporation on the copper (Cu) substrate to test the effects of substrate on the evaporation difference caused ions. The Cu(111) is employed. The L-J parameters for Cu atoms are ε_{Cu} = 0.186 kcal/mol and σ_{Cu}= 3.214 Å. The concentration of the $MgCl_2$ solution is 8.6%. Ions suppress the water evaporation on Cu(111) compared to the pure water, indicating that ions suppress evaporation is independent of substrates in our simulations.

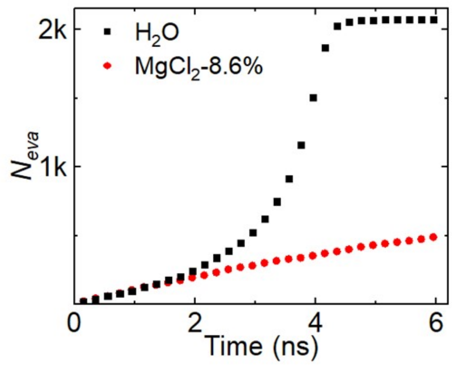

Figure S11. Evaporation difference from water droplet and $MgCl_2$-soultion droplet on Cu(111) surface.

8. The substrate with polarity

The polar substrate is the substrate in which some of atoms are charged as shown below. The different directions of the polarity have no striking effects on the evaporation rate.

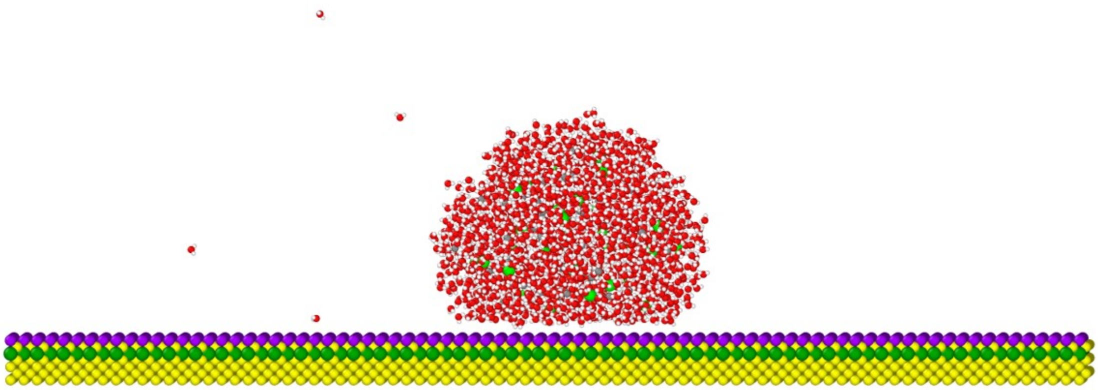

Figure S12. The substrate with polarity. The atoms in the substrate are the same with the non-polar one in our work. The violet spheres are the negatively charged atoms and green positively charged ones. The red and white spheres represent oxygen and hydrogen atoms in water molecules. The grey and green spheres are ions.

9. Cohesive energy on polar substrate

The cohesive energy of water molecules in the salty droplet on the polar substrate is shown below. The polarity is 0.1*e* (left) and 0.15*e* (right). A yellow region appears at the lower right-hand corner in the two panels. The values of cohesive energy at the two are -45.346 kJ/mol and -46.925 kJ/mol respectively. The evaporating energy barrier is smaller than that on the non-polar substrate, which results in the large evaporation.

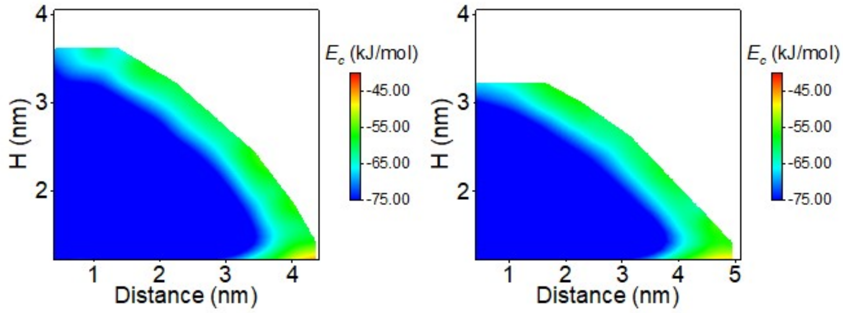

Figure S13. The profile of cohesive energy of water molecules in the salty droplet on polar substrate with 0.1*e* (left) and 0.15*e* (right).