

## *Supplementary Material*

### **Interaction of small ionic species with phospholipid membranes: the role of metal coordination**

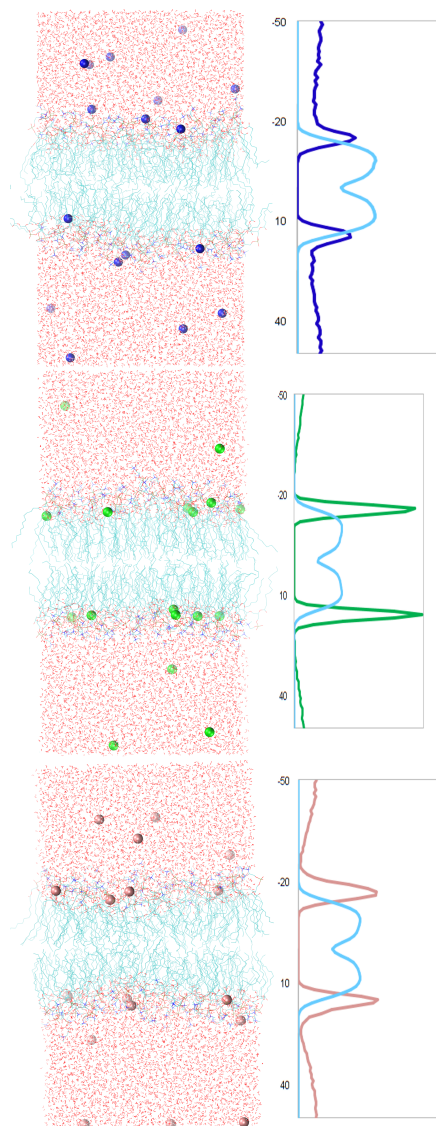
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## 1 Results of computer simulations

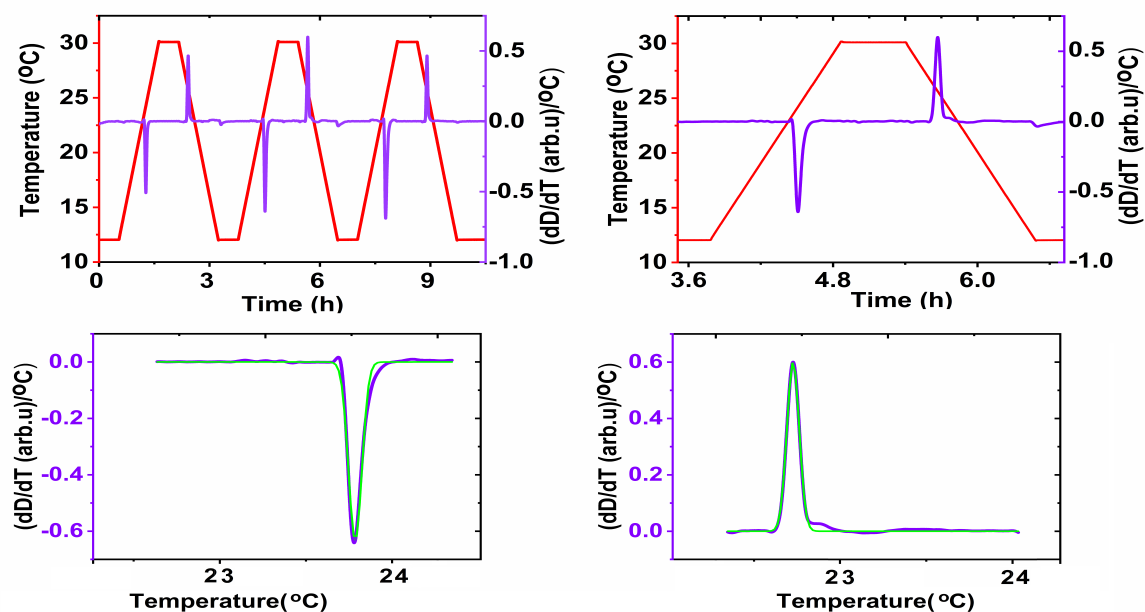


**Supplementary Figure 1.** Representative examples of the results of computer simulations. Snapshots of the last frames for  $\text{Na}^+$  (top),  $\text{Ca}^{2+}$  (middle) and  $\text{Mg}^{2+}$  (bottom), showing a side view and distribution plots. Colors: light blue: methylene; red: oxygen; dark blue:  $\text{Na}^+$ ; green:  $\text{Ca}^{2+}$ ; brown:  $\text{Mg}^{2+}$

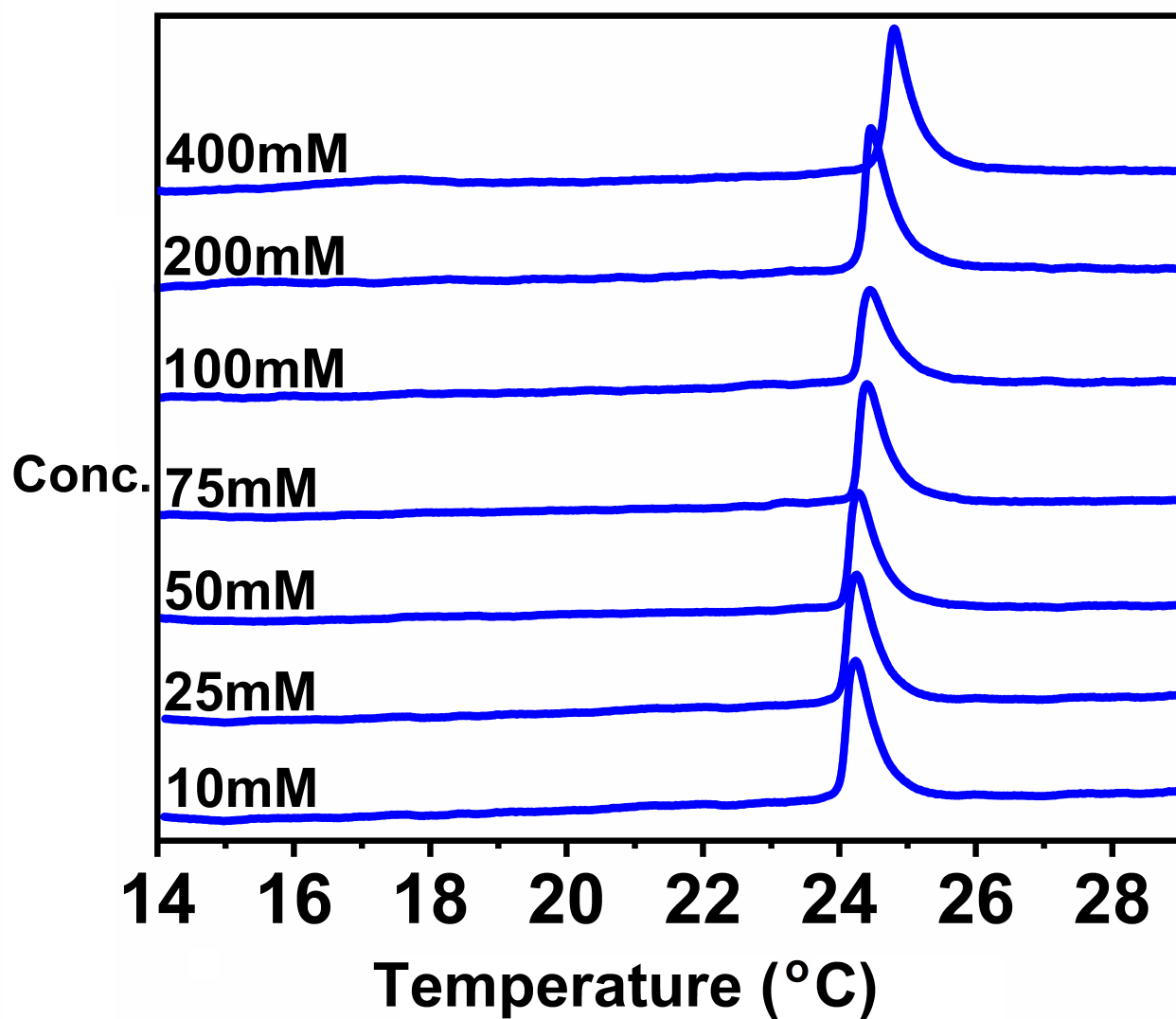
## 2 Phase transition measurements with QCM

In each experiment the MPA-modified chip surface was stabilized in water and then the salt solutions ( $\text{NaCl}$ ,  $\text{MgCl}_2$  and  $\text{CaCl}_2$ ) were introduced in different concentrations. DMPC supported membranes were formed via liposome deposition method in the respective salt solution. The temperature ramping

was conducted in three loops with identical parameters to the DSC experiments. In each case a control channel was used to record the dissipation changes in the salt solution (in the absence of a membrane), which was first subtracted from the membrane data before the first derivative was calculated. A processed dataset is shown in Supplementary Figure 2 top left and a single loop in Supplementary Figure 2 top right. Gaussian fitting of the phase transition peaks was performed in Origin software, and shown in the two lower panels of Supplementary Figure 2.



**Supplementary Figure 2.** Processed QCM dissipation data of the phase transition measurements: top left, a full dataset showing the three loops; top right, a single loop of temperature ramping data; bottom left, fitting for the endothermic process (heating); and bottom right, fitting for the exothermic process (cooling). Data shown for 75 mM  $\text{Ca}^{2+}$ .

**3 Phase transition measurements with DSC**

**Supplementary Figure 3.** An example of DSC measurements on DMPC liposomes in the presence of different concentrations of  $Mg^{2+}$ .