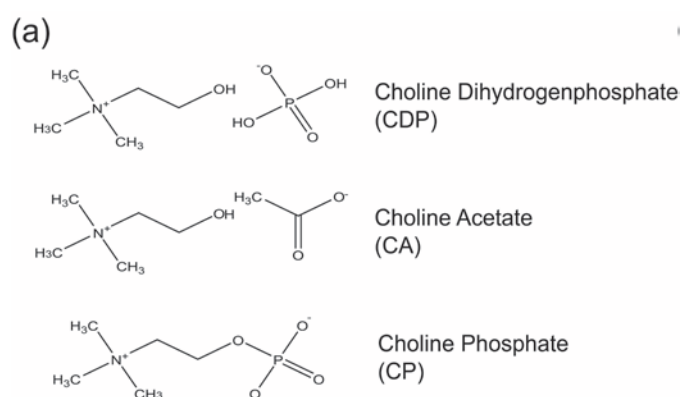


## Report to the beam time SC-4343:

### **Quantification of electrostatic interaction between biomembrane and ionic liquids**

The main goal of the proposed project was to quantitatively determine the ions density profiles across phospholipid monolayer in the presence of ionic liquids. We measured specular X-ray reflectivity (XRR) to extract the perpendicular structure of the lipid monolayer at the air/water interface on different ionic liquid subphases. We simultaneously recorded grazing incidence X-ray fluorescence (GIXF) to reconstruct the elements concentration profiles across the membrane surface.

We systemically measured the X-ray reflectivity and grazing incidence X-ray fluorescence of DOPC lipid monolayers on three different ionic liquids (figure 1). In addition, as control measurements we recorded the fluorescence spectra of DOPC monolayers on KCl containing buffer and on CaCl containing buffer. The DOPC were deposited at the air-water interface and then compressed to a surface pressure of 20 mN/m.

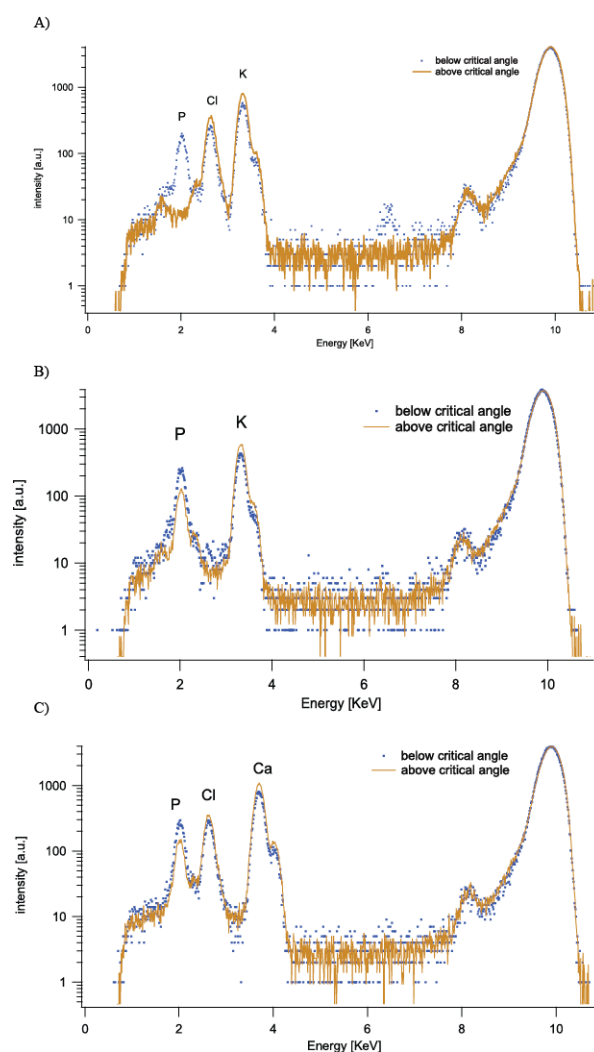


**Fig. 1** Chemical structures of choline dihydrogenphosphate (CDP), choline acetate (CA), and choline phosphate (CP).

Figure 2A depicts the fluorescence spectra of DOPC monolayer on KCl buffer below (blue curve) and above (orange curve) the critical angle. The fluorescence signals from phosphorus (P), chloride (Cl) and potassium (K) are visible. The signals from Cl and K recorded below the critical angle are slightly weaker than those recorded above the critical angle indicating that both Cl and K ions are depleted from the air-water interface. On the other side, the fluorescence signal from P is visible below the critical angle and disappears and from the spectrum taken above the critical angle. The P signal comes from the phosphate group within the DOPC head group implying the formation of stable lipid monolayer.

Figure 2B depicts the fluorescence spectra of DOPC monolayer on CDP ionic liquid below (blue curve) and above (orange curve) the critical angle. The fluorescence signal from P is stronger below the critical angle than the signal above the critical angle indicating that phosphorus is enriched at the air-water interface. This is due to the phosphorus content of DOPC lipids and to the enrichment of dihydrogenphosphate molecules near the DOPC monolayer. Similarly, the same tendency was observed in the measurements that were performed on CP ionic liquid (figure 2C).

However, detailed quantitative analysis is required in order to determine the later concentration of each element at the air-water interface.



**Fig. 2** (A) X-ray fluorescence of DOPC monolayer deposited on (A) KCl containing buffer (B on CDP ionic liquid and (C) on CP ionic liquid. The spectra were recorded below (blue curve) and above (orange curve) the critical angle of incidence. The fluorescence signals from the elements are indicated by their symbols.