

Role of ions in solid-liquid interfaces investigated by molecular simulations

Lidija Zivanovic¹

¹ *COMP Centre of Excellence, Department of Applied Physics, Aalto University, Helsinki, Finland*

To investigate the influence of ions on the different types of solid-liquid interfaces, we used MD simulations to study clinocllore and muscovite mica, and, as control systems, calcite and graphene, in the presence of high ion (NaCl) concentrations (>1M). On charged surfaces, solvated ions tend to accumulate close to the surfaces creating a clear electric double layer (EDL), reflecting the surface charge distribution in which ions are binding to specific surface sites. Furthermore, ions not only affect the water ordering within the first hydration layer but they are also increasing water ordering up to third and fourth hydration layers as ion concentration is increased. It is also important to investigate how ions affect on the mobility of hydration layers. To explore this further, we calculated water diffusivity in each hydration layer on mica and graphene surfaces. As expected, the first hydration layer created above graphene surface is more mobile then layer created on muscovite mica surface, assuming repulsive nature of interactions between water and graphene and attractive one between water and mica surface. Increased ion concentration has also affected on the mobility of each hydration layer. By calculating diffusion coefficient for each hydration layer on different type of surfaces, one can link mobility of hydration layers with the nature of the surface-water interactions.

