Molecular dynamics simulations of palmitic acid adsorbed on NaCl surface.

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The aerosol and gases e□ects in the atmosphere play an important role on health, air quality and climate, a□ecting both political decisions and economic activities around the world [1]. Among the several approaches of studying the origin of these e□ects, computational modeling is of fundamental importance in providing insights on the elementary chemical processes. Sea salts are the most important aerosol particles in the troposphere (10^9T/year) [2]. Our theoretical work consists in modeling a (100) NaCl surface coated with palmitic acid (PA) molecules at di□erent PA coverages. Molecular dynamics simulations were carried out with the GROMACS package[5], in the NPT ensemble at T= 235K. We have tested several force fields [3–4] to describe the molecular interactions in the fatty acid/salt crystal system. In this study, we focused on transition in molecular orientation of the adsorbate as a function of PA coverage, on the e□ect of humidity, by adding water molecules, on organization of the fatty acid at the salt surface, and especially on the occurrence of PA isolated islands.

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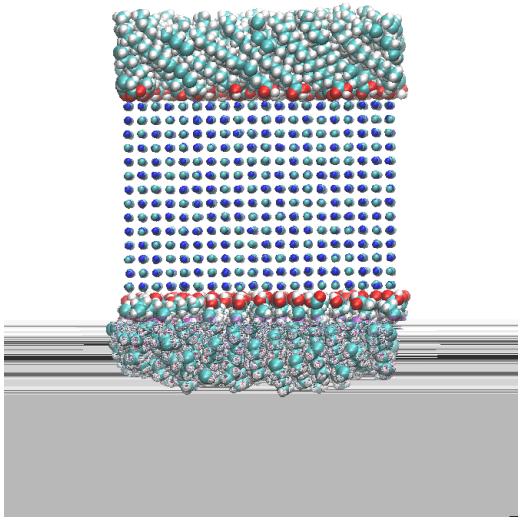

Figure 1: *Monolayer of palmitic acid adsorbed on (100) NaCl.*

References

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