



Molecular dynamics simulations of Palmitic acid adsorbed on NaCl

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The aerosol and gases effects in the atmosphere play an important role on health, air quality and climate, affecting both political decisions and economic activities around the world [1]. Among the several approaches of studying the origin of these effects, computational modeling is of fundamental importance, providing insights on the elementary chemical processes. Sea salts are the most important aerosol in the troposphere (109T/year) [2]. Our theoretical work consists in modeling a (100) NaCl surface coated with palmitic acid (PA) molecules. Molecular dynamics simulations are carried out with the GROMACS package [3], in the NPT ensemble at different temperatures, different PA coverages and various humidity. We focus on two aspects of the PA organization at the salt surface: the first one is related to transition in molecular orientation of the adsorbate as a function of PA coverage. The second one implies the effect of humidity, by adding water molecules, on the organization of the fatty acid at the salt surface, and especially on the occurrence of PA isolated islands as observed in the experiments [4]. For high humidity conditions, PA are removed from the salt surface and form islands on top of the water. This effect is enhanced when temperature increases.

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