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Computer simulations of SDS/dodecanol (hexadecanol) monolayers at water/air interface[1] HECTOR DOMINGUEZ, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico (UNAM). Mexico 04510, MARGARITA RIVERA, Instituto de Fisica, Universidad Nacional Autonoma de Mexico. Mexico 01000 — Simulations of monolayer mixtures of amphiphlic molecules were investigated to study the effects of the polar head groups in the structure of the monolayer at the water/air interface. The binary mixture was composed of sodium dodecyl sulfate (SDS) and dodecanol (hexadecanol) molecules For the low dodecanol concentration molecules two monolayer mixtures were prepared. In the first monolayer all the dodecanol molecules were placed together in the center of the simulation box whereas in the second monolayer those molecules were uniformly distributed in the surface area in such a way that they were a part from each other. Simulations of both systems indicate that the dodecanol tails in the first monolayer are more straight and more ordered than those in the second monolayer. When simulations of SDS/hexadecanol are performed it is observed that the tilt angle and the order of the tails are different respect to the SDS/dodecanol mixtures.

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