

Abstract Submitted
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Novel low temperature phase transitions in short grafted chains as a model for monolayers of amphiphile molecules with ionic heads¹ CARLOS GONZALEZ-CASTRO, GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, Universidad Nacional Autonoma de Mexico — We have carried out extensive Monte Carlo simulations in the NPT ensemble of a model for Langmuir monolayers of amphiphile molecules with ionic heads deposited on an interface. We considered a previously proposed coarse-grained model [1] in which the molecules are represented as short chains made up of beads with one slightly larger head confined at the interface. By analyzing the behavior of several order parameters as a function of temperature and pressure we obtained a liquid expanded phase and various ordered condensed phases with different molecular tilts. More importantly, we found a novel “untilted” to “collective tilted” to “small correlated tilted” phase transition at low temperatures, and different pressure values, as suggested by the behavior of two order parameters. One that measures the average molecular inclination and the other that measures the average projection on the x-y plane of the vector that joins the head center with the last monomer center of each molecule. The latter yields information about the correlation of the molecular tilt.

[1] C. Stadler, H. Lange and F. Schmid, Phys. Rev. E, Vol. 59, (1999).

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