THEORETICAL DESCRIPTION OF THE MOLECULAR FOOPRINT OF SELF-ASSEMBLED MONOLAYERS OF GOLD NANOPARTICLES AND SURFACES

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In the study of self-assembled monolayes at the nanoscale, the footprint plays a very important role, at both theoretical and experimental sides as well as for possible technical applications. This magnitude is gives the surface occupied per molecule. In this work, this magnitude is calculated theoretically for a self-assembled monolares of alkanethiol molecules on gold surfaces. Two-dimensional surfaces and spherical nanoparticles are considered in the calculations. The footprint is determined by calculating the surface tension in the simulations. The surface tension is obtained starting from its thermodynamics definition and working in the canonical ensemble. The dependence of the results on the molecular length and the surface curvature are discussed. A simple theoretical model is developed for the molecular coverage as a function of the nanoparticle radius. The results are compared with the experimental results obtaining a very good agreement.