

A simulation of the structure and AFM images of self-assembled monolayers on the gold (111) surface

A. Kalampokidis, M.L. Sushko, A.Y. Gal, A.L. Shluger

Department of Physics and Astronomy, University College London
London WC1E 6BT UK

Self-assembled monolayers of long-chain molecules are a promising class of systems with widespread potential applications in materials science. A potential application is to use them as a template for molecular imaging and to produce high-precision patterns with different methods, in particular, Atomic Force Microscopy (AFM).

Semi-empirical calculations have been performed on various systems of self-assembled monolayers of decanethiols $[S(CH_2)_9CH_3]$ on gold(111) surface. We have used the potentials developed by Hautman and Klein [1] with the interaction of the CH_3 , CH_2 , and S particles with Au atoms fitted by Tupper and Brenner [2]. The potential energy landscape of the full-coverage phase as a function of molecule orientation with respect to the surface has been studied and the barriers between different local minima have been determined. Lower-coverage phases have been optimized to obtain clusters of alkanethiol molecules on gold. The behavior of the system has been studied when local orientational defects and cavities are introduced into the system. Additionally, the effect of different tail-groups on the conformation of the monolayer has been investigated. Non-Contact Atomic Force Microscopy (NC-AFM) images of the optimized configurations were modeled. The resolution of the AFM images of the monolayers obtained with gold and with CH_3 modified gold tips will be discussed.

In conclusion, this study will help to understand the different conformations of self-assembled monolayers in different experimental conditions.

[1] J. Hautmann, M.L. Klein, J. Chem. Phys. 91 (8), 1989, 4994-5001

[2] K.J. Tupper, D.W. Brenner, Langmuir 1994, 10, 2335-2338