Nanoobjects microscopy

Hydrophilicity of Au(111) surface modified by alkanethiols: from molecule to material

Ya.Yu. Lopatina[1], V.Ye. Kutsenko[1], O.L. Kapitanchuk[3], S.V. Snegir[2], O.A. Marchenko[1]

[1]Institute of Physics, Nat. Acad. of Sci. of Ukraine. Prospect Nauki, 46, Kyiv-03039, Ukraine.
E-mail: yaroslava.lopatina@gmail.com

2 Chuiko Institute of Surface Chemistry, Nal. Acad. of Sci. of Ukraine, 17, General Naumov str.,Kyiv-03164, Ukraine

3 Bogolyubov Institute for Theoretical Physics, Nat. Acad. of Sci. of Ukraine,14-b, Metrolohichna str., Kyiv-03680, Ukraine

Aiming to achieve certain degree of hydrophilicity of the carrier the wetting properties of organic films of mercaptan molecules were studied. For this solutions of alkanethiols with different terminal group (-CH_3, –*OH,* –*COOH*) and dithiols with different chain length (1,9-nona, 1,4-buta) were deposited onto reconstucted Au(111) surface. The hydrophilicity of interface gold/mercaptan was investigated by measuring of contact angle. The structure of the monolayer absorbed on gold surface was determined by means of scanning tunneling microscopy (STM) and was confirmed by quantum-chemical calculations performed at the DFT level.

Our study revealed that contact angle is sensitive to the type of functional group of molecules self-assembled on the gold surface. Decrease of contact angle value with increasing of the polarity of terminal groups from 104° for -CH_3 to 22° for –*COOH* was observed.

It was found that wetting angle of the surface can be varied depending on morphology of the monolayer. In case of short 1,4-butanedithiol molecules the monolayer on Au (111) surface displayed low level of ordering resulting in lowering of contact angle in comparison with the monolayer formed by 1,9-nonandithiol molecules.

1. *Yung-Fang Liu, Yuh-Lang Lee.* Adsorption characteristics of OH-terminated alkanethiol and arenethiol on Au(111) surfaces. // Nanoscale. 2012.- **4.**-P 2093-2095.
2. *Devi J.M.* A simulation study on the thermal and wetting behavior of alkane thiol SAM on gold (111) surface // Prog. in Na. Sci.: Mat Intern.- 2014.- **24.-P.** 405-409.
3. *Förch R., Schönherr H., Tobias A. Jenkins A*. Surface design: applications in bioscience and nanotechnology. Germany: Wiley– VCH. – 2009. - 400 P.