

Nanostructured surfaces

Formation of disulfide bonds in alkyldithiol monolayers: STM study and DFT modelization

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Organic monolayers on metal surfaces have attracted considerable interest for many years due to wide use in molecular electronics and related applications. Most of experimental and theoretical works were focused on self-assembled monolayers (SAM) of alkanethiol molecules chemisorbed on gold surfaces Au(111). In such organometallic interfaces molecules are attached to the surface atoms through S-Au bonds. Physical properties of deposited SAMs depend on type of terminal groups.

We used alkanedithiols for attaching Au nanoparticles (AuNP) to Au(111) surface [1]. Our AFM study of attached NPs on the substrate revealed fast process of passivation of underlying monolayer which occurs within a 1-2 min after deposition. This can be explained by formation of –S-S- bonds between neighboring dithiol molecules which leads to their pairing. Association of molecules in pairs was also confirmed by STM investigations of initial stage of ordering. Instead of hexagonal structure typical for initial stage the double-rows of associated molecules were observed.

First principle DFT-calculations were used to study the changes in adsorption configuration and electronic properties upon the formation of disulfide bonds between alkyldithiol molecules in periodic slab. Stabilizing role of disulfide bonds was confirmed.

[1] *V. Kutsenko, et al., Alkylthiol self-assembled monolayers on Au(111) with tailored tail groups for attaching gold nanoparticles // Nanotech. – 2017. – 28 – P. 235603.*