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Assembling Cysteine Monolayers on Low-Index Gold Surfaces

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L-Cysteine ($\text{HO}_2\text{CCH}(\text{NH}_2)\text{CH}_2\text{SH}$) is an indispensable amino acid in biology containing a carboxylic acid, an amine and a thiol group. It is also essential as a ligand in stabilization of metalloproteins. Cysteine can assemble on gold surfaces and form stable monolayers due to gold–sulfur bond. Interestingly, surface structures of cysteine monolayers on Au(111) in aqueous solution are drastically different from monolayers formed in ultrahigh vacuum.

In this work we have studied monolayers of cysteine on the three low-index gold substrates in aqueous solution. In situ scanning tunneling microscopy (*in situ* STM) and electrochemistry have been employed to investigate the cysteine monolayers at molecular and submolecular resolution. Highly ordered monolayers have been achieved on low-index gold surfaces Au(111), Au(100) and Au(110). Surface structures such as network like clusters and strips have been disclosed, depending on the structure of the underlying gold substrates. Corresponding coverages of cysteine monolayers have been determined by voltammetry. We have further investigated the dynamics of self-assembled monolayer (SAM) formation of L-cysteine on gold electrodes. The adsorption is monitored by chronopotentiometry at sub-second time-resolution. Molecular packing, geometry and bond energy of the adsorbed molecules, as well as STM contrasts are addressed by molecular modelling based on the density functional theory (DFT) and support the experimental observations.

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