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The electrochemical stability of thiols on gold surfaces

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Abstract

In this paper we present a comparative analysis of the electrochemical stability of alkanethiols, aromatic and heterocyclic thiols on the Au(111) and Au(100) faces in relation to the theoretical energetic data. The peak potential and surface coverage are used as the key parameters to estimate the electrochemical stability while work function changes, adsorption energies and surface free energies calculated from periodic DFT, including van der Waals interactions, are used for the theoretical estimation. We find that the peak potentials do not correlate with work function changes and adsorption energies in particular for aromatic and heterocyclic thiols. In contrast, the reductive desorption potentials for the different thiols show a good correlation with the surface free energy of the SAMs estimated by density functional theory calculations. Surface coverage is a key factor that controls reductive desorption through van der Waals interactions.

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