

Prize Talk

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What is the structure of the thiol/gold interface in self-assembled monolayers? — ●DAVID WOODRUFF — University of Warwick, Coventry, UK — Laureate of the Max-Born-Prize

Perhaps the most archetypal of all self-assembled monolayer systems on surfaces are those formed by n-alkanethiolates ($\text{CH}_3(\text{CH}_2)_{n-1}\text{S}-$) on the Au(111) surface, and these have been subjected to a vast number of studies in the last 20 years or so. Despite this, the structure of the interface remains in doubt. Early theoretical (mainly density functional theory) calculations favoured a structure in which the S head-group atom bonds to a two- or three-fold coordinated bridging

or hollow site on an unreconstructed substrate, but more recently a wide range of experiments have shown that the S atoms occupy local atop sites. The solution to this dilemma appears to be that the thiolates induce a reconstruction of the substrate, plucking out Au atoms from the substrate to form Au-thiolate moieties; it is these moieties that 'self-organise' on the underlying Au(111) surface. There remains, however, controversy as to the exact nature and structure of these Au-thiolate species: specifically, are they Au-monothiolates or Au-dithiolates? In this short review I will describe the background to this problem and the experiments being conducted to resolve this controversy and provide a definitive solution to the structure of this interface.