

# Structural study of alkane thiols self-assembled on Au(111) surface

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## Abstract

The interaction between organic materials and solid surfaces is of great interest. The properties of self-assembled monolayers may lead to their industrial use as sensors, transducers, detectors, packaging and insulating layers for integrated circuits. It is well-known that long chain alkyl thiols (R-SH) bind strongly to surfaces of gold and silver. State-of-the-art density functional theory calculations have been performed for the interaction of the thiol head group with the Au(111) surface. The chemisorption site and energetics are calculated and compared to experiments. The effects of chain size have also been investigated and will be discussed.