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综述

Understanding and Predicting Thiolated Gold Nanoclusters from First Principles

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摘要：

This is an exciting time for studying thiolated gold nanoclusters. Single crystal structures of $Au_{102}(SR)_{44}$ and $Au_{25}(SR)_{18}^-$ (—SR being an organothiolate group) bring both surprises and excitement in this field. First principles density functional theory (DFT) simulations turn out to be an important tool to understand and predict thiolated gold nanoclusters. In this review, I summarize the progresses made by us and others in applying first principles DFT to thiolated gold nanoclusters, as inspired by the recent experiments. First, I will give some experimental background on synthesis of thiolated gold nanoclusters, followed by a description of the recent experimental breakthroughs. Then I will introduce the superatom complex concept as a way to understand the electronic structure of thiolated gold nanoclusters or smaller nanoparticles. Next, I will describe in detail how first principles DFT is used to understand the Au-thiolate interface, predict structures for $Au_{38}(SR)_{24}$, screen good dopants for the $Au_{25}(SR)_{18}^-$ cluster, design the smallest magic thiolated gold cluster, and demonstrate the need for the trimer protecting motif. I will conclude with a grand challenge: the real time monitoring of nucleation of thiolated gold nanoclusters.

关键词： Thiolate Gold Nanoclusters Density functional calculation Electronic structure Superatom complex

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