Electronic Properties of Ligand-Stabilized Au_{55} Cluster

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Ligand-stabilized metal clusters are of fundamental as well as of applied importance [1]. They are chemically stable and hence can in contrast to naked metal clusters be prepared under ambient conditions. Usually, for an investigation of the electronic structure in the valence band, UV photoelectron spectroscopy (UPS) or scanning tunneling spectroscopy (STS) is applied. However, in the case of ligand-stabilized clusters, UPS may only provide information from the ligand shell and the outermost layer of the cluster core. In contrast, STM accesses the whole cluster and can be performed locally on an atomic scale.

In this work low-temperature ultrahigh-vacuum scanning tunneling microscopy (STM) and STS were employed to investigate Au_{55} clusters stabilized by $[P(C_6H_5)_3]_{12}Cl_6$ ligands [2]. The clusters were deposited on Au(111) substrates from solution by spin coating. The STM images confirm that locally ordered cluster monolayers are produced [3]. At 7 K, the actual arrangement of the C_6H_5 rings of the ligand molecules can be imaged [4].

We have performed *I-V* measurements at two distinct locations on individual clusters (Fig. 1). Both curves exhibit an identical Coulomb blockade (CB) and a Coulomb staircase. The difference between them is the manifestation of a negative differential resistance (NDR) in curve B. All these features can be interpreted as being the result of charge-quantization phenomena [5]. The curves could be modeled by assuming a metallic particle, *i.e.*, the cluster, between two metallic electrodes, *i.e.*, tip and substrate. To model the NDR, a neighboring cluster has to be accounted for.

Locally resolved *dI/dV-V* spectra (Fig. 2a) reveal the energy quantization of the cluster core [4]. To deduce the individual energy levels, we performed a Monte-Carlo simulation of the electron transport through the double tunnel junction to fit the measured curves. For the CB regime a co-tunneling process was taken into account. Figure 2b shows the resulting density of states (DOS) near the Fermi energy. An average level spacing of *ca*. 160 meV can be derived.

We have also calculated the DOS of the Au_{55} cluster by using a parameterized density-functional tight-binding method [6]. The result is in good agreement to the experimental one with regard to the average level spacing.

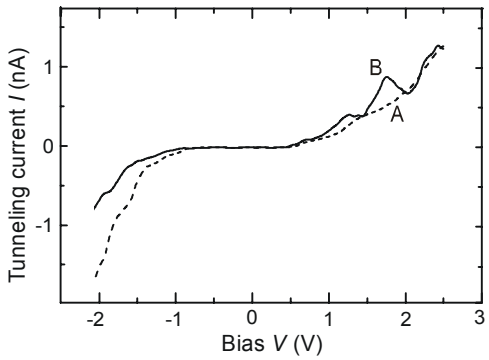

Fig. 1. *I-V* curves acquired right above a C_6H_5 ring (A) and next to the ring (B). Prior to data acquisition the tip-cluster distance was set at a substrate bias of 2 V and a tunneling current of 0.7 nA for both curves.

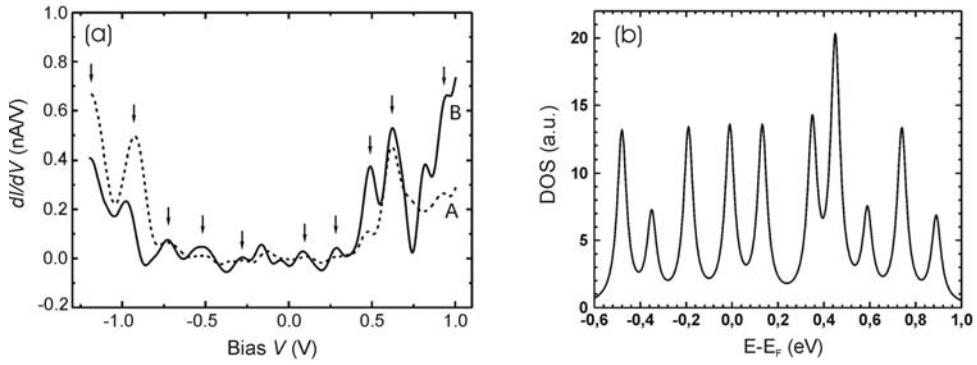

Fig. 2. a) Tunneling spectra acquired on the same locations as for Fig. 1. The arrows indicate conductivity peaks which precisely coincide for both spectra. b) DOS of the cluster core deduced from a) based on a Monte-Carlo simulation.

References

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