# Single atom tunneling junctions: Structure and magnetism

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A detailed understanding of electronic and magnetic properties of atomic-scale nanostructures is essential for future progress of magnetic data storage technologies. The scanning tunneling microscope (STM) has provided fascinating insights into properties of matter at the atomic scale. "Atomic engineering" based on the manipulation of single adatoms using the STM tip [1] has opened the possibility to build artificial atomic-scale nanostructures [2]. Atomic motion on metal surfaces can be controlled using the STM tip [3]. Magnetic properties of a single adatoms can be probed by placing the adatoms in tunnel junctions. Very recent STM experiments have demonstrated the ability to measure the spin excitation spectra of individual magnetic adatoms [4]. However, the location of the STM tip at the proximity of surfaces and adatoms can cause perturbations due to the tip-sample interaction. Here, we demonstrate that structural, electronic and magnetic properties of a single atom magnetic junctions are significantly affected by the tip [5]. Performing combined ab initio calculations and the molecular dynamics simulations we have revealed that the tip strongly changes the position of adatoms above the surface. Considerable atomic relaxations in the tip and the substrate have been found. As an example we present in Fig.1 our results for Co adatoms on Cu(001). We model the tip by a Cu pyramid consisting of 14 atoms. Calculations in a fully relaxed geometry show that the tip locally distorts the surface. One can see that the surface layer under the adatom is not flat anymore.

In order to get a deeper insight into the tip-adatom interaction, we have performed our calculations for different tip-substrate separations. Our results are presented in Fig.2.

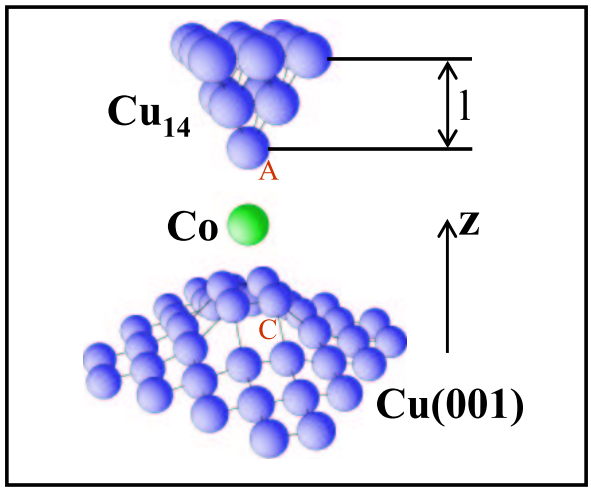


**Fig. 1:** One-atom magnetic junction in relaxed geometry

When the distance between the tip-apex and the substrate reduces, both the tip-apex and the adatom exhibit strong vertical displacements. Relatively small atomic relaxations also occur in the substrate underneath the adatom. In the range between 5.5Å and 4.5Å, the tip-apex is pushed down, while the adatom and the substrate atoms are pushed up. The attractive interaction between the tip and the adatom at this stage is the driving force for the observed atomic relaxations. However, at a closer tip-substrate distance (4.5-3.5Å), the repulsive interactions between the tip and the adatom, and between the adatom and the substrate begin to play an important role. At this stage the adatom and the substrate atoms are pushed down as much as 0.4Å and 0.15Å respectively. Considering that a distance reduction by 1Å typically results in a ten-fold increase of the tunneling current, it is obvious that the dynamics of the relaxation found here must have profound influence on the appearance of STM images.

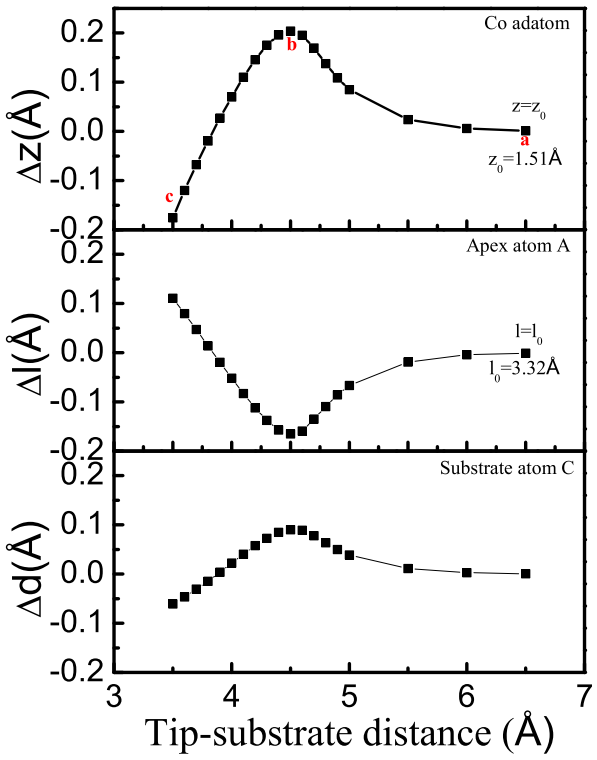


**Fig. 2:** Atomic displacements in the one-atom magnetic junction. $\Delta l = l_0 - l$ is the change of the tip length, where l and $l_0$ are the tip length with and without tip-adatom interaction; $\Delta z$ and $\Delta d$ are the displacements of the adatom and the substrate atom C along z axis, where $z_0$ is the relaxed adatom-substrate distance without tip-adatom interaction.

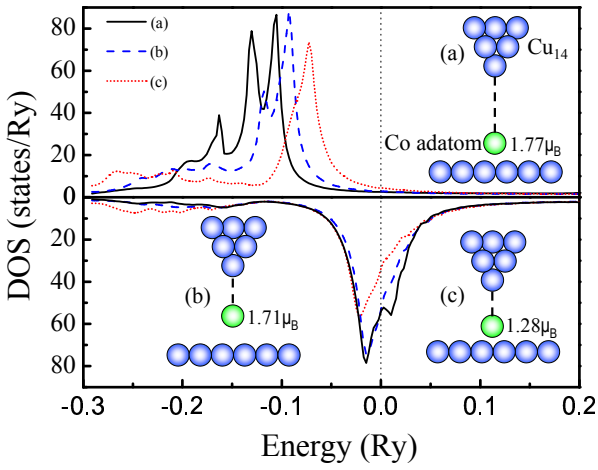


**Fig. 3:** Effect of the tip on electronic and magnetic properties of Co adatom on Cu(001)

To demonstrate the effect of the tip on electronic and magnetic properties of single magnetic adatoms, we have performed the ab initio calculations in a fully relaxed geometry for three different vertical distances between the tip and the Co adatom in the range between 6.5Å and 3.5Å (denoted a, b and c in Fig. 2). The local density of states (LDOS) on the Co adatom and its magnetic moments are presented in Fig.3. The results for both spin-directions are plotted with the energies given relative to the Fermi energy.

For the tip-substrate distances larger than 5Å, the interaction of the tip with the adatom is rather weak, and the LDOS on the Co adatom is very similar to the LDOS of a single Co adatom on Cu(001). However, at vertical distances between 4.5Å and 3.5Å the tip drastically changes the LDOS and the magnetic moment. We find that in this case the magnetic moment reduces from $1.71\mu_B$ to $1.28\mu_B$.

In summary, our results establish that tip induced changes in structure, electronic and magnetic properties of a single magnetic junctions significantly depend on the tip-surface distance. Effects found in our work may have consequences for the measured STM current in atomic junctions, and for understanding of single-atom spectroscopy experiments on magnetic adatoms.

## References

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