

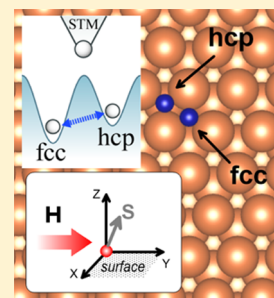
Tuning an Atomic Switch on a Surface with Electric and Magnetic Fields

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ABSTRACT: Controllable switching an adatom position and its magnetization could lead to a single-atom memory. Our theoretical studies show that switching adatom between different surface sites by the quantum tunneling, discovered in several experiments, can be controlled by an external electric field. Switching a single spin by magnetic fields is found to be strongly site-dependent on a surface. This could enable to control a spin-dynamics of adatom.



Bistability and multistability of internal states of a system have received a considerable attention in physics,^{1–4} chemistry,^{5,6} and biology.^{7–9} One can switch a system between two alternative states by an external stimulus. Progress in condensed matter physics has enabled us to study bistability (multistability) on the atomic scale. The first atomic switches were demonstrated by Eigler et al.¹⁰ and Lyo and Avouris.¹¹ The functionality of an atomic switch is determined by the motion of single atoms. In other studies, a charge bistability of single adatoms was reported. For example, Steurer et al. by attaching or detaching single electrons by the tip to the adatoms have achieved a charge bistability of single adatoms.¹² Recently, switching of Si dopants in GaAs(110) between a positive and a negative charge configuration has been observed by Smakman et al.¹³ The STM tip could serve for writing and reading the information on a single Si atom. Yang et al. have reported on the bistability of individual atoms in nanostructures.³ These results, suggest that single adatoms and single dopants can be used as a memory elements. A single-atom memory has been recently demonstrated by Schirm et al.¹⁴ They have provided evidence that a metallic atomic-scale contact can be operated as a switch. The switching process is caused by the rearrangement of single atoms. Locally bistable switching of magnetic states was found in the experiment on molecular magnets.¹ Magnetic bistability of adatoms on metal surfaces has been predicted by ab initio calculations and spin-dynamic simulations.^{15–17} The progress in STM made it possible to study single magnetic adatoms and determine their spin-polarization and magnetic anisotropy.^{18–21} Local control of adatoms position, their magnetic anisotropy, and the bistability of the magnetization might lead to them being used as memory bits. Lateral switching of adatoms between different lattice sites demonstrated by Stroscio and Celotta²² has opened a new possibility in realizing atomic switches. They have controlled the dynamics of the Co adatom on Cu(111)

that switches between neighboring (energetically nearly degenerate states) the fcc and the hcp sites at low temperature. Switching the Co adatom leads to a random two-state telegraph noise in tunneling current. The underlying mechanism driving a lateral atomic switch is based on the quantum tunneling of the Co adatoms.²² At first glance it seems to be improbable due to the large mass of the Co adatom. However, a small distance between the fcc and the hcp sites and small barrier height (<37 meV) can significantly enhance a tunneling rate. There have been several interesting studies on the quantum tunneling of large-mass adatoms. For example, Repp et al. have reported on the tunneling of a heavy Cu atoms on Cu(111) at low temperatures.²³ Surface diffusion of Cr adatoms on Cu and Au substrates by the quantum tunneling has been discovered by Ohresser et al.²⁴ and Bulou et al.²⁵ Heinrich et al. have found that the motion of CO molecules on Cu(111) can be initiating by the quantum tunneling.²⁶ Ronci et al. have presented evidence of the Sn adatom quantum tunneling at the α -Sn/Si(111).²⁷

The above-discussed works on atomic switches have demonstrated a remarkable possibilities for using a single atoms as memory bits; however, controlling the position and the magnetization of a single adatoms by an external stimulus has not been investigated so far. The aim of our paper is 2-fold (cf. Figure 1). First, performing ab initio calculations, we show that a lateral atomic switch can be tuned by an external electric field (EEF). We reveal that an EEF can significantly affect the rate for quantum tunneling of adatom between the fcc and the hcp sites. We concentrate on the Co adatom on Cu(111).

Second, we study the spin-dynamics of the Co adatoms in the fcc and the hcp sites on Cu(111) in an external magnetic

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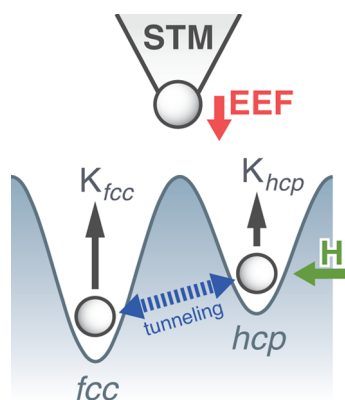


Figure 1. Adatom in an external electric and magnetic field.

field. Our results reveal a strong site dependence of the spin dynamics of the adatom. We demonstrate that the single spin can be switched on a time scale of several tenths of picoseconds.

Our calculations are performed by using the VASP code (Vienna simulation package),²⁸ with the projector augmented-wave technique²⁹ and the local Ceperly–Alder exchange and correlation functional (LDA).³⁰ We mimic the Cu(111) surface by 3×3 supercell of four layers. A criterion of force-on-nuclei convergence to within 10^{-4} eV/Å is chosen for geometry optimization. The energy cutoff of 450 eV for the plane-wave expansion and a $13 \times 13 \times 1$ Monkhorst-Pack grid for k-point sampling are used. A static electric field is introduced by a planar dipole layer and applied perpendicular to the surface.³¹

First, we present a spatial distribution of the screening charge around the Co adatom. As an example, our results for the Co adatom in the fcc site in the EEF = 0.9 V/Å are shown in Figure 2. It is obtained by subtracting the charge around the adatom in

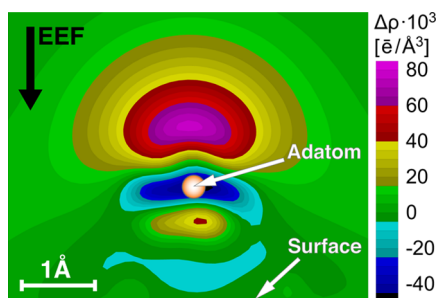


Figure 2. Spatial distribution of the screening charge around the Co adatom in the fcc-site. The results for the hcp-site are similar.

the EEF and without the EEF. One can see that an applied EEF induces a strongly inhomogeneous distribution of the screening charge. The screening of the bulk from the EEF occurs in a close proximity of the adatom (~ 1 Å). In our case the field is oriented to pull electrons out of the surface. A major part of the screening charge is found above the adatom. The screening density of electrons is not following the sharp contour of the adatom. This is the manifestation of the Smoluchowski effect.^{32,33} A strong depletion of electrons in the area between the adatom and the surface indicates that the electron corrugation of Cu(111) near the adatom should be affected by the EEF. As the result of such effect, the bonding of the adatom with the surface and the potential barrier between the fcc and the hcp sites could be also modified by the EEF. To

gain a detailed insight into this effect, we have calculated the barrier height in different EEF: $\Delta E(EEF) = E_{\text{fcc}(\text{hcp})}(EEF) - E_{\text{br}}(EEF)$, where $E_{\text{fcc}(\text{hcp})}$ is the energy of the adatom in the fcc(hcp) site in the EEF and $E_{\text{br}}(EEF)$ is the energy in the bridge position. Results presented in Figure 3b reveal that the

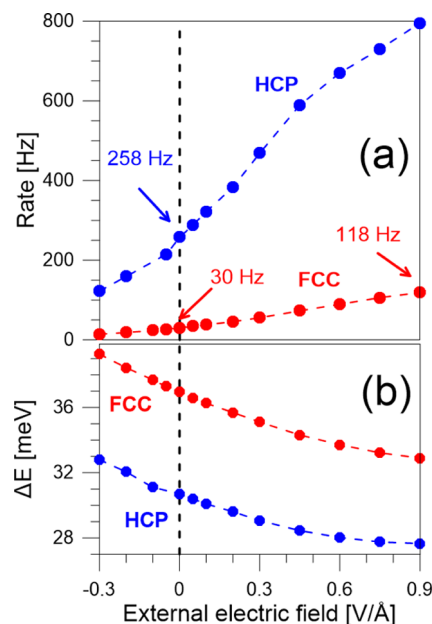


Figure 3. Rate of the quantum tunneling (a) and the barrier height (b) for the fcc and the hcp site in an EEF.

barriers for both sites decrease with increasing EEF. The physical mechanism responsible for this effect is related to the reduction of the corrugation of the charge density in a positive EEF due to spill out of electrons from the surface area (Figure 2). It was found that when the corrugation of the potential acting on adatoms decreases, the barrier between the fcc and the hcp sites also decreases.³⁴

Despite the fact that changes in the barriers are rather small (~ 7 meV), they can significantly affect the quantum tunneling of the Co adatom on the surface. We have calculated the rate for the quantum tunneling R_{fcc} and R_{hcp} between the fcc(hcp) and the hcp(fcc) sites. We have used the Wentzel–Kramers–Brillouin (WKB) approximation, similar to the work of Strosio and Celotta:²² $R_{\text{fcc}(\text{hcp})} = \nu \exp\{-d(2m\Delta E_{\text{fcc}(\text{hcp})})^{-1/2}/\hbar\}$, where $\nu = 10^{12}$ s⁻¹, $d = 0.74$ Å, the effective distance being a half the fcc-hcp separation, and ΔE is the potential barrier (see Figure 3). The results depicted in Figure 3a show that the rate of the quantum tunneling can be significantly enhanced for a positive EEF and suppressed by a negative EEF. These findings unambiguously prove that a switching of a single adatom between two surface sites by means of the quantum tunneling can be controlled by an EEF.

It is important to note that controllable switching an adatom between the fcc and the hcp sites can allow to engineer an electric conductance at a single atom level. Very recently, such experiments have been reported by Kim and Hasegawa.³⁵

Now, we turn to the discussion of the effect of an external magnetic field on the Co adatom. We find distinctive site-dependence of a single spin dynamics. These dynamics have been studied by the Landau–Lifshitz–Gilbert equation^{36,37}

$$\frac{\partial \mathbf{S}}{\partial t} = -\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}} + \frac{\alpha}{\mu_s} \mathbf{S} \times \frac{\partial \mathbf{S}}{\partial t}$$

Here μ_s is atomic moment, ($\mathbf{S} \equiv \mu_s / \mu_B$) is magnetization unit vector, $\gamma = 1.76 \times 10^{-11} \text{ T}^{-1} \text{ s}^{-1}$ is gyromagnetic ratio, $\alpha = 0.01$ is the damping parameter, and \mathbf{H}_{eff} is the effective magnetic field

$$\mathbf{H}_{\text{eff}} = \frac{\partial}{\partial \mathbf{S}} \left[S\mathbf{H} + \frac{K}{\mu_s} (S e_a)^2 \right]$$

where K is anisotropy energy of the atom and e_a denotes the direction of the easy axis.

Using the spin magnetic moments and the magnetic anisotropy energies (MAE) determined from our ab initio calculations, we study the time evolution of the magnetization of the Co adatom placed in the fcc and the hcp sites in external magnetic fields (Figure 1). Because of an increased coordination of the hcp site (the existence of the atom in the second layer below the adatom), the reduction of the MAE in the hcp site compared with the fcc site is expected. The adatom is excited by the magnetic field in the direction perpendicular to the easy axis (see inset in Figure 4). As an example, we present

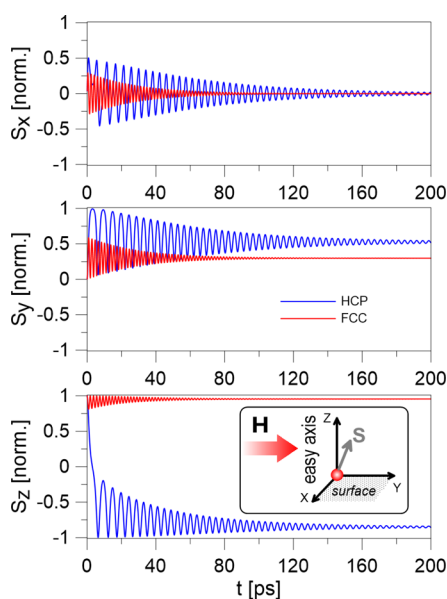


Figure 4. Dynamics of the magnetization projection of the adatom for the fcc and the hcp sites.

results for $H = 6.3 \text{ T}$ and $\text{EEF} = 0.9 \text{ V}/\text{\AA}$. An EEF reduces the interaction of the adatom with the substrate due to a spill out of electrons making the adatom more free-like. Therefore, the reduction of the MAE in the EEF oriented toward the surface is expected because a limiting case, a free atom, has a zero MAE.³⁸ Such EEF reduces the MAE from 1.8 to 1.2 meV and from 1.2 to 0.7 meV for the fcc and the hcp sites, respectively. The spin magnetic moment is practically unaffected by the EEF, being $\sim 2\mu_B$ for both sites.

The magnetic field triggers a precession motion of the magnetization. Results depicted in Figure 4 reveal a drastic difference between the spin dynamics in the fcc and the hcp positions. The striking result is the switching of the magnetization (S_z) in the hcp site. We have also observed the switching of the spin in the fcc site but for a significantly larger

magnetic field ($>12 \text{ T}$). This is due to a larger MAE in the fcc site. We would like to stress that the site-dependent spin dynamics of the adatoms is determined by the site dependence and the field dependence of the MAE. Electric and magnetic fields used in our calculations are experimentally achievable in modern STM experiments.^{38,39}

In summary, our findings have demonstrated the ability to affect quantum tunneling in the lateral atomic switch by an external electric field. Site-dependent spin dynamics in an external magnetic field is revealed for the Co adatom on Cu(111). We have shown that the adatom magnetization can be switched by the magnetic field. While we have used a particular system, Co adatoms on Cu(111) to demonstrate the possibility of tuning the quantum tunneling by an external electric field and the site-dependent switching of the magnetization of the adatom, the main conclusions of our work are of a general importance. It could be possible to control the position of adatoms and their spin states by an external electric and magnetic fields.

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Notes

The authors declare no competing financial interest.

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