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## TIP-INDUCED MODIFICATIONS IN SCANNING TUNNELING MICROSCOPY AND ATOMIC FORCE MICROSCOPY

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### Abstract

Tip-induced modifications of microscopic processes in scanning tunneling microscopy (STM) and atomic force microscopy (AFM) of the Si(100) surface are investigated with *ab initio* total energy pseudopotential calculations. The results of the calculations lead to a new understanding of the microscopic STM measurement process and the micro-mechanical changes (hysteresis and plastic deformation) in the AFM process. In particular, in the latter case, the results predict that the tip can be used to flip dimers on the surface, from one buckled configuration to the other, reversibly, and without inducing damage to either the intrinsic surface or the tip.

**Key Words:** Scanning tunneling microscopy, atomic force microscopy, Si(100) surface, surface reconstruction, hysteresis, plastic deformation, first-principles calculations, pseudopotential, density functional theory, local density approximation.

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### Introduction

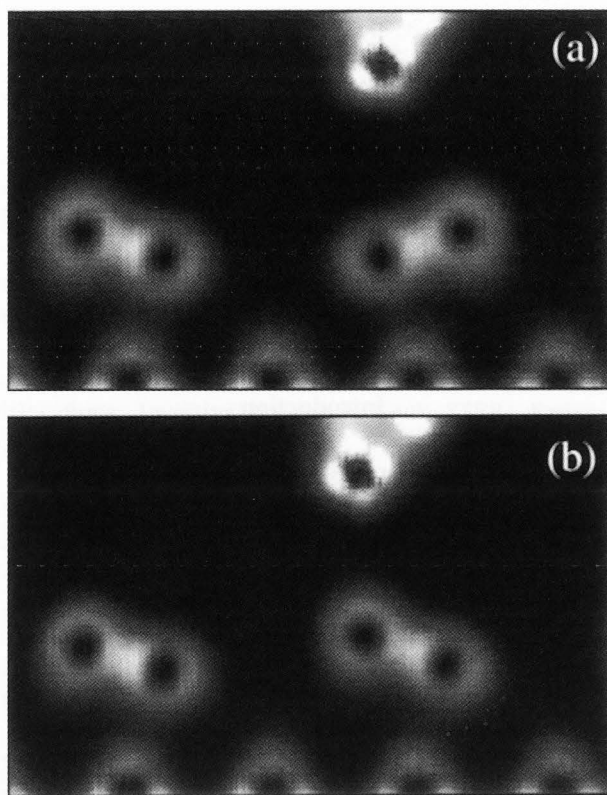
Scanning tunneling microscopy (STM) and atomic force microscopy (AFM) provide an image of a surface structure at atomic resolution [1, 2]. The basic principle of STM and AFM is to monitor the interaction between an atomically sharp tip and the surface, as the tip scans over it at a close distance. An STM (AFM) surface image is then generated as a collection of the tunneling current (force) between the tip and the surface, at each position of the tip on the corresponding surface area.

The conventional interpretations of an STM or an AFM image is that the image shows the *intrinsic* structure of the underlying surface. These interpretations are based on the assumptions made in the conventional theories of the STM and AFM images. The conventional theory of the STM image interprets the image as the convolution of the tip electronic wave function and the intrinsic surface electronic wave function based on the first order perturbation approximation [4, 9, 11]. On the other hand, the conventional theory of the AFM image interprets the image as the elastic response of the surface atoms to the interaction between the tip and the surface, so that the image is a mapping of the intrinsic stiffness of the surface atoms [for a review, see, 13].

Even though both of these simple interpretations are very good approximations for many surfaces, there are surfaces where the tip-surface interactions and the surface dynamics can significantly change the images from the intrinsic structure of the surface. In this work, we select the silicon (100) surface as an example of how the microscopic processes of an STM and AFM measurement can lead to a scanned image that does not represent the intrinsic structure of the surface. Our approach is to perform a first-principles study of the tip-surface interactions on this surface using a state-of-the-art density functional pseudopotential conjugate gradient scheme [10].

### Scanning Tunneling Microscopy at Room Temperature

The Si(100) surface consists of a dimer reconstruction. Each dimer is formed by moving two surface



**Figure 1.** The total valence electron charge density of the tungsten tip and the Si(100) surface system is plotted in the (011) plane. The cross section contains two asymmetric dimers and the apex atom of the tip. Top and bottom panels show different minimum energy geometry of the right-hand dimer, and the geometry of the bottom panel has lower energy by 0.2 eV.

atoms close together to form a covalent bond between them. The detailed nature of the dimer geometry has been a controversial problem since STM images revealed a symmetric dimer image at room temperature [7, 12], when theory had predicted a symmetric dimer geometry by about 0.1 eV [3, 6]. It was suggested that, at room temperature, the asymmetric dimer is thermally fluctuating between two equivalent geometries, thus leading to an averaged symmetric dimer image based on the assumption that the effect of the tip on the surface is negligible [6]. This assumption was tested by Huang *et al.* [8] with *ab initio* calculations of the tip-induced polarization of the Si(100) surface, using a model tip simulating the tip bias voltage, and the effect of the tip bias voltage on the dimer was found to be negligible. However, the effect of the actual tungsten tip was not included, and a full *ab initio* study of the tip-surface system using a realistic tip was yet to be reported. We resolve this controversy on the dimer geometry with full *ab initio*

calculations of the tip-surface system.

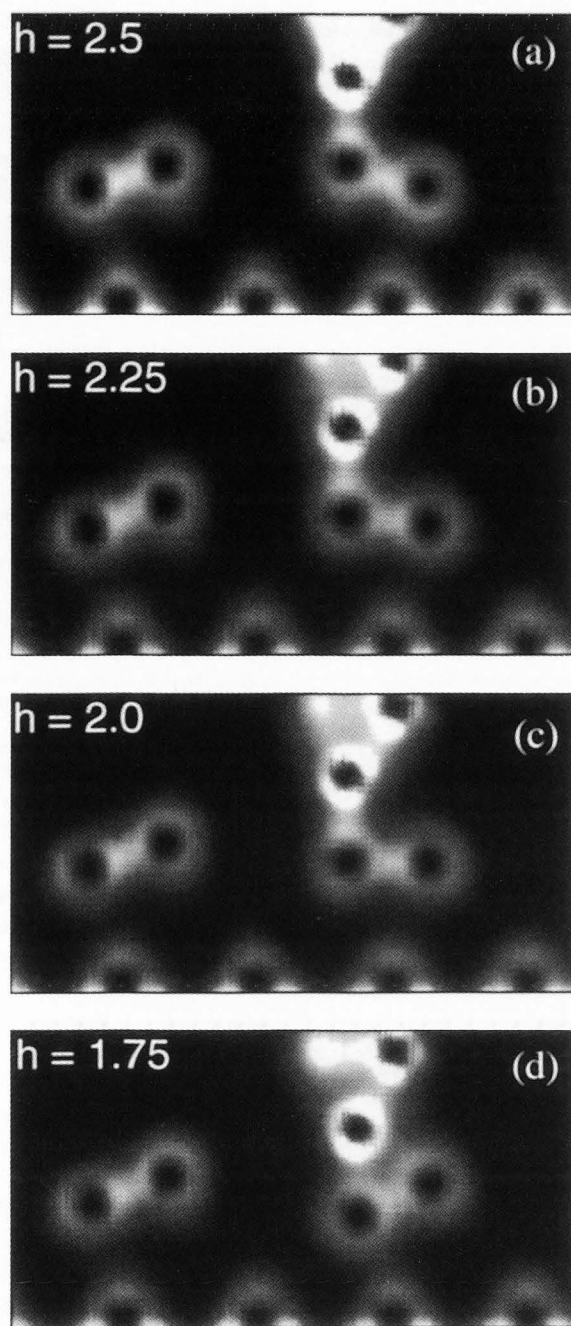
Let us investigate the tip-induced surface modifications at room temperature. At room temperature, the asymmetric dimer on the Si(100) surface can flip between two equivalent asymmetric geometries because the barrier of 0.1 eV is small enough to be overcome by thermal fluctuations. To study the influence of the tip on the dimer geometry, we place the tungsten tip above a dimer atom, as shown in the top panel of Figure 1. The thermal fluctuations lead to the flipping of the dimer geometry, as shown for the right-hand dimer at the top and bottom panels of Figure 1.

However, the calculation shows that the total energy of the tip-surface system is 0.2 eV lower for the geometry at the bottom panel of Figure 1 than for the geometry at the top panel. This energy difference leads to the capturing of the fluctuating dimer in the up-flip geometry, as portrayed in the bottom panel of Figure 1. Of course, as the tip moves away, the dimer reverts to its normal fluctuations. Consequently, the tip always measures a dimer atom in up-flip geometry, resulting in a symmetric STM image of the dimer. The details of these calculations are published in [5].

### Atomic Force Microscopy at Low Temperature

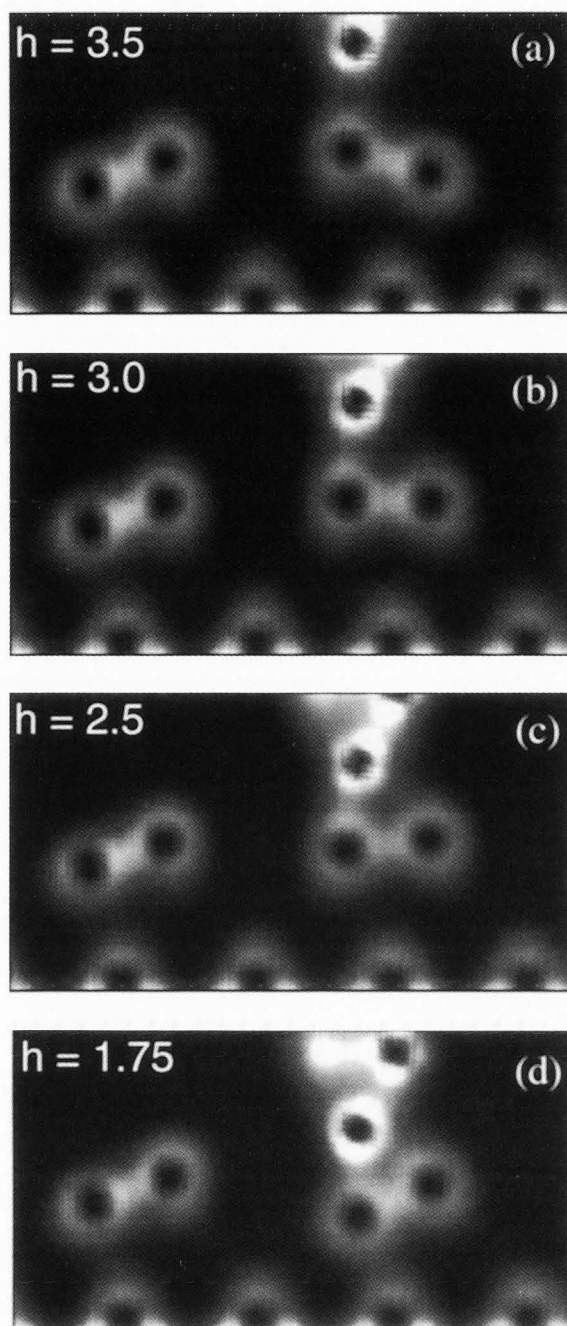
Let us now investigate the tip-induced surface modifications at low temperature, where the surface dynamics can be suppressed. Furthermore, let us test the validity of the universal interatomic interaction curve which is used in the conventional interpretation of the AFM image. In an AFM measurement process, the tip is interacting with a surface atom, and this surface atom is bonded to the other atoms of the surface. Depending on the tip-surface atom separation, these bonds are stretched or compressed to induce an attractive or a repulsive force on the tip.

The changes of the surface dimer geometry as the tip moves down to the surface and subsequently moves up from the surface are illustrated in Figures 2 and 3. Figure 2 shows the cross sections of the total charge density of the tip-surface system after the relaxation according to the tip-surface interaction forces. The four panels in Figure 2 correspond to the sequence of decreasing tip-surface distances, 2.5 Å, 2.25 Å, 2.0 Å, and 1.75 Å. This sequence shows that, as the AFM tip moves down, it *pushes down* and *flips* the surface dimer. The first three panels show a gradual decrease of the dimer angle (17°, 12°, and 2°), but the change of the equilibrium dimer-angle between the third panel and the fourth panel appears *discontinuous* (from 2° to -24°). To test the discontinuity of the equilibrium dimer-angle as a function of  $d_{\text{tip-surface}}$ , we perform the following exercise. We start from the relaxed atomic positions of



**Figure 2.** Sequence of the cross sections of the total valence electron charge density, as the tip moves down from the top panel to the bottom panel;  $h$  measures the height of the tip from the surface. (a)  $h = 2.5$ ; (b)  $h = 2.25$ ; (c)  $h = 2.0$ ; (d)  $h = 1.75$ .

the calculation at  $d_{\text{tip-surface}} = 2.0 \text{ \AA}$ , slightly move down the AFM tip to  $d_{\text{tip-surface}} = 1.9 \text{ \AA}$ , and let the tip-surface system relax. This small change of  $0.1 \text{ \AA}$  is found to be large enough to push the dimer over the stat-

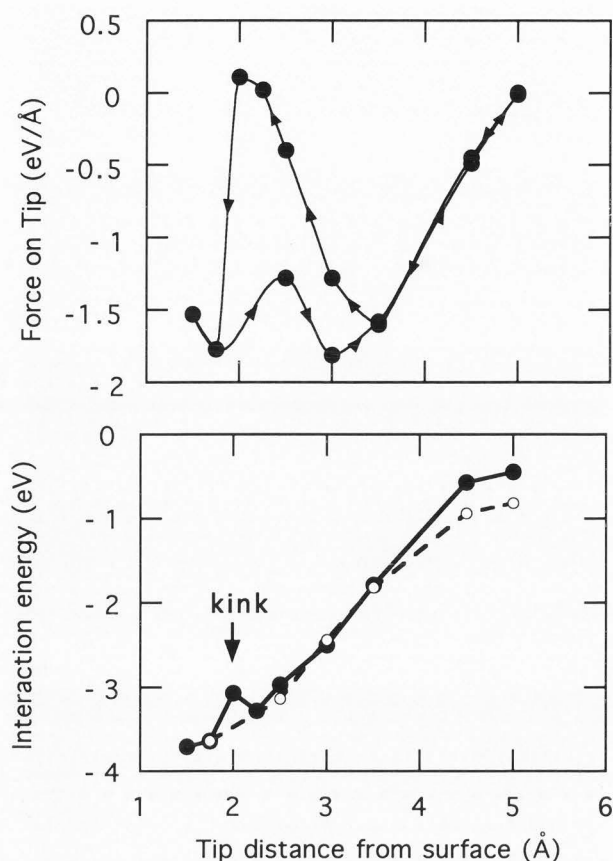


**Figure 3.** Sequence of the cross sections of the total valence electron charge density as the tip moves up subsequently from the bottom panel to the top panel;  $h$  measures the height of the tip from the surface. (a)  $h = 3.5$ ; (b)  $h = 3.0$ ; (c)  $h = 2.5$ ; (d)  $h = 1.75$ .

ic barrier of the symmetric configuration, and the dimer geometry relaxes toward the down-flip configuration.

However, as the AFM tip moves up, the dimer configuration changes continuously as shown in Figure 3.





**Figure 4.** The top panel is the calculated total force on the tip as the tip moves down and subsequently moves up as shown in Figures 2 and 3. The tip distance from the surface is the same  $h$  indicated in Figures 2 and 3. The bottom panel is the tip-surface interaction energy along the down-path (continuous line) and the up-path (broken line).

From the sequence of bottom to top, the tip-surface distance increases from 1.75 Å to 2.5 Å to 3.0 Å to 3.5 Å, and the dimer-angle increases gradually. This different behavior of dimer geometry clearly indicates that the dimer configuration follows two different local minimum energy paths as the tip moves down and up, and the dimer configuration shows not only a quantitative difference but also a qualitative difference in the down-up cycle.

In order to make direct contact with AFM experiments for this system, we have calculated the force on the tip for the two different pathways corresponding to lowering and raising the tip. The results are shown in the top panel of Figure 4. We note that the force-distance hysteresis loop exhibits a rather complex behavior. As the tip approaches the surface between 5.0 Å and 3.5

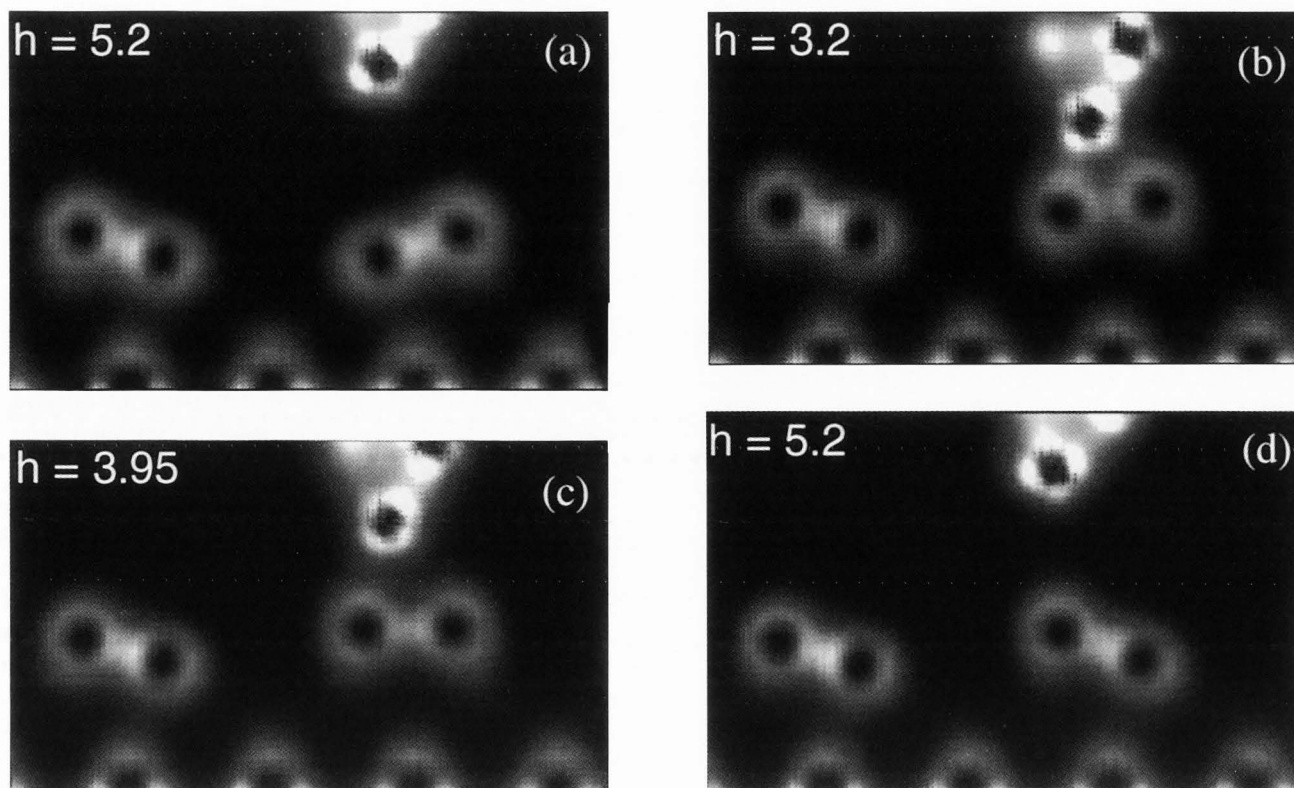
Å along the down-path, the force on the tip becomes more attractive and reaches a maximum at 3.5 Å. This corresponds to an inflection point in the interaction energy curve between the tip and surface as shown in the bottom panel of Figure 4. From 3.5 Å to 2.25 Å, one approaches a metastable equilibrium geometry for "adsorption" of the tip on the surface. At 2.25 Å, the force is zero and the interaction energy is at its minimum. As the tip approaches closer to the surface, the force now becomes repulsive, and at a distance of slightly less than 2 Å, the dimer has flipped with a discontinuous change in its equilibrium angle. This corresponds to a process of overcoming the *kink* in the interaction energy. At this point, the force is large and attractive since the tip would prefer to get closer to the down-dimer-atom. This corresponds ultimately to the global adsorption energy minimum geometry.

As we now raise the tip from a distance of 1.75 Å to 3 Å, the force initially becomes slightly less attractive up to 2.5 Å, and then reverts to becoming slightly more attractive from 2.5 Å to 3 Å. This corresponds directly to the tip atom being allowed to relax more during the first phase (1.75 Å → 2.5 Å). The relaxation of the tip is correlated to the change of the dimer geometry, and there is a larger change in dimer geometry position during the first phase than during the second phase. At 3 Å, the dimer angle has just changed sign, as shown in the second panel of Figure 3. As the tip-surface distance increases further, the dimer gradually reverts to its original flipped geometry and the force on the tip approaches zero.

### Plastic Deformation

As an extreme case of the hysteresis effect, one can induce a *plastic deformation* of the dimer geometry. This is achieved by capturing the lower dimer atom with the tip and pulling the dimer up (Fig. 5). This plastic deformation of the dimer geometry could have a practical application as a high density memory device. Since each dimer can be manipulated to exist in one of two equivalent states, it conceivably can be used to write and read one bit of information.

In conclusion, the scanning tip of STM and AFM can induce a significant modification of specimen surface structure during the measurement process, both at room temperature and at low temperature. Under these circumstances, one needs to include tip-induced effects in the interpretation of the scanned surface images. Finally, these calculations suggest the intriguing possibility that the scanning tip could be used together with the Si(100) surface to design an ultra high density memory storage device.



**Figure 5.** The sequence of the cross sections of the total valence electron charge density illustrates the plastic deformation process of the dimer. From the top panel to the second panel, the tip is lowered to capture the dimer, and the tip is brought up in the third panel and the bottom panel. (a)  $h = 5.2$ ; (b)  $h = 3.2$ ; (c)  $h = 3.95$ ; (d)  $h = 5.2$ .

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## Discussion with Reviewers

**Reviewer I:** It is a little bit unclear about the hysteresis curve in Figure 4. It appears that two diverging paths for approach and retraction of the tip do not occur until after going over the "kink" in interaction energy. If this were the case, a bit more physical explanation for how this "global adsorption energy minimum" position makes it any different from others in chemical bonding/structural relaxation, etc. would be helpful to readers.

**Authors:** The range of the hysteresis loop of the dimer geometry is not directly reflected in the curves of the force on the tip and the tip-surface interaction energy since the dimer geometry can follow two different local minimum paths with almost identical energies. The kink in the down-path energy curve only indicates the presence of an energy barrier for flipping the dimer in the down-path, rather than representing the range of the hysteresis loop. The diverging hysteresis paths of the dimer geometry begins at about 3 Å, before the down-path reaches the kink.

**H. Rauscher:** In the calculations of Huang and Allen [8], the symmetric appearance of the Si dimer is rationalized by a rapid thermally induced flipping of the dimer. Do you think that in an STM measurement the interaction of the scanning tip with the dimer is strong enough to stop this flipping temporarily or that such a thermal flipping is not relevant for STM measurements?

**Authors:** In an STM measurement, the interaction of the scanning tip with a dimer is different for the up-flip and down-flip configurations. Consequently, if one plots the energy of the tip-surface system as a function of the asymmetry angle, it becomes an asymmetric double potential well. At finite temperatures, the dimer can flip between the two local minima of the potential well. However, the difference of the local minimum energies leads to different average times for the dimer to stay in the up-flip or down-flip configurations. At room temperature, the dimer can flip many times (about  $10^5$  times) during a typical STM measurement time, and the ratio of the average time for the dimer in the up-flip and the down-flip configurations is about 2500. Consequently, the dimer stays in the up-flip geometry for all practical purpose, as if it is captured by the scanning tip.

**H. Rauscher:** Asymmetric dimers can be observed by STM in the vicinity of defects {bucking along the dimer row; see Wang *et al.* (1994)}. In this case, why is a flipping of the dimers (as postulated by the authors) not observed?

**Authors:** Asymmetric dimers are observed in room temperature STM measurements in the vicinity of the defects. This stabilization of the asymmetric dimers could have been caused either by an increase of the energy barrier between two asymmetric dimer configurations to suppress the thermal flippings or by the asymmetry of local minimum energies induced by the defect. Since the influence of a defect on a dimer in the vicinity is usually not symmetric to the two atoms of the dimer, the second mechanism is more likely to be in effect.

**H. Rauscher:** In AFM measurements, the interaction between the tip and the surface has a much longer range than in STM measurements. Usually, this interaction is considered to be relevant, not only for the outermost atom of the tip and "a surface atom" as stated by the authors, but between a number of atoms on the tip and on the surface. How do the authors see the possibility of fabricating a potential high density memory device (as stated in the text) by plastically deforming single dimers, and thus read and write single bits of information, in the light of these arguments?

**Authors:** In the usual AFM measurements, the scanning tip is pressed against the surface so that many tip atoms are in intimate contact with the surface atoms. In this case, the force on the scanning tip is repulsive. However, it is also possible to operate the tip at a larger distance with attractive force on the tip to satisfy the conditions described in the manuscript. The possibility of delicate control of a scanning tip, which can be used to realize the plastic deformation, was recently demonstrated by Salling and Lagally (1994).

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