Nanomanipulation of Au nanoclusters on the NaCl(001) surface by nc-AFM

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Introduction

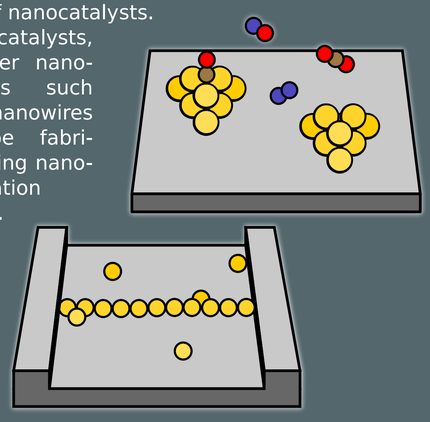
Non-contact AFM offers tools for intricate study of nanocluster properties and nanomanipulation enabling, e.g., exact design of nano-catalysts.

In this work, we experimentally demonstrate manipulation of Au nanoclusters on the NaCl(001) surface and examine the anisotropy seen in the movement of the clusters during manipulation.

Nanocatalysts & nanostructures

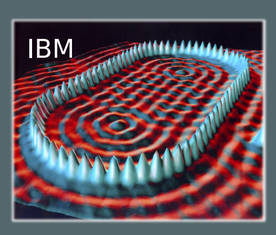
Metallic nanoclusters adsorbed on insu-lating surfaces are promising candidates for next generation catalysts in various important processes, and the size, shape and adsorption site of the clusters have profound effects on the reactive properties of such catalysts. Being able to control these variables would allow for optimization of the catalytic properties. Thus, the ability to manipulate clusters and single atoms on insulators is an invaluable tool in the study and design of nanocatalysts.

Besides catalysts, also other nano-structures such as nanowires could be fabri-cated using nano-manipulation methods.



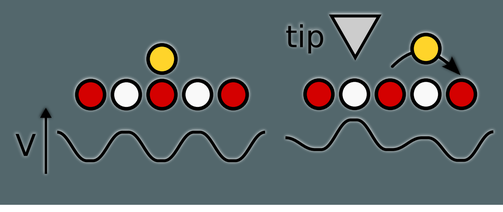
Nanomanipulation

Although manipu-lation of atoms using SPM tools is not new [Eigler & Schweizer, Nature **344**, 524 (1990)], it is still challenging on insulating surfaces where STM tools are ill suited. Working with such systems, nc-AFM is the method of choice.



Nanomanipulation of atoms with AFM typically works as follows. As the AFM tip is brought close to the surface, it affects the local potential energy landscape. If positioned suitably, the tip can lower the energy barriers between sites, allowng atoms to hop from one position to another - on surface or between the tip and the surface.

Large nanoparticles can be manipulated simply by pushing with the AFM tip. However, manipulation of clusters of some tens or hundreds of atoms is not as simple as the shape and size fo the clusters may be altered during the manipulation events, which may be undesirable.

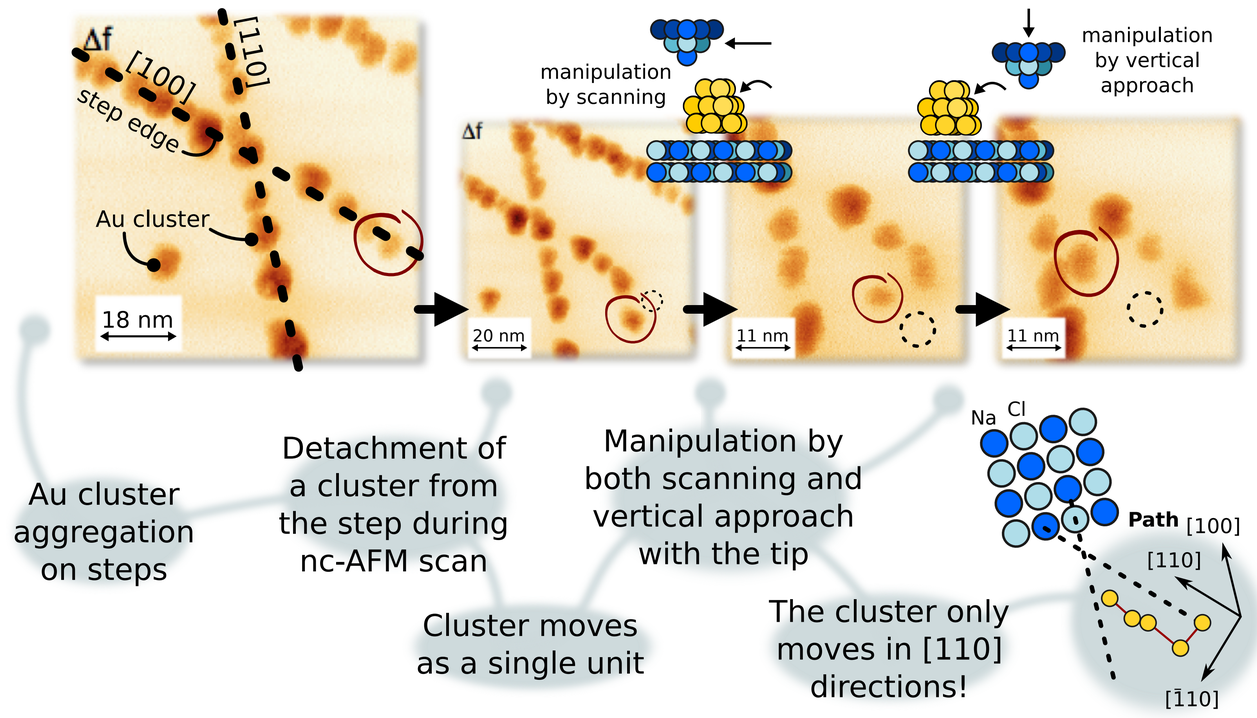


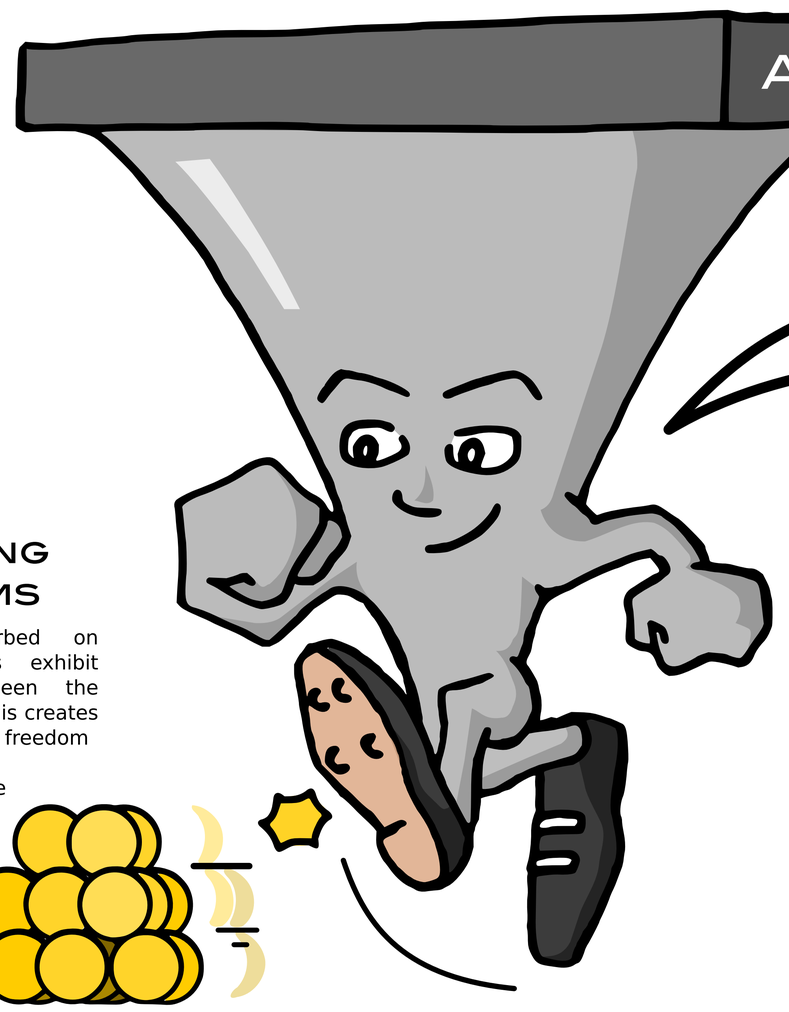
Experiments

Nanomanipulation of gold clusters on NaCl realized in experi-ments, movement of clusters anisotropic.

Method

- UHV cleaved+annealed NaCl(001) surface
- neutral Au atoms form clusters at steps
- cluster diameter few nm
- nc-AFM in constant height mode

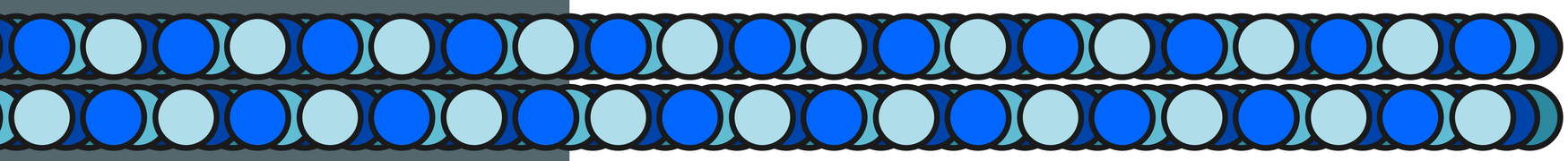




Insulating thin films

Metal clusters adsorbed on insulating thing films exhibit charge transfer between the cluster and substrate. This creates yet another degree of freedom for catalyst design.

So, as the next step, we are planning nano-manipulation studies on MgO/Ag...



Conclusions

Experimental

- nanomanipulation of Au clusters on NaCl(001)
- clusters move only in [110] directions, not [100]

Theory

- Au very mobile on perfect NaCl, vacancies anchor
- joint movement of Au and a Na vacancy prefers [110], as seen in experiments

Simulations

First principles calcu-lations determine the most stable configurations and preferred diffusion paths of clusters.

On perfect NaCl, the clusters are mobile with no preferred direction of move-ment, but the pre-sence of defects in-duces anisotropy.

Method

- plane wave DFT
- VASP code
- PBE functional
- Nudged elastic band algorithm (barriers)
- Au_{20} test cluster
- NaCl slabs of at least 106 atoms