Non-contact AFM offers during manipulation. Movement of the clusters anisotropy seen in the surface and examine the clusters on the NaCl(001) surface and examine the anisotropy seen in the movement of the clusters during manipulation.

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

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

Nanocatalysts & Nanostructures
Metallic nanoclusters adsorbed on insulating 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 nanostructures such as nanowires could be fabricated using nanomanipulation methods.

Nanomanipulation
Although manipulation of atoms using SPM tools is not new (Esler & Schwoerer, 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 correctly, the tip can lower the energy barriers between sites, allowing atoms to hop from one position to another - on surface or between the tip and the surface. Large samples can also be manipulated simply by pushing with the AFM tip. However, manipulation of clusters of some tens of hundreds of atoms is not as simple as the case above and the clusters may be altered during the manipulation events, which may be undesirable.

First principles calculations determine the most stable configurations and preferred diffusion paths of clusters. On perfect NaCl, the clusters are mobile with no preferred direction of movement, but the presence of defects induces anisotropy.

Conclusions
- Nanomanipulation of Au clusters on NaCl(001)
- Clusters move only in [110] directions, not [100]
- Au very mobile on perfect NaCl, vacancies anchor
- Joint movement of Au and a Na vacancy prefers [110], as seen in experiments

 SIMULATIONS

Method
- plane wave DFT
- VASP code
- PBE functional
- Nudged elastic band algorithm (barriers)
- Au23 test cluster
- NaCl slabs of at least 106 atoms