Nanoscale Analysis of Nano-Car and Buckeye Ball Structure and Diffusion

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Molecular machines have the potential to revolutionize a variety of fields, including material synthesis. More specifically, if the motion and structure of molecules is understood, it becomes feasible to develop nanoscale machines that transport molecules and facilitate bottom up synthesis. Characterizing the structural and diffusional properties of fullerenes and nano-cars is essential to advancing the field of molecular machines. In this project, we use ambient and ultra high vacuum scanning tunneling microscopy (STM) to analyze and compare the motion of pure fullerenes and fullerene wheeled nano-cars. Kandel et al. (*Journal of Physical Chemistry B* 2004) proposed an anchor model for fullerene diffusion on gold, as well as reported observing two distinct stable orientations of fullerene packs on gold. Additionally, Kelly et al. (*Nano Letters* 2005) used thermal excitation and STM tip manipulation to demonstrate the rolling motion of nano-cars on gold. We too have observed two distinct orientations of fullerene on gold. We plan to further confirm the aforementioned fullerene and nano-car models, and to extend these models to both different surfaces and different temperatures. Additionally, we plan to find the parameters for which we can use the scanning tunneling microscope to manipulate nano-cars under ambient conditions. Our characterization of the molecular structure and diffusion of fullerenes and nano-cars will expand our fundamental understanding of molecules and enhance the feasibility of molecular machines for engineering applications.

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Molecular Transport: The Fullerene-wheeled Nanocar

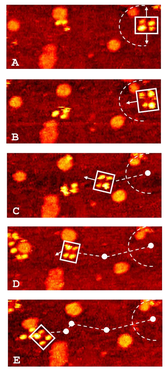


Figure 1: STM images of the Nanocar thermally translating across gold. It is only able to move perpendicular to its axles.[1]

Molecular transport makes possible processes like bottom-up synthesis, which is crucial to creating structures from nanomaterials.

The Nanocar is a molecular machine which, as illustrated in Figures 1 and 3, has demonstrated directed rolling motion on Au(111) and has the potential to facilitate molecular transport.[1]

To better understand the motion of the Nanocar, we need to understand the motion of its fullerene wheels.

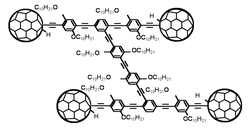


Figure 2: Chemical structure of the Nanocar. [1]

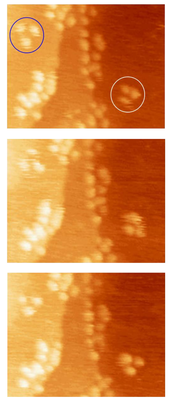


Figure 3: STM images of fullerene wheeled trimers pivoting when thermally excited.[1]

We test Kandel's model of fullerene diffusion using a scanning tunneling microscope (STM).

Kandel Model of Fullerene Diffusion

Kandel et al. created an anchorage model of cluster diffusion which accounts for variations in fullerene-fullerene and fullerene-Au(111) bonding based on its orientation.[2]

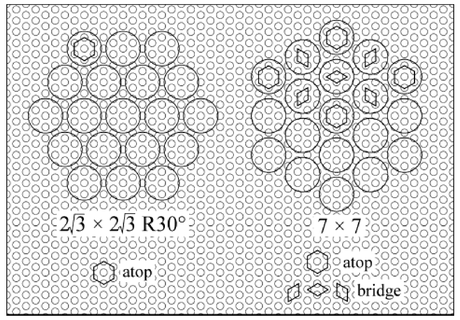


Figure 4: Two orientations of fullerene. [2]

The two orientations of fullerene on Au(111) are shown in Figure 4.[2]

For $2\sqrt{3} \times 2\sqrt{3}$ R30°, the variations in fullerene-Au(111) binding energy are significant to diffusion.[2]

For, 7 x 7 both the variations in fullerene-Au(111) and fullerene-fullerene binding energy are significant to diffusion.[2]

Anchorage Model: The diffusion of the least stably bound fullerene on an island destabilizes neighboring fullerenes and causes them to diffuse at an exponential rate leading to apparent cluster diffusion. [2]

Scanning Tunneling Microscope (STM)

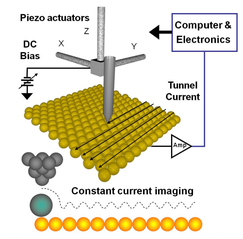


Figure 4: Basic schematic of STM.

The STM uses quantum tunneling of electrons to obtain high resolution topographic data about a surface.

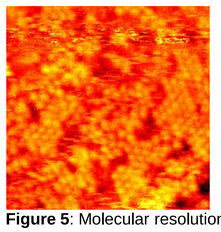


Figure 5: Molecular resolution image of fullerene evaporated on gold.

We use the UHV STM to collect images of fullerenes that have been evaporated onto Au(111) at 200nA and 30s.

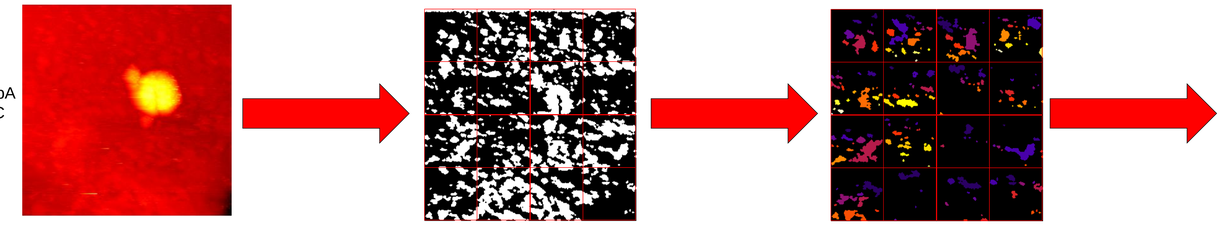
Testing the Anchorage Model

Before testing the diffusion model, we used RHK's software to correct for the drift of the piezoelectric tube.

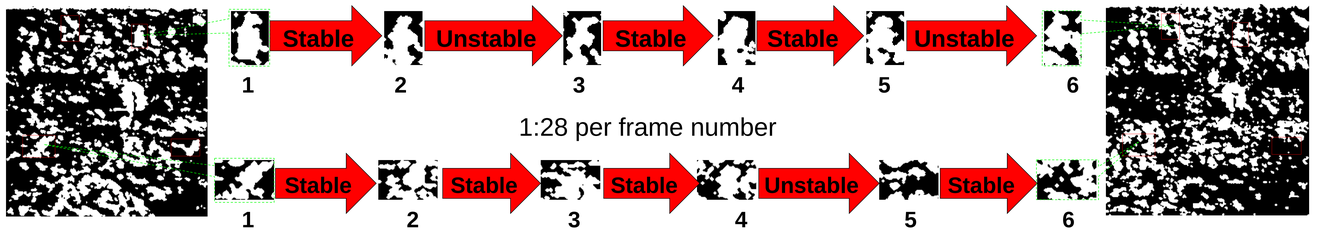
To track cluster diffusion from islands we generated the following algorithm:

1. Converts original image to binary and isolates the clusters that remain within user defined regions. This allows one to easily locate and monitor specific islands and clusters.

IV: .4V; 5pA
T: 43°C

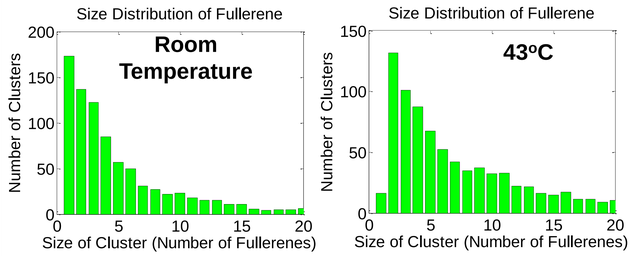


2. Finds areas with largest fullerene islands based on the image created in step 1 and tracks these areas over time.



According to the anchorage model, fullerene islands should display periods of stability on the time scale of the STM, followed by sudden instabilities too fast for the STM to image. This is exactly what we see.

Implications of the Anchorage Model



Size distributions at room temperature and 43°C show that most diffusion occurs in clusters.

The anchorage model accounts for most fullerene dynamics on Au(111).

Distributions begin to show the temperature dependence of fullerene-fullerene and fullerene-Au(111) bonding energy, but we need more data points to draw conclusions.

Confirmation of Kandel Model

The anchorage model for cluster diffusion is confirmed.

A group of Nanocars in close proximity is likely effected by both fullerene-Au(111) bonding and van der Waals forces between fullerene wheels.

An algorithm similar to ours could be used create a quantitative model of fullerene diffusion

References and Acknowledgements

1. Y. Shirai et al. *Nano Letters* **2005** *5* (11), 2330-2334
2. Kandel et al. *The Journal of Physical Chemistry B* **2004** *108* (37), 14074-14081

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