# Controlling Molecules on Surfaces

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The motion of one molecule on a surface can cause the subsequent motion of another molecule, and so on in a cascade of molecular motion. We call such an engineered motion a "molecule cascade". A molecule cascade is similar to a row of toppling dominoes. It offers a unique chance to study the physical mechanism of hopping molecules as well as interesting applications for information transport and computation [1].

Carbon monoxide molecules were arranged in atomically precise configurations on the copper (111) surface with a low-temperature scanning tunneling microscope (STM). We found that one configuration of three CO molecules at nearest neighbor sites is stable enough to be investigated but unstable enough to decay on the timescale of seconds. This "chevron" configuration is shown in Fig. 1. A cascade of motion is achieved by placing pairs of CO molecules such that a preceding hop sets up another chevron and so on in a chain of arbitrary length.

We never saw molecule cascades moving backwards and therefore concluded that the energy loss per hopping molecule is larger than $k_BT$. This triggered a thorough investigation of the hopping mechanism of chevron-based cascades. We studied the hopping rate as a function of temperature from 0.5 Kelvin to about 10 Kelvin. The lower temperature limit of 0.5K is given by our new STM.

At low temperatures we found a hopping rate that is independent of temperature from 0.5K to about 6K (2.5s for $^{12}C^{16}O$) indicative of quantum tunneling. To further test this hypothesis we studied the hopping rate as a function of carbon and oxygen isotopes. We relied heavily on the use of inelastic vibrational spectroscopy to distinguish the different isotopes in-situ [2]. A molecule cascade built from heavy carbon proceeds about 4 times slower than light carbon whereas the oxygen mass plays a smaller role in this tunneling process. At temperatures above 6K we observed thermally activated hopping with very low exponential prefactors for all isotopes suggesting tunneling from thermally excited vibrational states. The Oxygen isotope does not influence the propagation speed nearly as much. A linked chevron cascade with $^{18}O$ propagates about half as fast as the $^{16}O$ cascade. Hence, a mass change on the Oxygen is less efficient in tuning the propagation speed of the cascade than a mass change on the Carbon.

Cascades of any type can be used to transmit information from the beginning of the cascade to its end. In a molecule cascade this is inherently binary: either the molecule is in the initial or in the final state. In analogy, the dominoes are either standing upright or have fallen over.

Figure 2 shows a molecule cascade based on the linked chevron design in the initial and final configuration. After triggering the cascade with the controlled motion of one molecule, all remaining hops occur spontaneously.

Through the use of empirical rules we were able to engineer the intersection of molecule cascades to demonstrate logic functions such as AND, OR, fanout, and crossover. We were able to drive the input of one gate directly from the output of another, demonstrating that operating a nanoscopic circuit is possible, a first step towards integrated nanocircuits.

The most complicated circuit built with molecule cascades is a three input sorter where three outputs count the number of inputs that have been triggered. By designing the same logic circuit in current CMOS technology the vast potential for nanotechnology becomes apparent: the molecule cascade circuit is 260,000 times smaller in surface area.

## References

[1] A.J. Heinrich, C.P. Lutz, J.A. Gupta, and D.M. Eigler, Science **298**, 1381 (2002)
[2] B.C. Stipe, M.A. Rezaei, and W. Ho, Science **280**, 1732 (1998)

## Figures

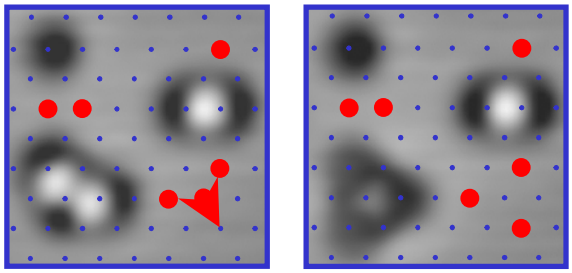

**Fig. 1** Six CO molecules (red circles) on Cu(111) (blue dots indicate substrate atoms). The chevron on the left is unstable and decays by the hopping of one molecule. The final and stable configuration is shown on the right.

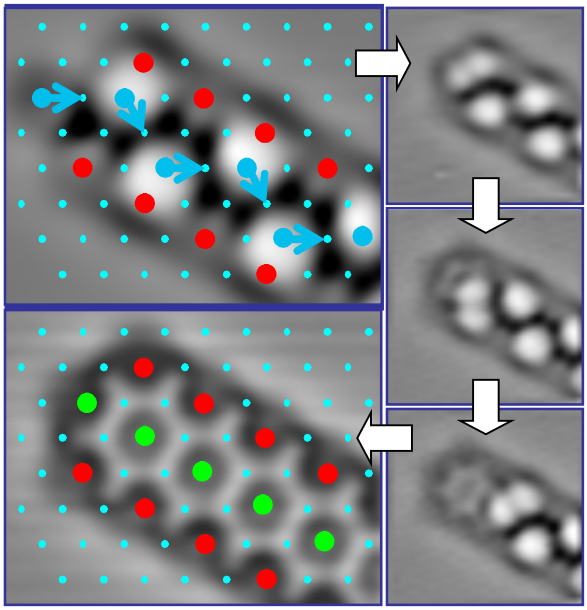

**Fig. 2** Linked chevron molecule cascade on Cu(111). Upper left shows the initial configuration, lower left the final configuration after all molecules have hopped. Images on the right are intermediate steps of the cascade, from top to bottom: after the initial trigger, after stage 1 hops, and after stage 2 hops.