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Measuring and Controlling Molecular-Scale Properties for Molecular Electronics

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1. Introduction

We use intermolecular interactions to direct molecules into desired positions to create nanostructures [1,2], to connect functional molecules to the outside world [2], and to serve as test structures for measurements on single or bundled molecules [2-4]. We use and develop scanning probe microscopes to determine both local structures and the electronic and other local properties [5]. We have applied these tools to isolate molecules with electronic function to determine the mechanisms of function, and the relationships between molecular structure, environment, connection, coupling, and function [3,4,6]. We have been able to demonstrate that single molecules can function as multistate switches, and have determined important aspects of the mechanism, function, and persistence of switching. We will discuss the origins of switching and the relevant aspects of the molecular structure and environment required.

2. Approaches

We apply selective chemistry and self-assembly in combination with conventional nanolithographic techniques to reach higher resolution, greater precision, and chemical versatility in the nanostructures that we create [1,2]. The key to these approaches is using precise, robust molecular layers that attach selectively to specific patterned substrate materials. In one approach, we apply precise-thickness multilayers (termed "molecular rulers") to nanolithographically created structures and use these multilayers as resists for lift-off [2]. The thickness and thus the spacing of the resultant structures can be controlled down to 5 nm, with control to 1 nm or better. We have demonstrated this approach both with e-beam generated structures as well as those based entirely on self-assembly. An additional advantage of molecular rulers is the inherent capability to displace the molecular resist chemically, and thus to remove the resist material simply and completely. We can also use molecular rulers with carefully designed parent structures to create complex structures that would be difficult to generate by conventional means. These can be made still more sophisticated by the selective application and use of sacrificial intermediate or parent generation structures. We will discuss our approaches to pattern design and creation using this method.

Another method that we use to study functional molecules and nanostructures involves controlling the types and densities of defects in self-assembled films in order to control the degree to which molecules can be added to or exchanged from the film, as well as the extent of mobility within the film [1].

This has allowed us to place functional molecules into defects for measurement, as well as to change their environment in order to explore the effect of their surroundings on the properties of interest [3,4]. Defects control both the number of inserted molecules and the tightness with which they are held. Both these variables can be used to advantage. The means of control and their application will be discussed.

3. Observations

We have followed the behavior of single molecular switches using scanning tunneling microscopy [3,4]. We have developed analysis tools to track many individual switches or bundles in the "field of view" of the microscope in order to measure the effects of changing the switch molecules, their environment, or the measurement conditions on distributions of single molecule or isolated bundles of switches.

We have varied the functional groups included as well as the backbone of the molecule. We have further varied the tightness of the molecular matrix around the switches. We have shown under what conditions we find stochastic switching and how to induce switching with an applied electric field. These experiments have enabled us to identify the mechanism by which the molecules switch, and to eliminate many other suggested mechanisms.

In other experiments we have used nanolithographically designed structures in combination with self-assembly of bifunctional molecules in order to create nanostructures to be used to hook up functional molecules to the outside world [2]. These structures have precise spacings tuned to match the length of the molecules connected. We will present examples, current capabilities, and limitations of this method in its current state of development.

4. Conclusions

We use self- and directed assembly to create and to modify functional nanostructures. These nanostructures can be further tailored and tuned through molecular design of both the functional and structural components.

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