Nano- and mesoscale molecular junctions: Control of defects, chemical bonds and surface topography at metal-molecule interface

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Using molecules in electronics has an enormous appeal. Reaction chemistry offers vast diversity of molecular substructures and chemical transformations. However, wiring the molecules in a macroscopic circuit remains a challenging problem.

I present three approaches that we use to build small molecular structures. The first group of experiments is targeted toward wiring of a single or just a few molecules. We found that the conductance mechanisms observed in such ultrasmall devices differ dramatically from the predicted transport through molecules. The electronic states mediating the transport are low energy defect states rather than the electronic states of the molecules. To detect the conductance associated with the molecular states, we have developed high-yield process based on prefabricated nano-templates to screen the properties of larger molecular junctions with characteristic size of ~50–300 nm. The approach readily permits to experiment with the topography, the chemical bonding at metal-molecule interface and to significantly reduce the defect density. For the first time, we directly compare the properties of conjugated versus saturated molecules with the length of ~1.5 nm. Finally, we build molecular junctions by imprinting ~100 nm Au pads on top of self-assembled monolayers. The pads are contacted by conducting AFM. Surprisingly, the results of all experiments show that the conductance of molecules is 4–5 orders of magnitude smaller than is commonly believed.