Single Molecule Electronics

Stuart Lindsay
(Stuart.Lindsay@asu.edu)
Department of Physics and Astronomy
Arizona State University
Tempe, AZ 85287
U.S.A.

The contact between a metal or semiconductor surfaces and a molecule is a key issue in the development of molecular electronics because electron transfer is exponentially sensitive to small changes in the bonding arrangement at these interfaces. In order to explore this problem, we have developed a scheme for making reliable contacts to single molecules[1]. The ëtestí molecule is embedded in an inert matrix with one end chemically bonded to a gold surface and the other end chemically bonded to a gold nanoparticle (NP). The structure is produced by self-assembly, and the top NP contacted by a gold-coated conducting AFM probe. In this way, we have obtained highly reproducible data from a number of (single) molecules. First principles simulations give results that are quite close to experiment[2].

The NP is not a passive participant in the process, and evidence of its electronic structure is seen in measured single-molecule I-V curves. Somewhat surprisingly, we find that the covalent bond between the molecule and metal is unstable, fluctuating significantly at room temperature to give rise to stochastic ìon-offî switching of the wired molecule[3].

These methods have also been applied to electrocative molecules, some of which exhibit negative differential resistance[4, 5].

1. Cui, X.D., A. Primak, X. Zarate, J. Tomfohr, O.F. Sankey, A.L. Moore, T.A. Moore, D. Gust, H. G., and S.M. Lindsay, Reproducible measurement of single-molecule conductivity. Science, 2001. 294: p. 571-574.

2. Tomfohr, J. and O.F. Sankey, Complex bandstructure, decay lengths and Fermi level alignment in simple molecular electronic systems. Phys. Rev. B, 2002. 65: p. 245105-245105-12.

3. Ramachandran, G.K., T.J. Hopson, A.M. Rawlett, L.A. Nagahara, A. Primak, and S.M. Lindsay, A Bond-Fluctuation Mechanism for Stochastic Switching in Wired Molecules. Science, 2003. 300: p. 1413-1415.

4. Rawlett, A., T.J. Hopson, L. Nagahara, R. Tsui, G. Ramachandran, and S. Lindsay, Electrical measurements of dithiolated electronic molecules via conducting atomic force microscopy. Applied Physics Letters, 2002. 81: p. 3043-3045.

5. Ramachandran, G.K., J.K. Tomfohr, O.F. Sankey, J. Li, X. Zarate, A. Primak, Y. Terazano, T.A. Moore, A.L. Moore, D. Gust, L.A. Nagahara, and S.M. Lindsay, The Electron Transport Properties of a Carotene Molecule in a Metal-(Single-Molecule)-Metal Junction. J. Chem. Phys. B, 2003. 107: p. 6162-6169.