Molecular electronics

This issue of PNAS contains a series of articles on molecular electronics. These papers deal with several crucial aspects of a field that has become very active in the last decade. The core field of molecular electronics comprises the fundamental chemical physics and energetics of signal transport, switching, logic, and storage at the molecular level. It also includes optoelectronics, magnetoelectronics, and bioelectronics at the molecular scale, although none of those topics is addressed here. Most of the publications concern the electronic response of a molecule in a molecular transport junction, on a length scale from the mesoscopic to the atomic. Molecular electronics also involves applications of molecular materials in computational electronics. Here, the most advanced ideas involve use of molecules as individual logic or memory units.

Current work in molecular electronics usually addresses molecular junction electronic transport properties, where the molecule can be viewed as a barrier for incoming electrons. This is the fundamental Landauer idea of "conduction as scattering" generalized to metal/single molecule/metal molecular nanojunction structures. The experimental contributions from the Gourdon and Hersam groups focus on the tunneling process in molecular transport junctions, using powerful and elegant techniques involving both demanding single-molecule junction synthesis and scanning tunneling microscopy and spectroscopy. The paper by Ho's group extends these experimental methods to examine vibronic components in the STM-geometry conductance, using precisely engineered surface structures. The contribution by Fisher and Ness addresses those inelastic effects in junction transport from a theoretical point of view. The papers from the Mayor and Kushmerick groups address such transport issues as fluctuation and vibronic features of molecular electronic wires by using break-junction and monolayer test beds.

These contributions reflect the drive to develop a truly planar atomic scale technology to prepare the molecule/electrode binding geometry with a precision better than 0.1 nm. A major unsolved problem in the structure determination is that there currently are no robust methods to image and determine the precise adsorption site and conformation of the molecule on this length scale. Such technology may open a new era for molecular electronics, when intramolecular quantum behaviors will be more accessible. Such understandings and control might then enable the use of the large quantum state space of a molecule for applications in computation or robotics. At the current stage of structural uncertainty, one expects to see fluctuations from measurement to measurement, or even within the same test system over time. Such fluctuations have been observed and are a clear consequence of the very small length scale and the resulting static and dynamic structural modifications of current molecular junctions. This occurrence of such fluctuations seems to be endemic to structures of this size, and therefore will be a concern in all sorts of electronics, molecular or other.

The introductory paper starts with this quantum engineering point of view. We discuss how a molecular structure can be viewed as a guiding quantum medium for superexchange interaction between the two nanoelectrodes that act as the quantum source and detector within the junction. Because molecules generally exhibit relatively strong vibronic coupling, we also discuss the decoherence and relaxation processes. These should be more significant with increasing molecular wire length and decreasing injection energy gap.

Molecular electronics is a technology-facing area of science. Its remarkable growth in the last two decades is a direct reflection of the synthetic capabilities arising from surface functionalization and bonding at interfaces, and of the invention of the scanning probe microscopies that permit both manipulation and measurement at the nanoscale. In the most favorable situations, such as those that have been developed and explored by many groups, including groups whose contributions are found in this special feature, it is possible to make measurements in a junction containing exactly one molecule. Such studies constitute the logical place for the science of molecular electronics to begin. We hope that the molecular electronics papers in this issue of PNAS will demonstrate the breadth and excitement of the field in 2005.

This collection of papers on molecular electronics is part of a series of PNAS special features highlighting forefront areas of multidisciplinary science, with a particular focus in the chemical sciences. Previous topics for special features have included Supramolecular Chemistry and Self-Assembly, Asymmetric Catalysis, Rapid Climate Change, Astrobiology, Science and Technology for Sustainable Development, Social and Behavioral Sciences, Natural Product Synthesis, Long-Range Electron Transfer, and Chemical Theory and Computation. An objective of these special feature issues is to advance the journal's initiative to expand its coverage of mathematics, physical sciences, and social sciences. PNAS continues to encourage submission of exceptional research articles in all areas of the natural sciences, social sciences, and mathematics.

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