

If Moore's law, which predicts that integrated circuit components tend to halve in size every 18 months, is to continue, such components will soon have to be single molecules with nanometer size. Such is the aim of *unimolecular electronics*.

The basic components will be molecular wires and molecular diodes.



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FCT

PTDC/FIS/72831/2006

Unimolecular Electronics — UNIME

The ongoing technological improvement in today's electronics/microelectronics (based on inorganic semiconductors and metals) has been mainly driven by an increase of integration density, which has been limited by the patterning tools - the so called top-down approach. Dimensions are approaching nanometer size, where quantum physics starts to play a key role, which may, in turn, lead to a different "electronics".

A different approach, trying to mimic processes in nature, relies on the assembly of individual molecules to play various electronics functions: the bottom-up approach. While nature has had millions of years to evolve, we are still in the infancy of the (uni)molecular electronics. While chemists design new molecules, playing with different chemical structures in an effort to tune the electronic properties of the molecules, we still miss the right tools to assemble and characterise the unimolecular electronic devices we may construct with such molecules. The aim of this project is to address this key issue, combining synthesis of molecules, their assembly in the appropriate substrates, building the right simple structures (wires, diodes), and characterise them in terms of current-voltage characteristics. While we are extending to the molecular level the properties we find in the macroscopic materials, it may well turn out that new electronic devices and logic will be at the core of a new electronics age.



Example of a threaded molecular wire (F. Cacialli et al, Nature Materials, 1, (2002) 160)





The aim of the project is to combine the synthesis of new molecules, their assembly to form wires and diodes, and, finally, to measure their current-voltage characteristics.

In a first approach we are addressing self-assembled molecular monolayers (SAMs). The final goal is the assessment of the electronic properties of individual molecules.

Molecular wires:

The molecules under preparation are conjugated oligomers (able to transport charge) with functionalisation at both terminals which will allow their perpendicular alignement on specific conducting substrates (such as gold and doped Si). In order to avoid lateral interactions between the molecules deposited as monolayers on a given substrate, they will be threaded with insulating molecular sheets.

To measure their conductance, a conducting probe-atomic force microscope (CP-AFM) and a scanning tunneling microscope (STM) are in use. AFM further allows us to determine the monolayers topography, providing information about their structure and order.

Additional tools, which may be used to measure the conductance, will be the mercury drop and broken junctions.

Molecular diodes:

The molecules for this type of devices combine electron accepting groups with electron donating groups, separated by "non conducting" bridges, thereby creating an asymmetry in terms of current flow. Their assembly on conducting substrates requires the molecules terminal groups to have different chemical functionalities to favour the formation of oriented monolayers, leading to cooperative phenomena.

We are first addressing monolayers but the final aim will be the characterisation of single molecules.

The characterisation tools will be the same as those used in the characterisation of the molecular wires.

Further information at http://www.lx.it.pt/~alcacer/TM_Group/

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