Molecular electronics - a future for electronic devices ?

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Abstract

Molecular electronics is a recent field of physics at the interface of atomic, molecular, and solid-state physics with the purpose of studying electric conduction of molecules. We give a few examples of this type of scientific research.

One of the most important goals in the engineering of electronic devices is the miniaturization. The present technologies of microstructuring semiconductor material, especially silicon, are expected to reach their limits in the next decade. The smallest transistors are of about 100 nanometers wide, and tens of millions of them may be integrated on a single chip. Below this size the controlled doping becomes more and more difficult. The next important step in the miniaturization might be done by reducing the electronic devices to the scale of molecules. This new field of physics is called molecular electronics.

The chemical bonding of atoms in molecules is long studied and it is one of the most important subject of quantum mechanics. In the context of molecular electronics the basic question is to what extent the chemical bonds can be used by electrons to travel through a molecule composed of several atoms, and to carry electric charge. The answer begins with the structure of the atomic orbitals. According to the quantum mechanics the motion of an electron inside an atom is described by a wave function, which can be imagined as a sort of cloud (called atomic orbital) surrounding the nucleus [1]. Atomic orbitals can have a spherical shape (s orbitals), or can be like two spheres aligned in a space direction x, y, or z (p orbitals, or p_x, p_y, p_z), as shown in Fig. 1, or even more complicated. The energies of the electrons have discrete values, and usually the more pieces an orbital has, the higher the energy.

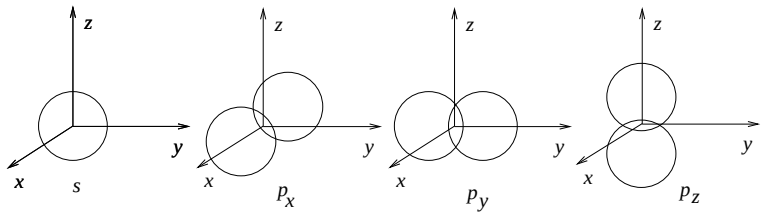

Figure 1: Atomic orbitals of s and p type. The origin of the axes is in the center of the atom.

When two atoms come close together, the electrons with the highest energies may extend their orbits to the other atom, yielding molecular orbitals, which make the chemical bonds. The molecular orbitals may have various shapes, depending on the form of the original atomic orbitals. Two examples are shown in Fig. 2, where O_1 and O_2 are the centers of the two atoms. The atomic orbitals of the type s or those of type p oriented along the direction O_1O_2 combine into molecular orbitals called σ, distributed in between and outside the atoms. The atomic orbitals of type p oriented perpendicular to the direction O_1O_2 generate π orbitals, which are elongated and distributed lateral from the atomic centers [1]. The molecular orbitals shown in Fig. 2 are called bonding orbitals. But both σ and π orbitals may be also broken it the middle, in which case they are called antibonding orbitals, and are denoted by σ^* and π^*. Typically the antibonding states have higher energies than the bonding states.

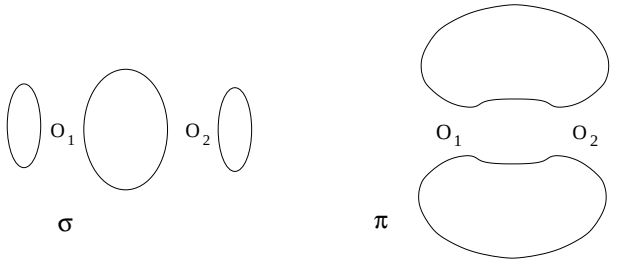

Figure 2: σ, π molecular orbitals. O_1 and O_2 are the centers of two atoms.

As recent experiments and calculations show, the π orbitals are the most favorable for the charge transport through a molecule. One such experiment [2] used benzene molecules. A very thin gold wire was covered by a solution containing benzene, and then slowly stretched until it breaks into two tips with the benzene solution in between them. Then the solvent which hosted the benzene molecules was evaporated, and the tips where brought together down to a distance of about 8-9 Å. A voltage was then applied to the gold electrodes, and a conduction was established through a single ben-

zene molecule connecting the tips. The benzene molecules had sulfur atoms at the ends, which bound to the closest gold atoms of the tip electrodes, Fig 4.

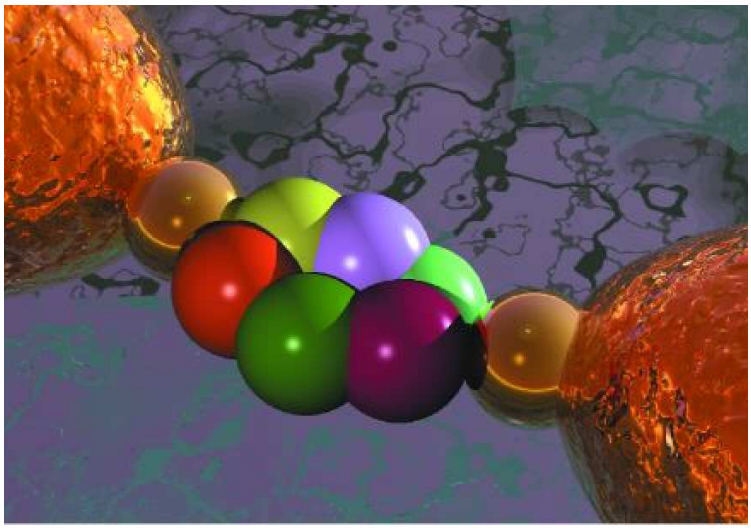

Figure 3: An artists view of a molecule between two gold electrodes. Picture borrowed from Ref. [3].

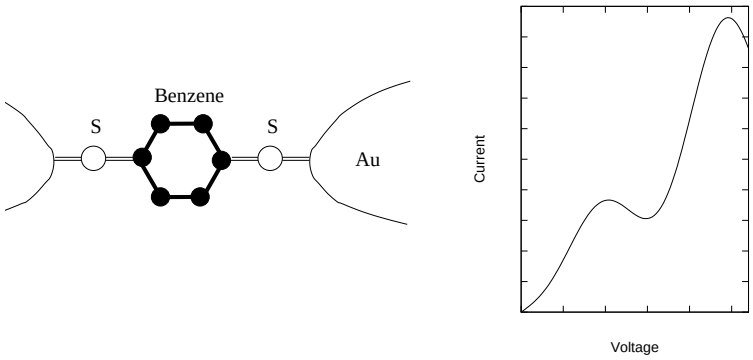

Figure 4: A two-terminal device made of the benzene molecule terminated with S atoms and Au electrodes, and the qualitative I-V characteristic.

The observed I-V characteristic has been explained by the calculations of Pantelides et coll. [3]. An electric charge can be transferred through the molecular orbitals only if their energy is aligned with the energy of the electrons in the gold electrodes. The calculations showed that by increasing the voltage across the Au electrodes, first the energy of the π^* orbitals of the benzene ring increases close to the energy of the electrons in the gold tips,

and they become available for the transfer of one electron between the electrodes, resulting in the first peak of a current. The second peak, at a higher voltage, is produced when the the energy of the π orbitals increases to the conduction energy. The calculations also showed that the magnitude of the current (in the experiment fractions of nA, for a voltage of a few V) changes if extra atoms are inserted between the sulphur atoms and the electrodes. In other words the atoms connecting the benzene molecule and the gold electrodes behave like electric impedances, depending on how their atomic orbitals couple with the electrons in benzene.

The conduction may also be strongly influenced by another molecule attached to the benzene ring, for example an NO_2 group replacing a hydrogen atom. In this case the I-V characteristic is sensitive to the orientation of the NO_2 group, in the same plane as the benzene ring, or perpendicular [3]. This situation opens questions on the behavior of the benzene molecule as a three-terminal device [3, 4], i. e. with an additional pair of electrodes acting like a capacitive gate, and giving an electrostatic field perpendicular to the direction of the gold electrodes of Fig. 4. The result is a molecular transistor, with an I-V characteristic with peaks that shift and change height with the gate voltage [4].

In another recent experiment Chen et al. [5] measured the electrical conduction in chains of three benzene molecules, and found a surprising I-V characteristic with a single and very pronounced peak, like a spike. The reason for it is the self-blocking of the conduction through the π orbitals at some large voltages, when the electrons are quickly absorbed in the contacts.

A very tempting idea is to consider biomolecules, i. e. molecules with a role in biologic phenomena, as candidates for future molecular devices. The reasons are their possibilities of self assembling and recognition. This means the electric contacts between molecules in a circuit could be by built by natural processes. Di Felice et al. [6] studied guanine molecules, and showed that conduction occurs when they stack in columns, again through the π orbitals, and have similar behavior as in a wide-gap semiconductor. This structure is similar to the structure of DNA. Due to its complexity DNA has many types of electric conduction, from semiconductor behavior [7], to superconductivity [8], depending on the composition, temperature, or surrounding solution. Amazing sturctures have already been achieved by self assembling of the building blocks of DNA. Their electrical properties are not well studied, but one idea is to use these structures to organize simpler molecules into nano-electrical-circuits.

The use of molecules for engineering ultrasmall electronic devices offers thus many possibilities. But the currents are weak, and very sensitive to many factors, which have to be very well controlled for robust applications. The future role of molecular electronics is only to be cleared by intensive experimental and theoretical research in physics and chemistry with an in-

terface to biology.

References

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