



Molecular Junctions: Introduction and Physical Foundations, Nanoelectrical Conductivity and Electronic Structure and Charge Transfer in Organic Molecular Junctions

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Abstract

There are fewer components in the nanoelectronics industry that do not use some kind of molecular junctions or interface. In general, many nanoelectronic devices have layered structures, and the behavior of the electron at the interface affects the electron properties of the final component, because the electron transfer mechanisms at the interface and multiple junctions are significantly different from the bulk material. Their junctions were studied. It was shown that to study the mechanisms of electron transfer and parameters affecting the conductivity of the junctions, various molecular junctions such as broken junctions can be used. It has been suggested that the solution temperature, shape, material, and spatial arrangement of the molecule used, the material, properties and surface nature of the metal electrodes, and the band structure of the junction's components can affect the conductivity of these systems. Attempts have been made to introduce the salient features of each of these junctions and to discuss examples of real Nano electronic components and molecular junctions used in them. We will see that the conventional mechanisms for electron transfer in these devices strongly depend on the electronic structure of the molecules used and generally include direct tunneling, fullerene tunneling. Molecularly deals with the effects of various factors on it. controlling the conductivity of a molecular bond by changing its physical, chemical and mechanical properties and optimizing the electrical properties of the final nanoelectronic component. Organic molecular junctions, as a special form of molecular junction, are used in many organic nanoelectronic devices. Therefore, it is very important to study the nature of the interface between these junctions and their electron transfer mechanisms. Conductivity of junctions is analyzed based on the band structure of their components. Therefore, in this paper, organic molecular compounds are introduced and their electronic structure is discussed. As you will see, certain phenomena also occur in these junctions, the most important of which are the formation of organic dipoles at the interface of the organic molecule/metal and the CNL parameter. Attempts have been made to put these phenomena into plain language without addressing mathematical models and the heavy concepts of quantum physics, and to discuss their effect on charge transfer and the electronic structure of organic junctions.

Keywords Molecular junctions · Physical foundations · Electrical conductivity · Nanoelectronic · Metal electrodes · Electronic mutation

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1 Introduction

Most nanoelectronic devices have layered structures in which two homogeneous or heterogeneous materials come into contact with each other. For example, we can refer to the structure of the layers of solar cells. The study of the electronic structure of bulk materials and their interface shows that the potential behavior of electrons as well as charge transfer mechanisms in the interface regions are completely different from the volume of matter [1–3]. Therefore, the study of the electronic structure of the interface used in the field of nanoelectronics is one of the important tools to understand the nature of electron transfer in these structures. In the present article, in order to facilitate the discussion and avoid readers' confusion, the interface is examined in two molecular and trans molecular scales (bulk) [4, 5]. Areas of an interface that consist of only two or more specific molecules are called molecular junctions, and a group of interface formed by the contact of bulk solids with each other is called an interface [6–8]. Although some of the charge transfer mechanisms in both types of junctions chains are relatively similar, the nature of these processes is completely different and, depending on the type of junction's interface and its strip structure, lead to unique electrical properties [1–3].

Molecular units used in the manufacture of molecular junction's can be selected from organic or inorganic materials, depending on the type of application and the nature of the charge transfer. Most of these junctions are made from organic or biological molecules [1, 8]. However, nanometer-sized materials such as DNA, carbon nanotubes, and graphene can also be used to make them. Electrical conductivity in molecular junction's is defined in a special way and its meaning is slightly different from the conventional definitions for bulk material. Numerous factors also affect the conductivity of these systems. Some of these factors are inherent and depend on the nature of the molecular units or electrodes used, and some are non-intrinsic factors and go back to the environment or temperature of the complex [4, 5].

Studies show that the nature of electron transfer in bonds based on organic molecules is slightly different from previous discussions. In these junctions, the contact of the molecular unit with the metal electrode causes the formation of electrical dipoles in the joint and facilitates the load transfer process [2, 3, 8]. In this type of junctions, approximations and parameters can also be used to simplify the study of load transfer. For example, an important CNL parameter is defined and the electrical conductivity of these junctions is evaluated based on this variable [6].

2 Molecular Junctions

By definition, a molecular junction is a set consisting of one or more organic or inorganic molecules, and these molecular units are stretched between two macroscopic electrodes. In molecular nanoelectronics, these junctions are very important [4]. For example, a molecule with three electron donors, an acceptor, and a bridge can move charge carriers through its electron levels. The most important factors that affect the voltage curve of molecular junctions can be the type of molecule used, the geometric shape and chemical composition of the electrodes, the set temperature, the bond of molecules with metal electrodes, the electric field applied to the system, and finally the environment in which the junctions are made [5]. For example, the molecule-electrode junctions interface in molecular junctions can, under certain conditions, limit the electric current or completely improve the electrical response of the junction [6, 7]. Figure 1 shows a diagram of organic molecular junctions made by placing one or more arrays of organic molecules between two metal electrodes.

In practice, there is no definitive method for determining whether only a single molecule is placed between two electrodes or that the desired junctions consist of several molecules with a specific spatial arrangement [8]. Also, the contact surface of the electrode with the molecules at the atomic scale is not smooth and uniform, so if the electrode is made of soft and flexible metals such as gold, the measurement of changes in electrical current with voltage may cause severe physical distortions on the electrode surfaces [8, 9]. Therefore, the lack of full understanding of the nature of the electrode/molecule contact surface and the arrangement of molecules in the junctions are among the most important sources of uncertainty in research in this field [1]. Studies have shown that the attachment of organic molecules to the surface of a metal electrode causes the formation of electrical dipoles in the regions of the interface, and the electronic structure and, consequently, the electrical behavior of the system are completely affected, because the chemical nature of the molecule/electrode junctions can change the energy of the molecular levels and the electron density of the molecular orbitals, thereby significantly altering the conductivity of the molecular units [1, 3].

Depending on the type of molecular bond and the structure of the organic molecule used, electron transfer in molecular units is done by different mechanisms [2]. The most common load transfer mechanisms in molecular junctions are direct tunneling, Fowler-Nordheim tunneling, thermionic emission, and hopping conduction [4].

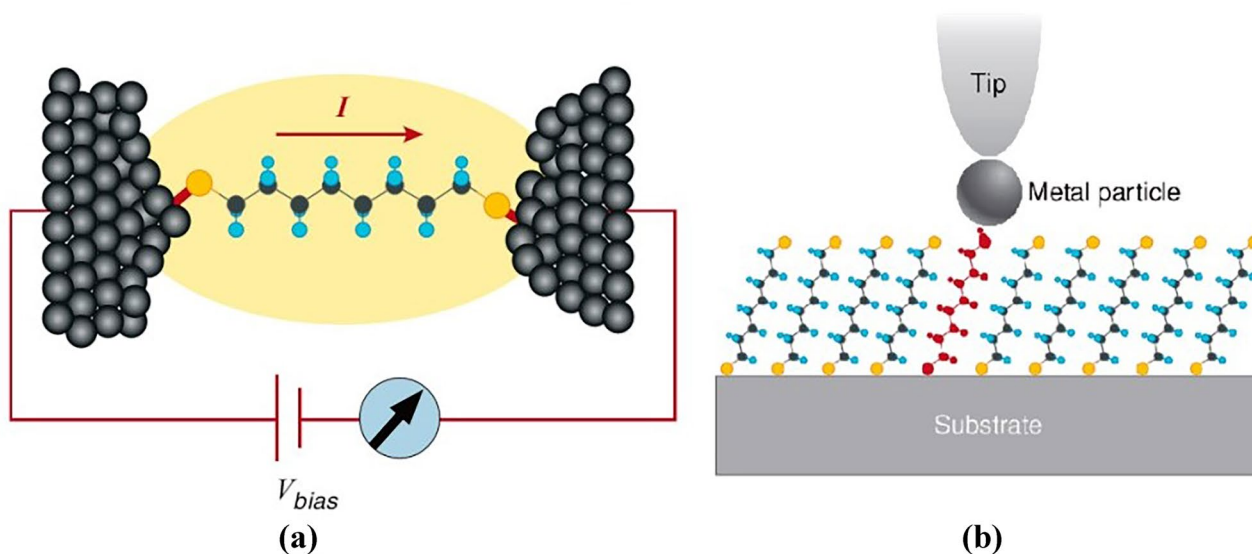


Fig. 1 Scheme of molecular junctions including **a** single organic molecule and **b** regular arrangements of organic molecular units [1]

In general, many geometric parameters of organic molecular bonds are unclear due to the very small size and random arrangement of molecular units, and there is a great deal of uncertainty in determining the number of organic molecules used and how they are arranged [6]. Therefore, it seems that the use of quantum chemistry calculations and macroscopic measurements of electrical conductivity of junctions can be very helpful in determining the conductivity of molecular junctions [10–13]. However, molecular junctions can be used based on the type of structure of the molecular unit and the order of placement

of organic molecules and electrodes can be divided into several general categories [8]. An overview of the types of these molecular junctions, the energy diagram of the electron balances, and an example of the type of molecule used in each junction are given in Fig. 2.

- Molecular junctions consisting of two metal electrodes in which one of the electrodes acts as an electron donor and the other acts as an electron acceptor (Fig. 2a). The organic molecules used in these junctions are often linear chain alkane molecules. Based on theoretical electron

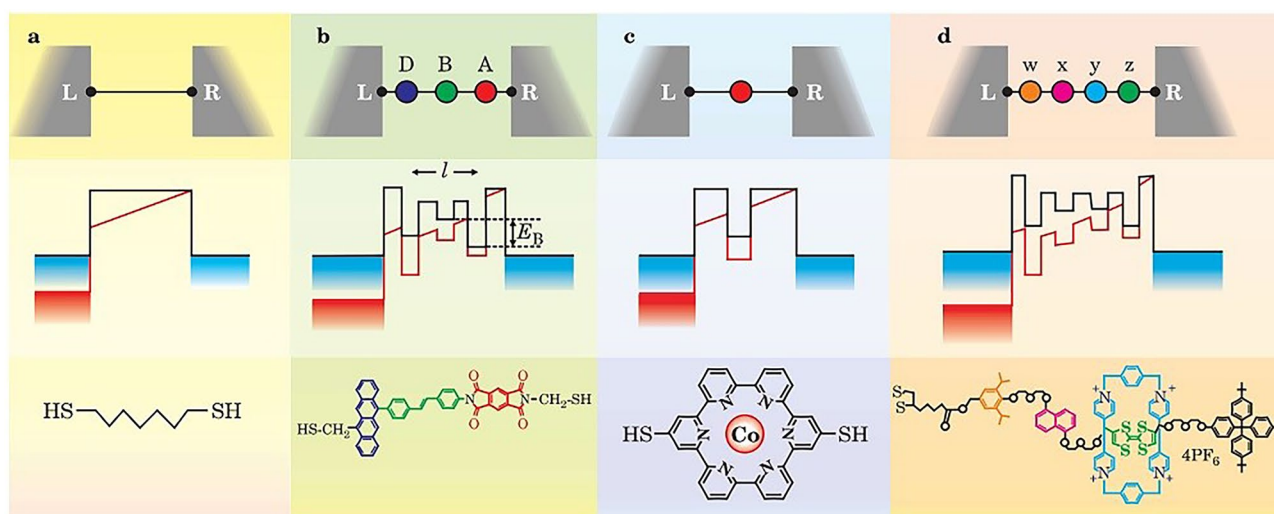


Fig. 2 Examples of molecular junctions to establish electrical charge transfer, including electron jump paths and steps (top row), how the molecular alignments and electrodes (middle row) are positioned, and the molecule used in the molecular junction (bottom row). The dashed lines indicate the energy levels of the various parts of the molecular unit by which the electrons can move along the bond, thus defining the path of charge carriers. The red lines also show the same

energy levels for a state where an external electric field is applied to the junction: **a** a molecular junction consisting of an organic molecule and two electrodes; **b** molecular junction donor-communication bridge (DBA); **c** molecular junction with the base of quantum dots or single molecules; **d** Molecular binding including large molecules such as proteins, oligomers and DNA [2]

transfer relationships such as the Harden McConnell relationship at very small applied voltages and for a given chain length of alkane molecule, the current passing through the bond decreases exponentially with increasing chain length and the alkane molecule effectively acts as a barrier, it acts energetically [11].

- Organic molecular junctions that include the electron donor functional group-communication bridge-electron acceptor functional group (DBA) (Fig. 2b). In this type of molecular junctions, it is possible to observe different mechanisms of charge transfer and the variety of conduction mechanisms, the ability to change the electrical properties of molecular junctions by adjusting these properties during synthesis processes [12]. For example, by changing the synthesis conditions and design of molecular junctions, the level of energy levels of molecular units and the current of electric charge shifting between the receiving and receiving electron sites can be controlled [13]. The structure of DBA can be used as a suitable model to study such things as the operation of electron transfer mechanisms in solution systems and the study of the electrical conductivity of semiconductor molecular junctions [14].
- Molecular junctions with a base of molecular quantum dots (Fig. 2c). This type of junctions is one of the simplest molecular junctions because its molecular levels have a lower energy distribution than other types of junctions (including DBA junctions) and are therefore very suitable for modeling molecular junctions [15]. For example, quantum dot-based junctions can be used to study electrode-molecule interactions and to study quantum effects on the transfer of electrical charge through molecular junctions [16]. The molecules used to make these types of junctions have specific functional groups [2]. These functional groups facilitate the attachment of the molecule to the electrode and enable communication between the two electrodes. It should be noted that in organic chemistry, functional groups are specific groups of atoms or bonds that, in a molecular unit, are responsible for performing specific chemical reactions with other molecules [3].
- Molecular junctions in which the bridge between two electrodes consists of a large molecule composed of several different functional groups (Fig. 2d). Today, these molecular junctions, like DBA molecular junctions, have received as much attention. The most important molecules used in the junctions of this group of junctions are protein molecules, oligomers, rotaxane molecules and DNA [12].

Molecular junctions can also be categorized based on the number of molecules used in their structure. Based on this, molecular junctions are divided into the following two general categories [2–4]:

- Ensemble junctions
In this type of junctions, molecular units with a specific spatial arrangement are used. The most obvious example of these junctions is when the tip of an atomic force microscope (AFM) probe is formed on a layer of self-assembled monolayers (SAMs). Another way to make multi molecular junctions is to use melt droplets as electrodes [14–16].
- Single-molecule junctions
The structure of this type of junctions consists of a single molecule placed between two metal electrodes. The most common method of making complementary junctions is to use the break junction method. The most common single-molecular junctions are mechanical broken junctions and electrochemical break junctions [2, 3].

3 Types of Molecular Junctions

Molecular junctions are often divided according to the number of molecules used and their spatial arrangement. According to this classification, molecular junctions can belong to only one of the following main groups [11, 12].

3.1 Multimolecular Junctions Based on Melt Droplets as Electrodes

These junctions are made using molten droplets, often to investigate the self-assembly properties of molecules or to measure the electrical conductivity of molecular junctions [13, 17, 18]. Figure 3 shows how to form a multi molecular bond. As can be seen, the droplet of melt allows it to advance to the threshold of separation from the main column of the melt. In this case, the diameter of the junctions of the drop to the molten column will be so small that only a few molten molecules will be able to be in this area independently [6, 10, 11].

3.2 Mechanical Break Junctions

The method of making a controlled junction with mechanical load is to place a thin grooved film of gold metal on a flexible and soft polymer substrate. The groove on the gold film becomes a very small gap (within a few angstroms) due to the piezoelectric charge [13, 18, 19]. This is shown in Fig. 4. When the system is placed in a solution containing thiol groups, several molecules can pass through the gap at the same time [12, 13]. Therefore, by controlling the piezoelectric load, the dimensions of the gap can be adjusted so that only a single molecule can be placed in the space between the gaps [20–22]. This creates an MCBJ junctions. The most important advantage of this method is the possibility of studying the electromechanical properties of molecular junctions

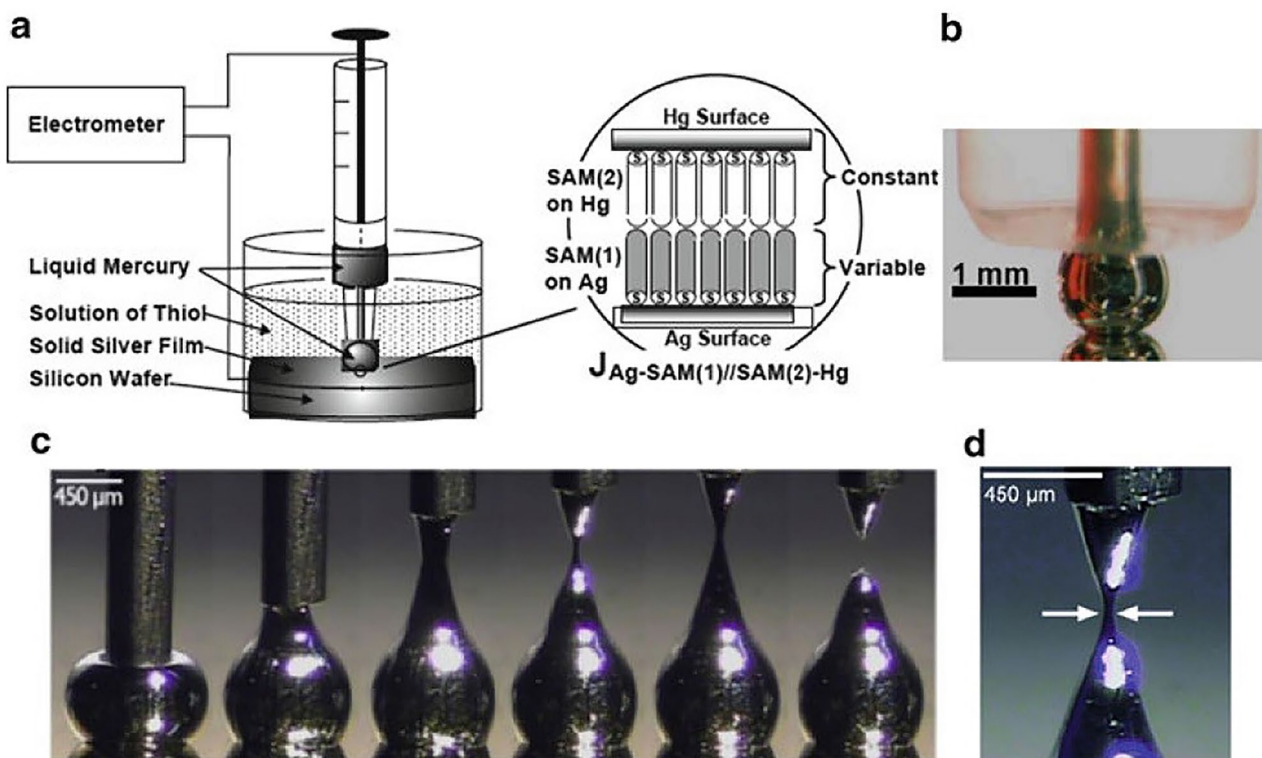


Fig. 3 The process of forming multi-molecular bonds using the melt droplet technique: **a** the controlled droplet generation system, **b** a schematic of molecules arranged in the neck of the molten droplet, **c**

the practical process of forming and controlling the dimensions of the molecular bond region, and **d** SEM image of the molecular junction region with a fraction of a micrometer in diameter [3]

and investigating the effect of junctions dimensions on the electrical conductivity properties. In other words, by changing the intensity of the piezoelectric force, the dimensions of the junctions can be changed and the desired properties can be attributed to the geometric dimensions of the junctions [23–26]. Another advantage of mechanically broken joints is the possibility of using different solution and gas environments to place molecular units in the gap. For example, a drop of the desired solution can be dropped on the

junction slit and, by drying, the desired molecular unit can be placed in the junction core. The gas absorption process by metal electrodes can also be used for this purpose [14, 15].

3.3 Electrochemical Break Junctions

Broken electrochemical bonding is similar to controlled mechanical bonding, except that mechanical bonding, unlike mechanical bonding, which is often used in a vacuum

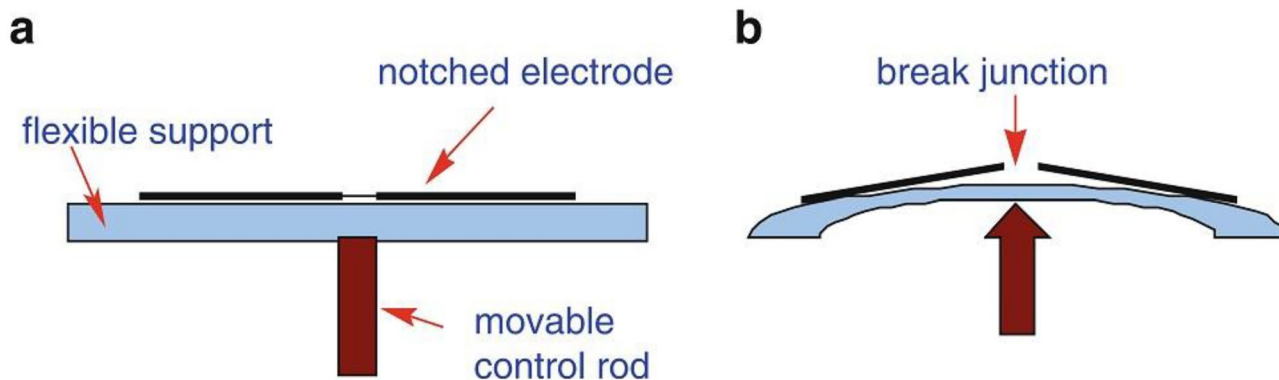


Fig. 4 (a) and (b) the method of creating a controlled junction with a mechanical load [5, 6]

environment, is used inside chemical solutions, and it is the soluble molecules that have a chance of being in the gap [15, 27–29].

3.4 Molecular Sampling Based on STM

This type of junctions is called in situ junctions or scanning tunneling microscope (STM). This type of junctions is made by placing the tip of a scanning tunneling microscope probe in the vicinity of a single set of self-assembling molecules (Fig. 5). According to Fig. 5, by examining the changes in current intensity passing through the junctions with the distance of the probe tip from the self-assembly, the correct formation of this junctions can be detected. The method is that the electrical conductivity for a situation where only one molecule is trapped between the top of the probe and the substrate is $G_0 = 2e^2/h$. Now, if it is possible to plot the changes in the distance of the probe tip from the substrate according to the intensity of the current created, many steps and sudden jumps will be observed in it. If the tip of the probe is too far from the substrate, the intensity of the current will decrease and the conductivity will not be significant if several molecules are at this distance. Also, as the tip gets too close to the substrate and all molecular units are removed, a short circuit will occur in the circuit and a very large current will be recorded [2, 16].

The most important advantage of this method in making molecular junctions is the ability to create thousands of molecular junctions repeatedly in a short period of time, in which molecular units are junctions to two metal electrodes and the conditions for studying the conductivity properties of molecular junctions with a very high statistical population are provided [30–32].

It should be noted that molecular junctions are used in various electronic fields as components of circuits and molecular devices. Molecular junction has unique geometric and electrostatic properties that are specific to nanometer-sized materials, and these properties distinguish them from conventional electrical junctions [33–36]. In molecular joints, the control of the movement of charge carriers is a very important issue and extensive research has been done in this field. By engineering electrical junctions, it is possible to have precise control over the movement of load carriers and make unique changes in the electrical, optical, thermal, and mechanical properties of conventional materials [37–40]. Figure 6 shows some of the most important molecular devices made using molecular junctions. These devices are designed based on the movement of electrical charges in molecular junctions [3, 12]. Figure 6a shows photovoltaic devices comprising molecular junctions consisting of an array of semiconductor (red) nanowires in contact with a transparent and conductive electrode. Figure 6b also shows a type of field effect transistor in which molecular junctions including carbon nanotubes are used. In field effect transistors, the electric current generated between the source electrode (high electrode) and the discharge (low electrode) is controlled by the gate electrode. Figure 6c shows a type of biochemical sensor that has molecular junctions consisting of antibody-activated nanowires. Antibodies can bind to specific protein molecules and thus affect the conductivity between two metal electrodes. Figure 6d shows a type of Li-ion battery, which is made of molecular junctions, including arrays of anode (brown) nanowires coated with solid gold electrolyte. These nanowire arrays are surrounded by a cathode background (pink). Figure 6 shows a diagram of molecular electronic devices designed based on the thermoelectric phenomenon. In this

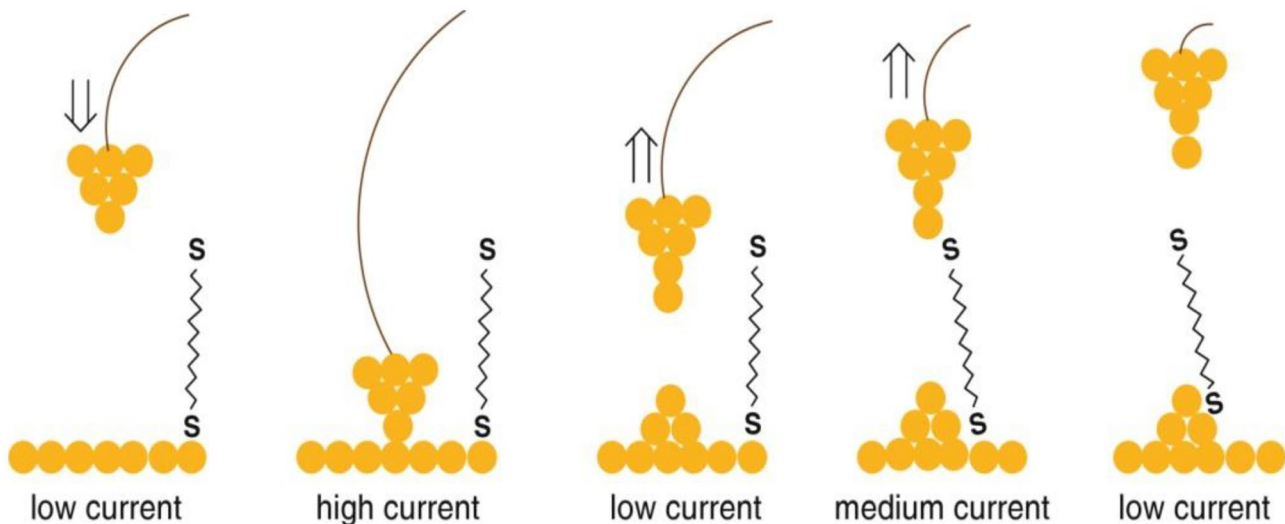


Fig. 5 Different stages of forming an in situ junctions using the tip of a STM microscope probe [5]

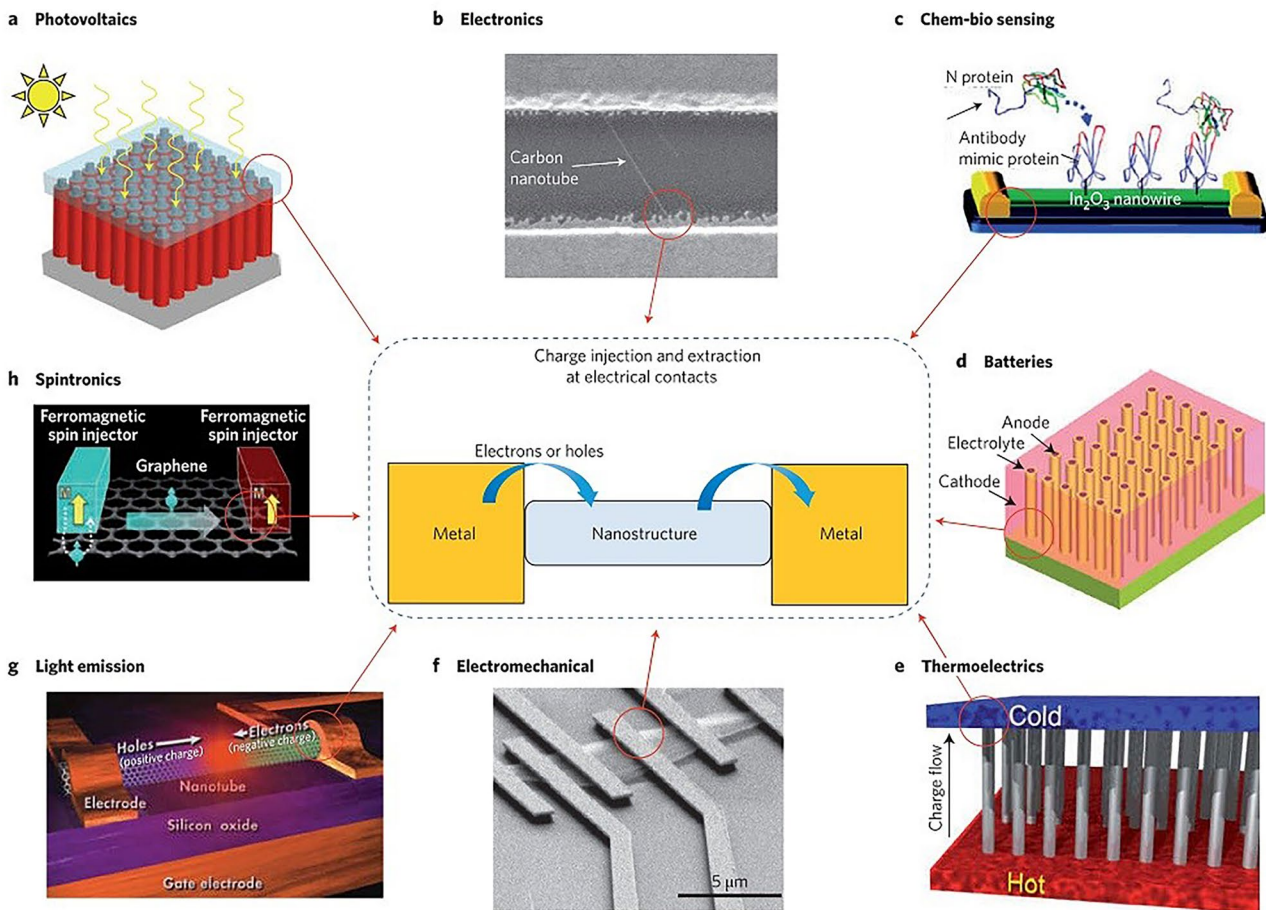


Fig. 6 **a** Photovoltaic devices such as solar cells. **b** Field-effect transistors with carbon nanotube bases. **c** Biochemical sensors. **d** Ion-lithium batteries. **e** Thermoelectric devices. **f** Electromechanical sys-

tems with graphene base. **g** Electron-emitting optical devices with carbon nanotube base. **h** Graphene-based spintronic devices [6]

type of device, by creating thermal gradients along an array of nanowires, a considerable electrical driving force can be created in the nanowires to allow the flow of electric charge carriers along the nanowires, and thus, the electrical current in the system. In contrast, a temperature gradient can be created by inducing an electric charge in a molecular bond [11, 17]. Figure 6 shows a schematic of a graphene-based electromechanical system. In this system, the graphene layer begins to vibrate when an oscillating voltage is applied by the gate electrode. The degree of vibration and displacement of the graphene membrane can be determined by measuring the current generated in it. Figure 6 shows the electron emitting devices with a carbon nanotube base. In this connection, the two electrodes are separated by carbon nanotubes. The phenomenon of light scattering occurs due to the collision and recombination of electrons and the output cavities of two different electrodes. A gate electrode can also be used to adjust the intensity of the emitted light. Figure 6 shows the graphene-based spintronic devices [13, 41–43]. This junction consists of two ferromagnetic electrodes

connected by a graphene layer. In this junctions, the ferromagnetic metal electrode injects charges with polarized spin into the graphene lattice, and then, by moving electrical charges toward the second ferromagnetic electrode, the electrons are removed from the junctions by random spin.

3.5 Factors Affecting the Electrical Conductivity of Molecular Junctions

In the mechanical methods developed for making molecular junctions, there are many parameters that can be controlled to achieve completely different conductivity properties in molecular junctions [60–62]. The most important of these parameters are the environment around the junctions, local heat due to the passage of electric current in the junctions, the geometric shape of the electrode-molecule junctions, the matching of energy levels in the electrodes and molecular units, and external forces applied to the junctions. In this section, the effect of each of these factors on the conductivity properties of molecular junctions is investigated [23, 24].

3.6 Geometric Shape of Metal/Molecule Junctions

In the proposed mechanical methods for making molecular junctions, the number of atoms or molecules that are placed in the common phase of the two electrodes depends on the distance of the metal electrodes from each other and the piezoelectric force applied to the junctions. This factor makes the geometric shape of broken mechanical junctions completely different from each other [63–66]. Studies show that the electrical conductivity of junctions depends significantly on the number of atoms or molecules that make them up, their geometric shape, and their spatial arrangement. Assuming that the atomic weight of the junctions is constant, Guo et al. have studied the electrical conductivity of a large number of quantum dot joints with different geometric shapes [25–27]. Figure 7 shows a diagram of the studied junctions and a diagram of their conduction changes with the geometric arrangement of metal atoms. The results indicate that the number of atoms that make up the junctions and their spatial arrangement can affect the electrical conductivity of the junctions.

In another study, Salmon et al. were able to obtain the energy levels of electrons located at the HOMO level of C5S2H2 molecules with completely different spatial structures. The results are summarized in Fig. 8. In this figure, the Fermi energy level of the metal electrodes is assumed to be zero and the HOMO level energy in the C5S2H2 molecules relative to the zero point is determined. As can be seen, changes in the spatial structure of molecules can greatly affect the level of energy levels and the band structure of molecular bonds.

3.7 Electrode/Molecule Junctions Strip Structure

Conductivity of molecular junctions depends on the degree of alignment of the energy levels of the HOMO and LUMO molecular orbitals with the Fermi energy of the metal electrodes. As a general rule, to establish an electric current in molecular junctions, the surface of the metal electrode Fermi levels must be within the energy gap width of the molecular unit strip structure, because if the HOMO or LUMO levels of the molecular unit are close to the formal electrode formaldehyde, electron transfer is possible. It is provided between them and the molecule is momentarily oxidized or reduced. In practice, the energy level of the HOMO and LUMO levels of molecular units can be changed by applying a gate voltage to the junctions [28, 29, 67–69]. Figure 9a and b show a diagram of a single-molecular junctions and its associated band structure. As can be seen, the application of gate voltage (V_g) causes the band structures of molecular units to shift. Figure 9c also shows the changes in current intensity across the junctions in terms of gate voltage. According to this diagram, increasing the gate voltage limits the electron transfer between the electrode-molecule. The main reason for this is that the closer the HOMO and LUMO levels are to the Fermi level of the electrodes, the greater the likelihood of oxidation and electrochemical reduction of the molecules. In those molecules that are reversibly oxidized and reduced, the application of gate voltage can significantly affect their electrical conductivity. These effects are studied using the band structure of molecular junctions. It should be noted that the alignment of energy levels is determined by controlling the intrinsic properties of molecules and electrodes as well as the interactions between them [70–73].

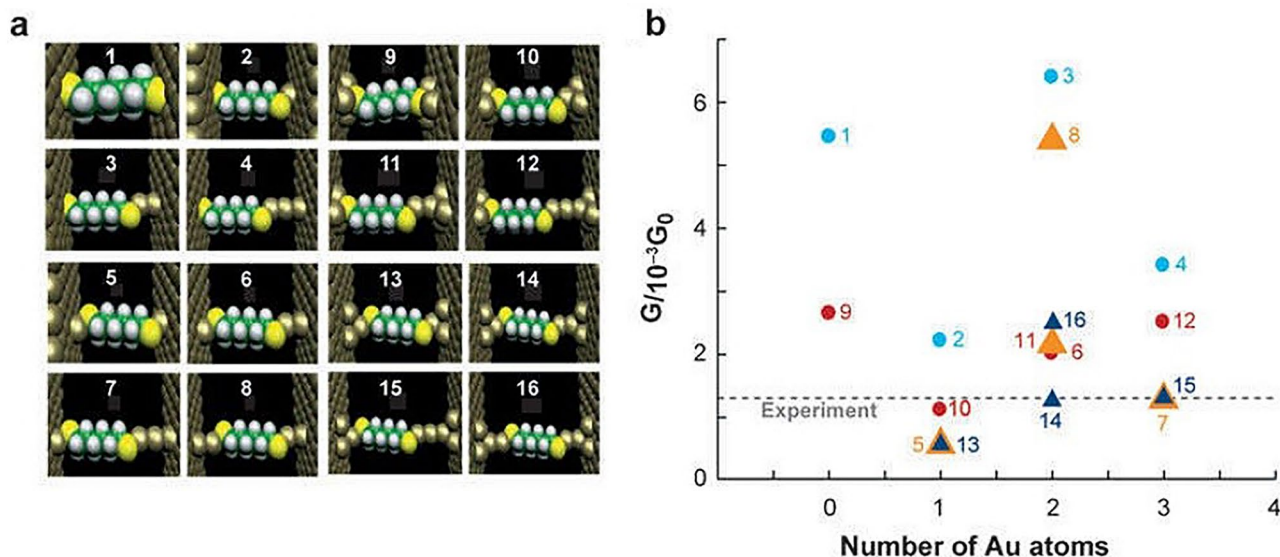


Fig. 7 **a** Completely different geometric shapes of 6,1-hexanedithiol quantum dot junctions with gold electrodes. **b** The process of changing the conductivity properties of the junctions according to the number of metal atoms in the junctions and their different geometric shapes [1]

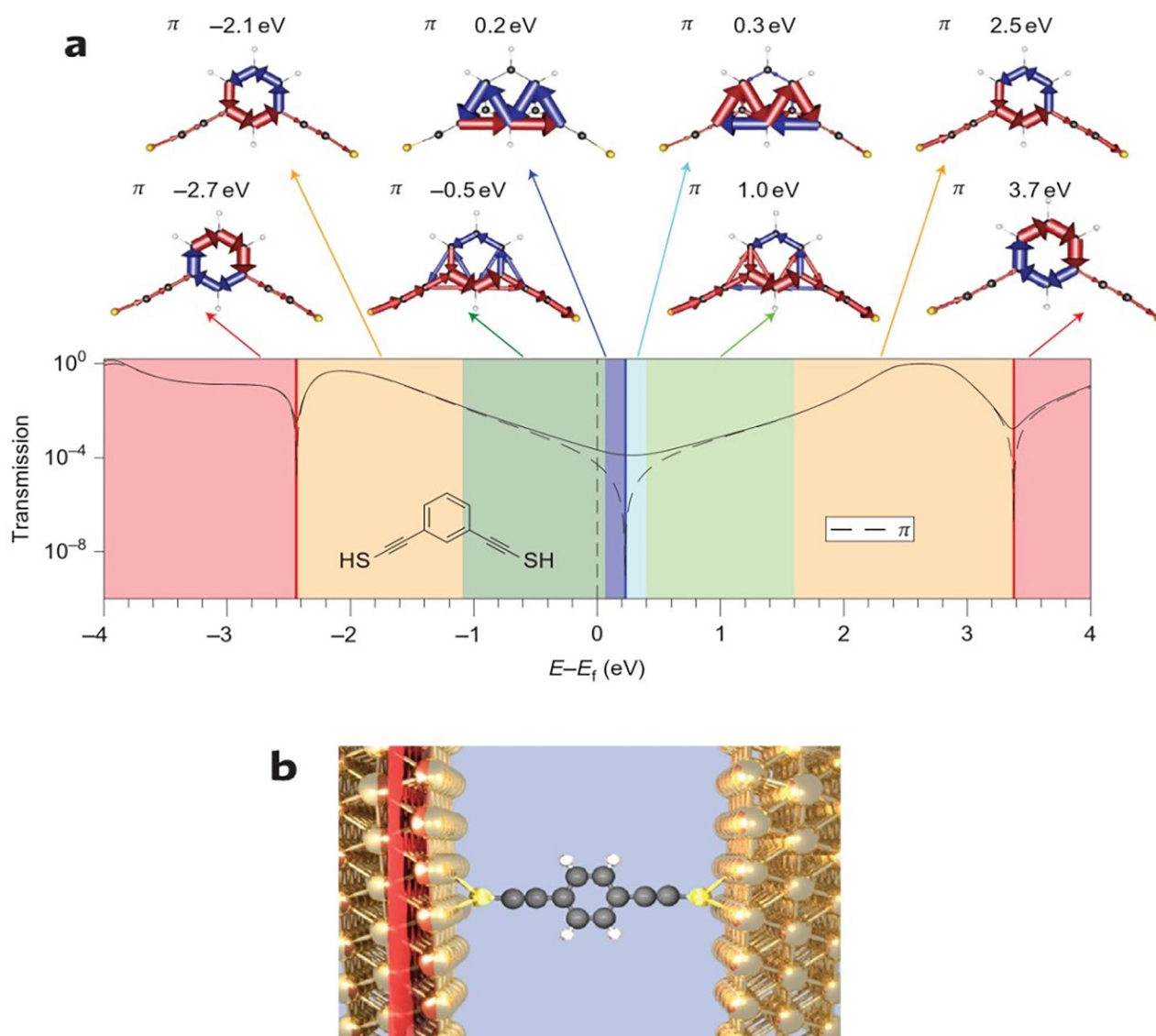


Fig. 8 **a** The different spatial structures of the HS-C₆-SH molecule and the energy of its HOMO levels. **b** The bond used to measure the electron properties of the molecule in question [3]

3.8 Foreign Forces

In STM and AFM-based molecular junctions, the two metal electrodes are fully movable and their separation distance can be changed. Now, if, according to Fig. 10a, there is a molecule between the substrate and the AFM microscope probe, the force required for separation and the electrical conductivity of the resulting molecular bond can be measured as the probe separation distance increases [74–76]. The diagram of the force changes required to increase the junction's length and its electrical conductivity as a function of the separation distance is shown in Fig. 10b. As can be seen, increasing the separation distance causes a simultaneous decrease in the required tensile force and electrical

conductivity of the molecular bond. The reason for the continuous decrease in force is due to the fact that in the early stages of tension, the molecular bond tries to separate from the region of the common molecule–metal season instead of breaking from the molecular branch. Each of the steps in the force-tensile diagram corresponds to the flow of metal atoms in the common molecular bonding phase. Finally, the tension continues until the metal electrode atoms are unable to maintain bond with the molecular unit and bond failure will be the predominant phenomenon. It is obvious that increasing the separation distance increases the electron transfer path during molecular bonding and the electrical conductivity will decrease in proportion to the gradual decrease in force [30, 31, 77, 78].

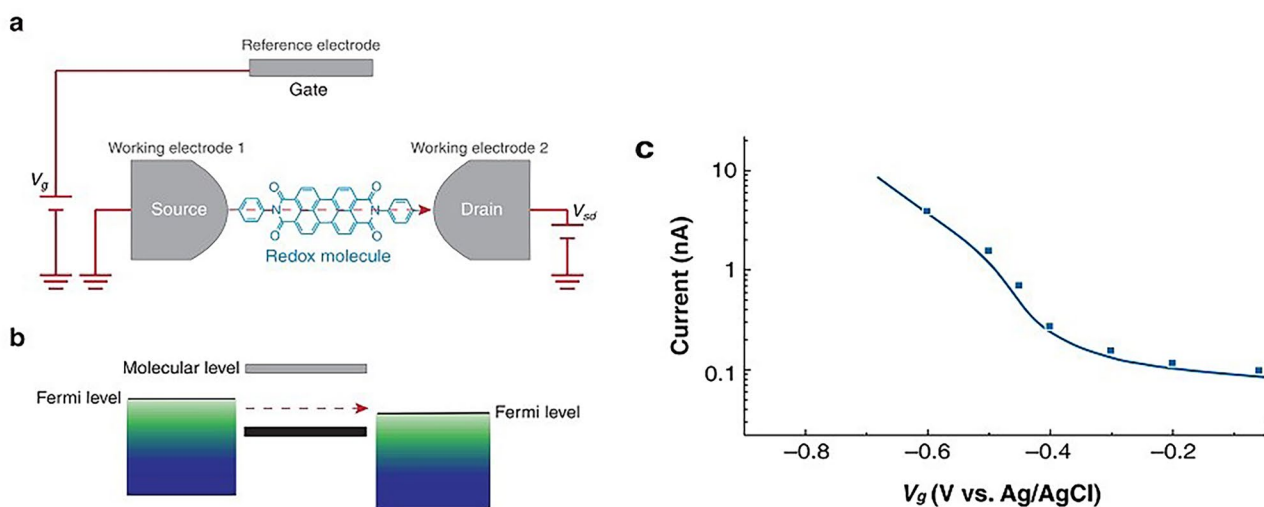


Fig. 9 **a** Schematic of single-molecular junctions within an electrochemical cell. **b** Molecular junction strip structure. **c** The current passing through molecular junction A as a function of the gate electrochemical voltage [1]

4 Electrical Conductivity of Molecular Junctions

The most important quantity that describes the electrical properties of bulk materials is electrical conductivity. Electrical conductivity in bulk materials (σ) is defined as follows [17]:

$$\sigma = (I/V) \times L/A \quad (1)$$

In this regard, I is the intensity of the transmitted electric current, V is the applied bias voltage, L is the length,

and A is the cross-sectional area of the material. In principle, accurate determination of parameters A and L is not possible for small molecules, and Eq. 1 must be redefined to study the conductivity of molecular bonds [17]. For this purpose, a parameter called conductance (G) is defined for molecular units such that

$$G = I/V \quad (2)$$

One of the challenges in this field is to determine the electrical conductivity of junctions in which the molecular units used are made of metal electrodes themselves. The

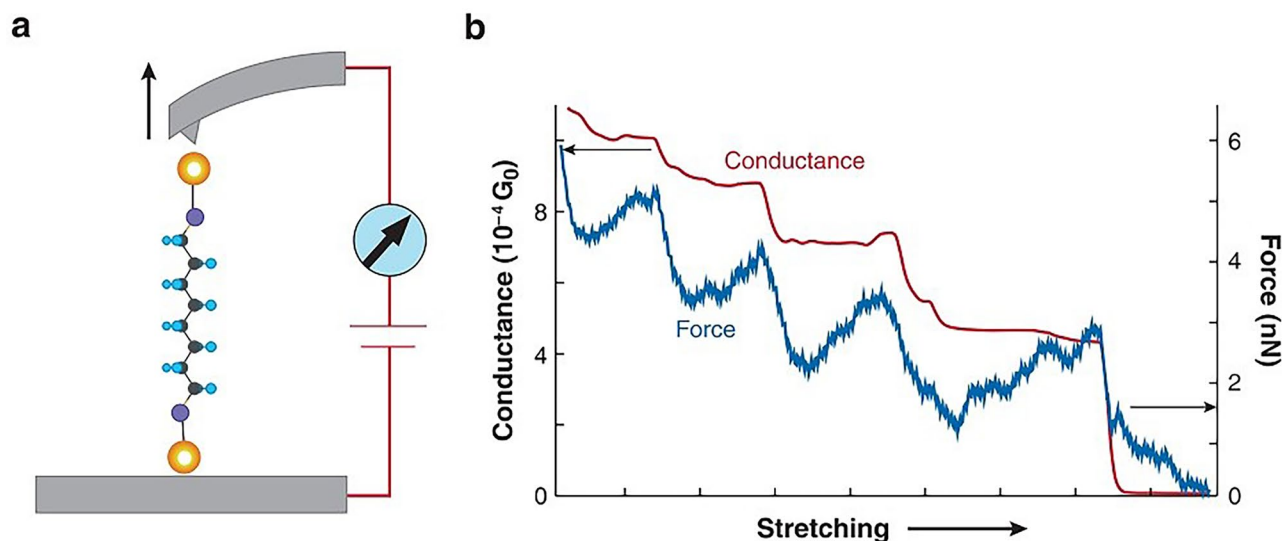


Fig. 10 **a** Schematic of AFM microscope-based molecular junctions. **b** A graph of the force changes required to stretch the molecular bond and its electrical conductivity in terms of separation distance [1]

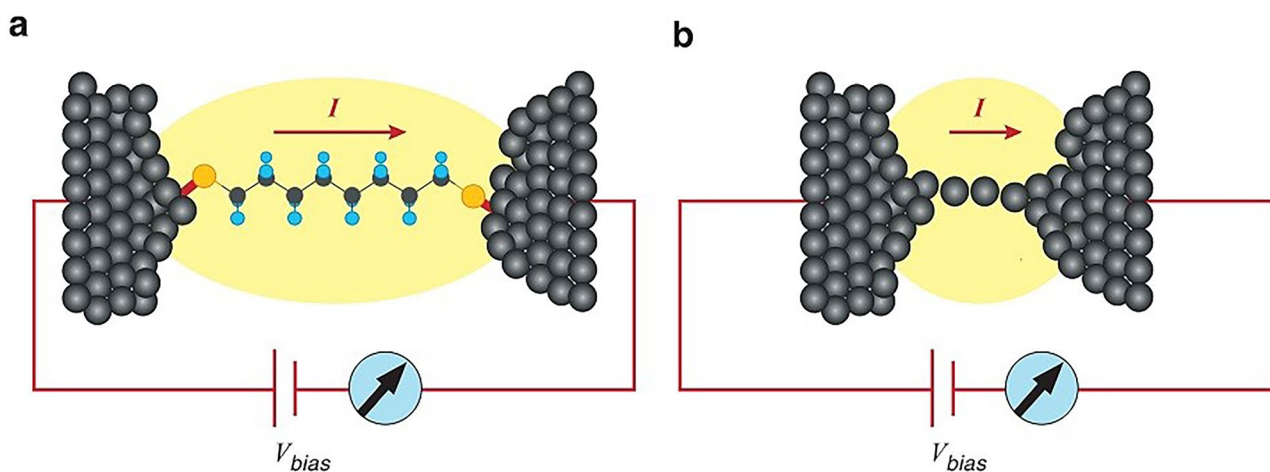


Fig. 11 Schematic of quantum dot junctions. Molecular units include clusters of metal electrodes [1]

most important of these junctions are gold nanoparticle-based junctions with gold metal electrodes. By definition, junctions that consist of a single atom or atomic clusters of metal electrodes are called quantum point junctions [13, 44–48]. Examples of these junctions are shown in Fig. 11.

It is proved that for metals, the electrical conductivity of quantum dot joints will be $G_0 = 2e^2/h$ [13, 17]. In this relation, e is the charge of the electron, h is the Planck constant, and S is the unit of electrical conductivity.

According to quantum physics, G_0 means the 100% transfer of electrons from one electrode to another using a quantum dot. Therefore, it is possible to express the electrical conductivity of a molecular unit or molecular junctions in unit G_0 , and thus, the electrical behavior of the desired junctions will be comparable to the conductivity of metal base junctions. The electrical conductivity of molecular junctions is often measured using an I - V or J - V diagram (J current flow) [49–52]. It is also possible to evaluate the reversibility or non-reversibility of electrical charge transfer reactions in the junctions by measuring the intensity of the electric current for the negative and positive values of the applied voltage. Obviously, the symmetry of the I - V diagram with respect to the $V=0$ axis means that the process of transferring electrical charge in molecular junctions is reversible (Fig. 12) [11].

The most important challenge for research in this field is to choose the type of complementary junctions, because the geometric shape of the junctions has a significant effect on its electrical conductivity [53–56]. In general, most studies on the experimental measurement of electrical conductivity of molecular junctions have been performed using one of the two methods, “mechanically controlled break” and STM. But what these two methods have in common is that in both cases, the final junctions structure will consist of a metal array/molecular unit/metal. In this case, the conductivity behavior of the single molecule can be evaluated by applying the potential difference between the two metal electrodes [12, 13, 21]. It is preferable to use a single molecule and otherwise a molecular self-assembly to measure practical conductivity. For example, to make such a junction, a thin wire of gold metal must be broken within a few angstroms by means of a controlled load with mechanical load, broken, and the dimensions of the fracture zone using piezoelectric force [57–59]. To create a self-adhesive monolayer on a metal wire, the surface of the gold metal must be exposed to a chemical solution of tetrahydrofuran (THF). Under such conditions, a regular array of benzene-4,1-dithiol molecules are formed perpendicular to the surface of the gold metal. Now it is possible to change the intensity of the piezoelectric force to provide a condition in which only one specific

Fig. 12 Current–voltage characteristic of four devices [11]



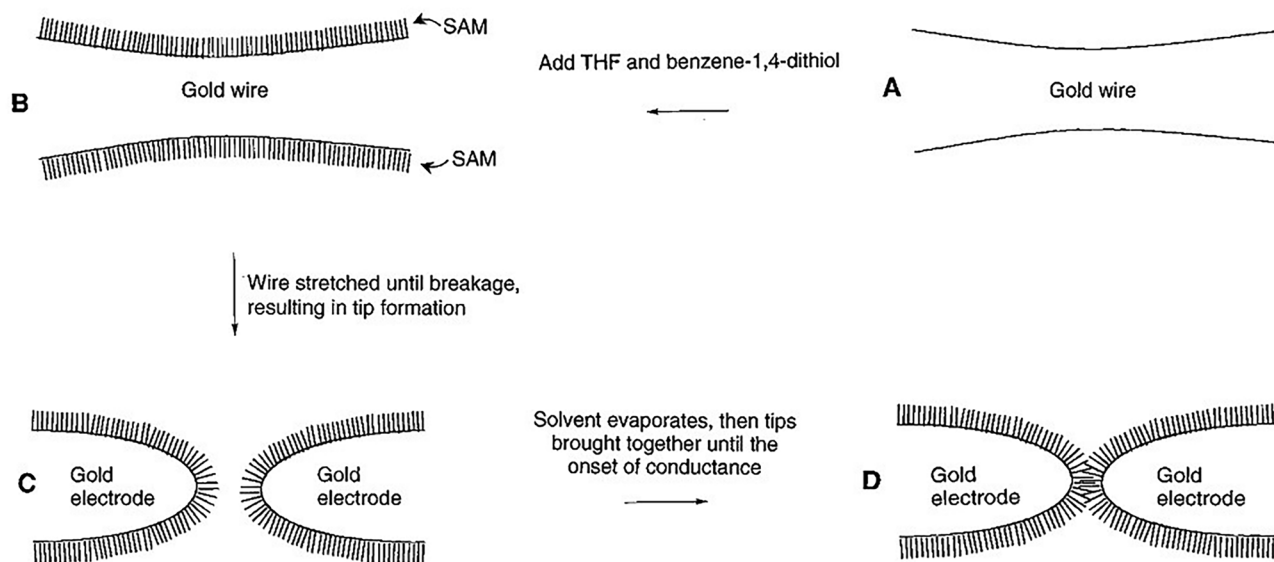


Fig. 13 Schematic of the process of making organic molecular compounds based on benzene-4,1-dithiol [8]

molecule is placed between two metal electrodes. The steps for making such a junctions are shown in Fig. 13. Figure 14 also shows the two-dimensional arrangement of organic molecules in the interface of two metal electrodes. By applying the voltage difference to the mentioned molecular junctions, I-V, J-V diagrams and electrical conductivity can be drawn according to the applied voltage. The experimental results obtained for this junctions are shown in Fig. 15. As can be seen, increasing the applied potential difference increases the transmission current and, consequently, increases the electrical conductivity of the junctions.

5 Study Environment

In general, the environment around molecular junctions (including organic molecular junctions) can severely affect their conductivity due to some changes in the electrical charge transfer process. The most important environmental variables can be mentioned as follows [32, 33].

5.1 Solution pH

Changing the pH of the molecular bond environment can significantly affect their electrical conductivity. For example, the trend of changes in the conductivity of cyst amine-glycine-cysteine-based junctions is shown in Fig. 16. As can be seen, the electrical conductivity of these junctions is much higher in acidic environments than in gaseous environments. The reason for this is due to the direct dependence of the process of oxidation or reduction

of molecules on the pH of the environment [34, 79–81]. Changing the pH can affect the redox reaction of the NH_2 and COOH functional groups and alter the conductivity of the target molecule [1].

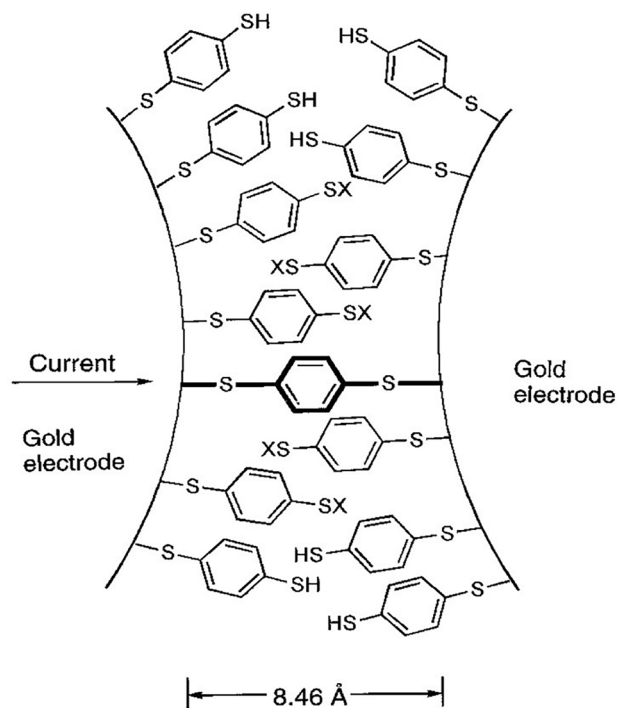
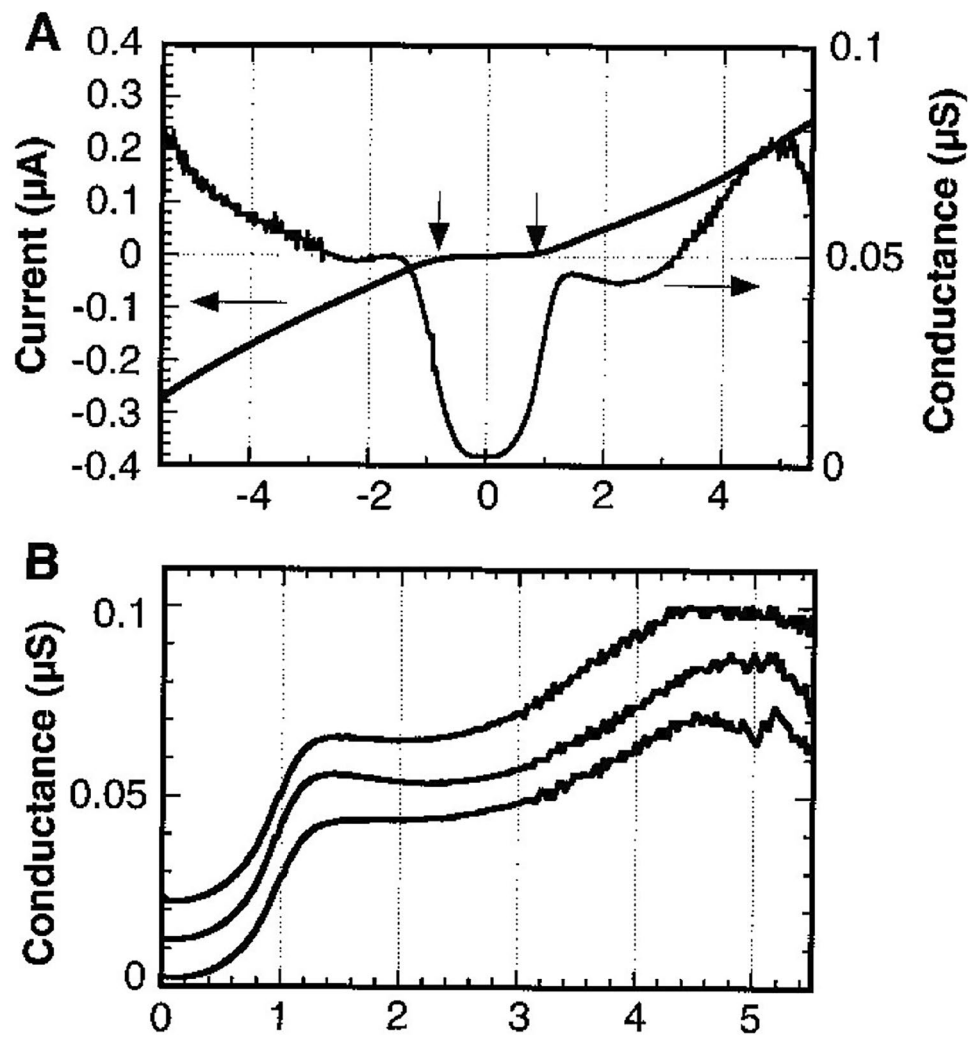


Fig. 14 Schematic of a benzene-4,1-dithiolite self-assembly monolayer between two gold metal electrodes [8]

Fig. 15 Diagram of changes in A current and B electrical conductivity (G) in terms of applied voltage for the molecular organic bond of benzene-4,1-dithiolite/gold [8]



5.2 Presence of Metal Ions in the Environment

The presence of some metal ions such as Cu^{2+} and Ni^{2+} in the solution environments around the joints can significantly

increase their electrical conductivity. For example, an increase of up to 300-fold has been reported for Cyst amine-Gly-Cys molecular junctions. The proposed mechanism to justify this increase is that the existing metal ions are able

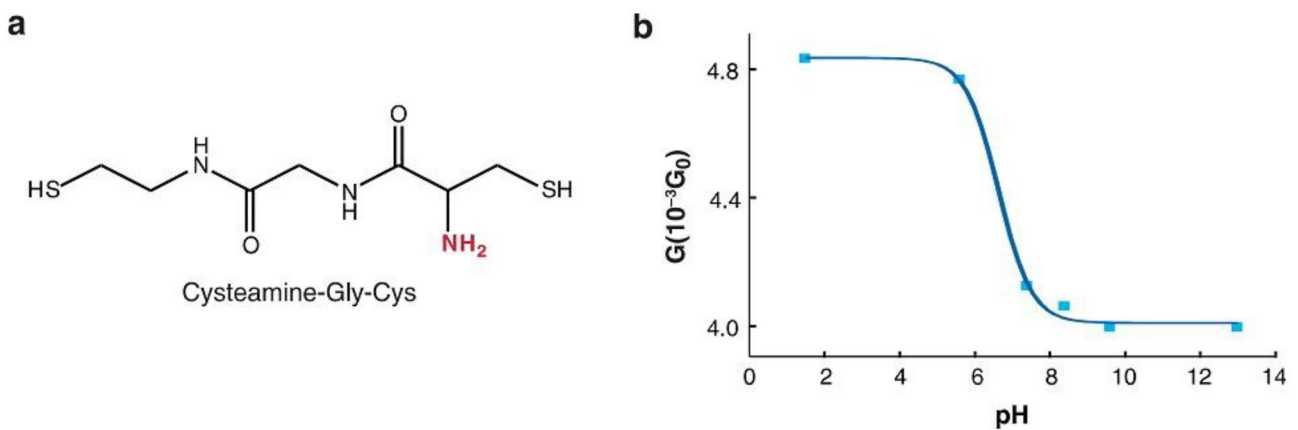


Fig. 16 a The structural formula of the cystatin-glycine-cysteine molecule. b The dependence of the current passing through the molecular junction of paragraph A on the pH of the surrounding environment [1]

to easily bond with the functional groups of the molecules and thus increase the electrical conductivity of the bond. The extent of this increase also depends on the length of the molecules and the nature of the metal ions. Chemical bonds between metal ions and molecules can increase the electrical conductivity of molecular bonds in several ways:

- (A) The formation of chemical bonds causes the transfer of electrons from the functional groups of molecules to metal ions, followed by the oxidation of molecular bonds. The same phenomenon affects the band structure of molecular units and changes the distribution of electric charge along molecular branches. Studies show that changes in the distribution of electrical charge in molecules also lead to changes in the height of the tunnel barrier of charge carriers and affect the conductivity of molecular junctions [35, 36].
- (B) The presence of metal ions causes the formation of additional energy levels in the band structure of molecular units and facilitates the tunneling process of electrons.
- (C) The formation of bonds between metal ions and molecular units leads to a change in the spatial arrangement of the molecules (molecular conformation) and, consequently, to a change in the conductivity of the junctions. As mentioned earlier, the spatial structure of molecules can affect the electrical conductivity of molecular junctions [82, 83].

5.3 Existence of Doping Conditions

In some cases, the acidity or alkalinity of the binding medium can change the doping conditions in molecular units [84–86]. For example, in one study, the conductivity of the molecular binding of hepta-aniline oligomer to gold electrodes was measured in both toluene and acidic electrolyte media. Based on the results, the current–voltage diagram of this connection is linear ohmic in toluene solution and inverse ohmic with a negative slope in acidic solution. The downward trend of the *I*-*V* diagram for acidic solutions indicates that the placement of this molecule in acidic environments and the occurrence of electrochemical oxidation phenomenon leads to an increase in the electrical conductivity of hepta-aniline oligomer bonds [37]. In fact, the acidic environment due to electrochemical oxidation of the molecule plays the role of doping agent in polymeric materials (Fig. 10).

5.4 Local Heating of the Junctions Due to the Passing Current

The local heat generated in molecular joints is one of the important parameters in the design of nanoelectronic devices. In other words, electronic devices must be designed

and constructed in such a way that the heat generated by the passage of electrical current through molecular connections does not cause physical damage or system malfunction [87–89]. As a general rule, in nanometer junctions, the length of the electron mean free path is relatively large compared to the physical dimensions of the junction, resulting in a very small fraction of the energy of the electrons as they pass through the junction (phonon). Local heat is lost. Therefore, the heat generated in molecular joints due to current density is very high. In recent years, extensive research has been conducted to quantify local heat in molecular junction [38]. Based on the obtained results, the actual molecular junction temperature (T_{eff}) can be expressed as a function of bias voltage (V_{bias}) as follows:

$$T^{\text{eff}} = T_0 + \gamma^4 V^2 \text{bias} \quad (3)$$

In this regard, T_0 is the room temperature and γ is a constant parameter that expresses the contribution of the bias voltage to the local heat generation. For example, it is proved that for benzene rings with *n* carbon atoms, $\gamma = 375 \exp(-0.19n) \text{ K/V}^{1/2}$ and for octane diol molecules $\gamma = 82 \text{ K/V}^{1/2}$. Based on the above equations, the temperature of octane diethyl molecular junctions per bias voltage 1 V (equivalent to 20 nA) will be about 25 K above room temperature.

6 The Nature of the Metal Electrode/Organic Molecular Unit Interface

As a general rule, the band structure of a molecule attached to two metal electrodes is quite different from the band structure of a single molecule. The reason for this difference is due to changes in electrostatic potential within the molecular junctions. When two materials with different Fermi surfaces come in contact with each other, a stream of electrons is created between the two materials so that the energy levels of the charge carriers at the points near the common section reach relatively equal amounts. If the molecule is organic, due to this electrostatic equilibrium, dipoles form in the junction's metal/organic molecule, causing potential differences within the molecular component [38, 90–93]. In other words, this potential change is due to the charge transfer between the molecule and the electrodes, and its intensity depends on the bipolar strength created at the molecule/metal interface. When molecule/metal coupling is relatively weak, electron transfer does not occur well and there are no noticeable changes in molecular orbitals. The stronger the polarity created in the metal/molecule junctions section, the greater the displacement of energy levels of the molecular orbitals in the vicinity of the junction's section.

Some studies have proposed a new macroscopic model to investigate the effect of the formed bipolar strength on the electronic properties of molecular bonds. According to this model, changes in electrical potential and charge density in the metal/molecule junction's season can be considered completely localized, because the junction's season is quite sharp and the junction's properties change abruptly as it passes through it [95–98]. Therefore, the molecular units used in molecular junctions can be divided into two parts: the coupled region and the extended molecule. In order to calculate the effect of the bipolar region on the electronic properties of molecular junction's, a parameter called extra electrostatic potential for the polarized region can be defined. In general, the binding of the organic molecule to the metal electrode results in the formation of a polarized region in the molecule/metal interface and shifts the energy levels of the molecular unit relative to their original position [36–38]. Also, the formation of electric dipoles causes the molecular orbitals to become wider, because the discontinuous levels of the molecular component are affected by the interactions of the interface and shift to their original state by junction's to the electrode with perfectly continuous electron levels. As a result of this displacement, a phenomenon called “energy level broadening” of the molecule occurs. This phenomenon is shown in Fig. 17.

7 Electronic Structure and Charge Transfer in Organic Molecular Junctions

The most important parameter that controls the electrical conductivity of linkers in molecules is how the Fermi energy level (EF) of a component is positioned relative to the Fermi level of other components. Usually in inherent semiconductors, the Fermi energy level is located exactly at the center

of the energy gap [99–102]. However, the addition of dopant atoms to intrinsic semiconductors leads to the displacement of energy levels in the material, and the amount of this displacement can be controlled by changing the amount of additive. Relatively similar conditions exist in organic molecular junctions. In these systems, in addition to the Fermi level, a level of energy called “charge neutrality level” (CNL) is defined, which can be compared by comparing the energy level of this level with the Fermi level of metal electrodes or their working function, the transfer phenomenon predicted the load on molecular junctions. In other words, the difference between the CNL parameter and the Fermi surface of the metal electrode controls the intensity of the electrical dipoles formed in the common metal/organic semiconductor phase. By definition, the neutral charge surface is the level of molecular energy below which the number of energy distribution states between the charge carriers is equal to the number of electrons per molecular unit. This definition can be understood by considering the concept of the electronic state density of a system or DOS. According to this definition, the CNL energy level is located between the two levels of HOMO and LUMO in the band structure of the molecule. Numerous and complex statistical and experimental methods have been developed to calculate the CNL energy level. Figure 18 shows the electronic structure of a bond based on an organic molecule and two gold electrodes. As can be seen, to study the charge transfer at the metal/organic semiconductor interface, instead of dealing with the band structure and different energy levels, it is sufficient to compare the Fermi energy level with the CNL level of the organic molecule and the electric dipstick intensity and force estimated the stimulus for electron flow between the two substances [103].

The position of the metal Fermi energy level relative to the CNL level of the organic molecule controls the amount of electrical charge transferred from the metal electrodes

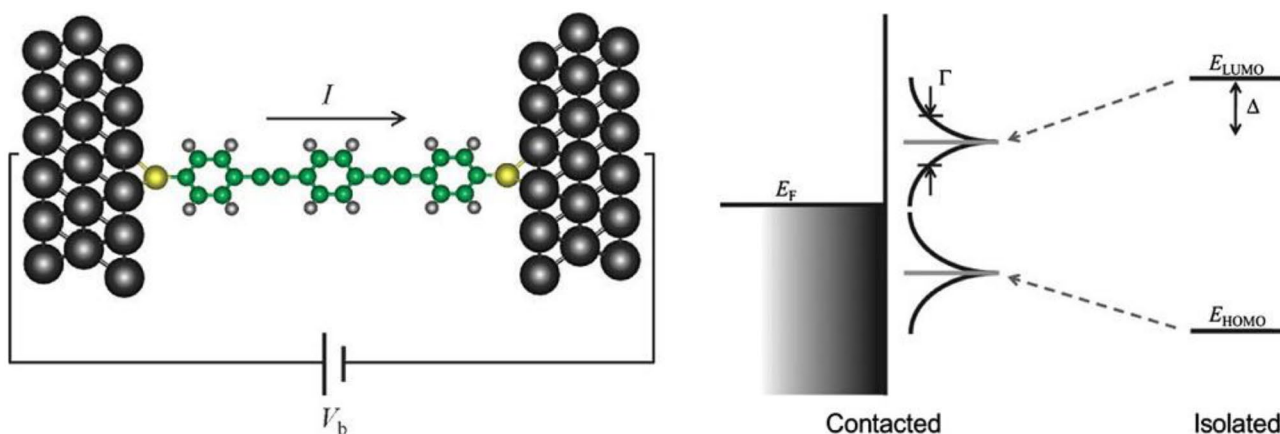


Fig. 17 Scheme of organic molecular junctions and the phenomenon of energy surface expansion at points near the common electrode/molecule season [14]

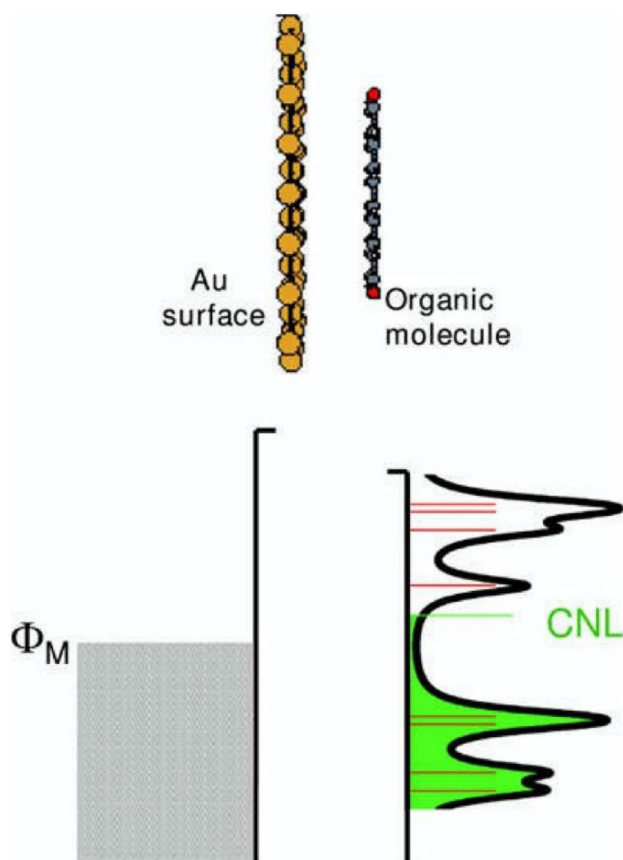


Fig. 18 Electronic structure and electron state density (DOS) for an organic molecule-based bond and gold metal electrode. By comparing the CNL energy level of organic molecules and the Fermi energy level of metal, the charge transfer mechanism can be studied [15]

to the junction's bridges of the molecular units in the junction's. In other words, the driving force of this charge transfer is the difference between the CNL energy level and the Fermi level of the metal electrodes [14, 15]. Figure 19 shows a diagram of molecular junction's and Fermi levels (E_F) and CNL and their band structure in the presence of bias voltage. As you know, the Fermi energy of any substance under constant conditions is always a certain amount. However, applying a voltage difference between the two metal electrodes changes the Fermi energy level in the two metals. This difference in energy level will create a stream of electrons along the junction. Under such conditions, in the presence of a voltage difference, the electrons move from the molecular states occupied in the high-formaldehyde metal to the common molecule/metal phase, and finally to the lower-level metal electrode occupied by the nonoccupied molecular orbitals in the molecular units. These unoccupied molecular orbitals as intermediate states of energy can aid in the process of tunneling electrons between two electrodes. Therefore, molecular orbitals can be considered as channels for the passage of electron current. It is emphasized that if

the bias voltage is not applied to the two metal electrodes, no charge current will be observed at the junction and the only common phenomenon will be the formation of dipoles at the metal/molecule interface [14, 15].

8 Application of Bias Voltage and Gate Voltage in Organic Molecular Junction

Based on what has been said so far, the motion of electrons along molecular junctions is a function of the relative state of the electronic structure of the organic units and metal electrodes used, and their displacement relative to each other changes the nature of the electron transfer. In practice, the displacement of the band structure of a common molecule/metal chapter is often accomplished by applying a secondary voltage called a gate voltage. This is shown in Fig. 20. According to this figure, in addition to the voltage difference V_b , which is applied to the source and discharge terminals to create energy differences between the Fermi surfaces of metal electrodes, the secondary voltage V_G or voltage gate can also be used to adjust the band structure of molecular units in the junction. In this figure, V_G is assumed to be zero and the path of electron motion between the energy levels of the molecular bond is shown.

In practice, the application of gate voltage and bias voltage to molecular junction can be done in different ways, the most common of which is to keep the electrical potential level of one of the metal electrodes (e.g., electrode A) constant by junction it to ground and finally applying gate voltage along the unit. It is molecular. Under such conditions, the application of gate voltage will displace the electrochemical potential of another electrode (e.g., electrode B) and the molecular steps used in the junction. In other words, the main role of the gate voltage is to oppose the displacement of the energy levels of the junction components due to the bias voltage V_b and to reduce the degree of dependence of this displacement on the bias voltage. Therefore, the final effect of gate voltage is to change the number of conductor channels that participate in the load transfer process under a certain bias voltage. To clarify the discussion, consider Fig. 20. In this figure, it is assumed that electrode A is grounded and its Fermi energy level always remains the same. In this case, applying a positive bias voltage (Fig. 20a) or negative (Fig. 20b) to the two electrodes causes the Fermi energy level of electrode B to shift by $|V_b|e$ will be. As a preliminary approximation, it is assumed that the energy level of the CNL or the Fermi level of the molecular unit is exactly at the center of the gap between the Fermi levels of the metal electrodes. What follows from Fig. 20 is that in each of the above cases, the molecular bridge can act as a conducting channel, and the current generated by the passage of load

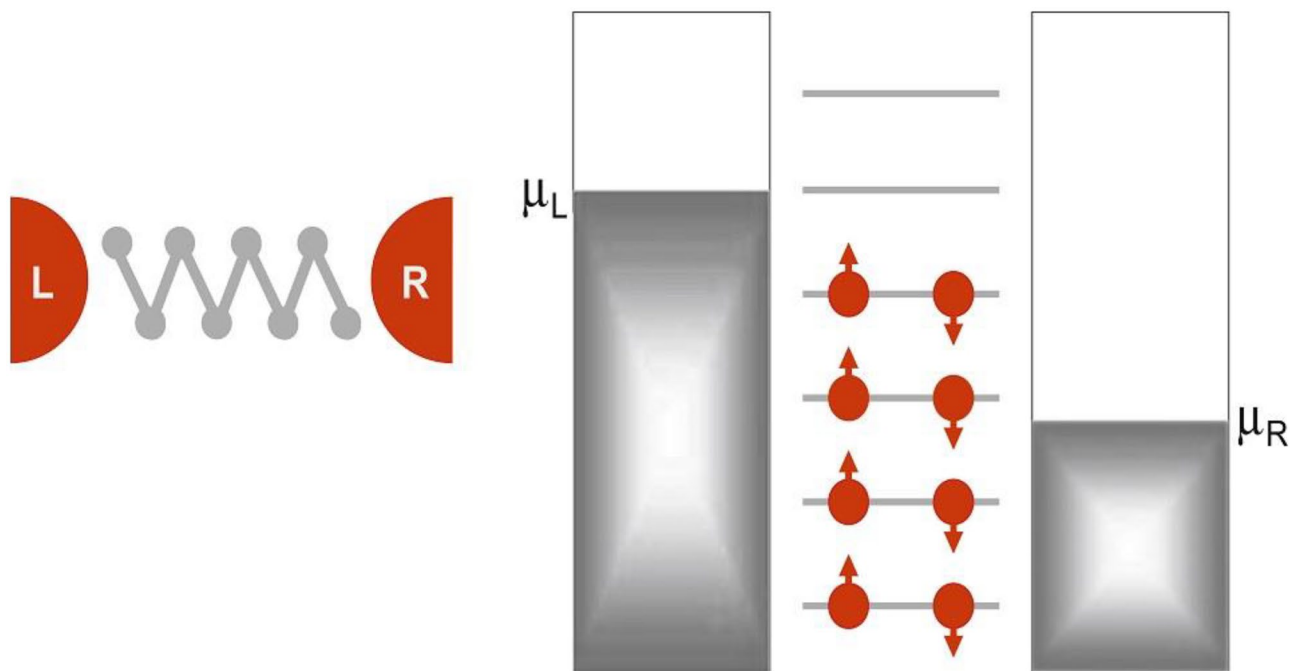


Fig. 19 Schematic of molecular junction and their band structure in the presence of bias voltage [16]

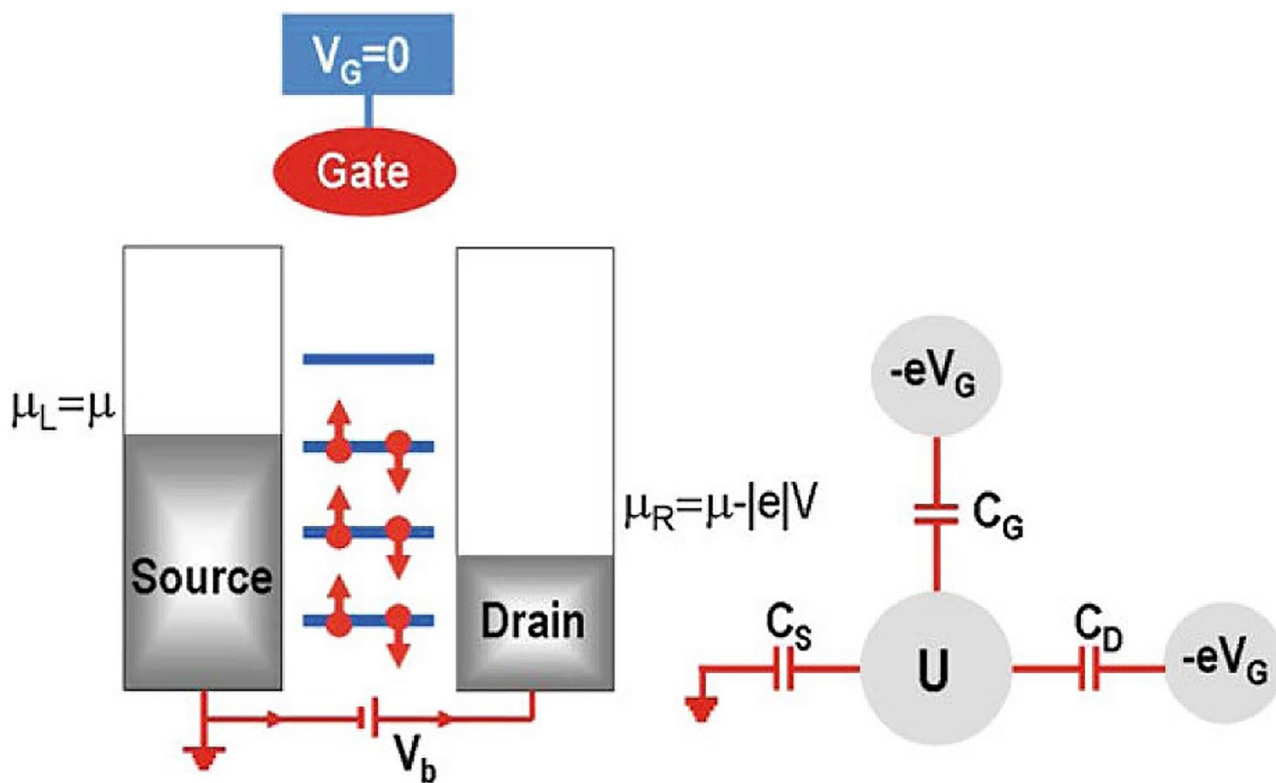


Fig. 20 a Schematic of metal–molecule–metal molecular junctions with V_G gate voltage and b equivalent circuit of molecular junction A. Applying gate voltage reduces the LUMO level energy level and facilitates the process of transferring electrical charge in this junctions [16]

carriers through these channels will be exactly the same in both of these junctions. This statement only applies if no gate voltage is applied to the junction [14–16].

Applying a certain gate voltage to the molecular junction will shift the energy level of the molecular unit and change the conductivity of the junction. In other words, the gate voltage at the junction $V_b > 0$ will cause the energy level of the molecule to shift to higher energy levels (Fig. 21c) and at the junction $V_b < 0$ will cause it to shift to lower energy levels (Fig. 21d). In the first case, in addition to the fact that the Fermi level of the molecular unit, similar to its initial state, will remain between the Fermi surfaces of the two metal electrodes, it will be even closer to the Fermi level of the more negative electrode. Under

such conditions, molecular units can act as conduction channels and facilitate the transfer of charge from a more negative electrode to a more positive electrode [104–108]. However, applying the same gate voltage to the second state junction causes the Fermi surface of the molecular unit to exit the width of the energy gap between the two electrodes. This creates a huge potential barrier to the movement of load carriers and significantly reduces electrical conductivity. In this case, the molecular junction will act as a diode. Therefore, by applying the gate voltage and changing the polarization of the bias voltage, the electrical conductivity of the molecular junction can be controlled and the current intensity in the two opposite directions can be determined [14–16].

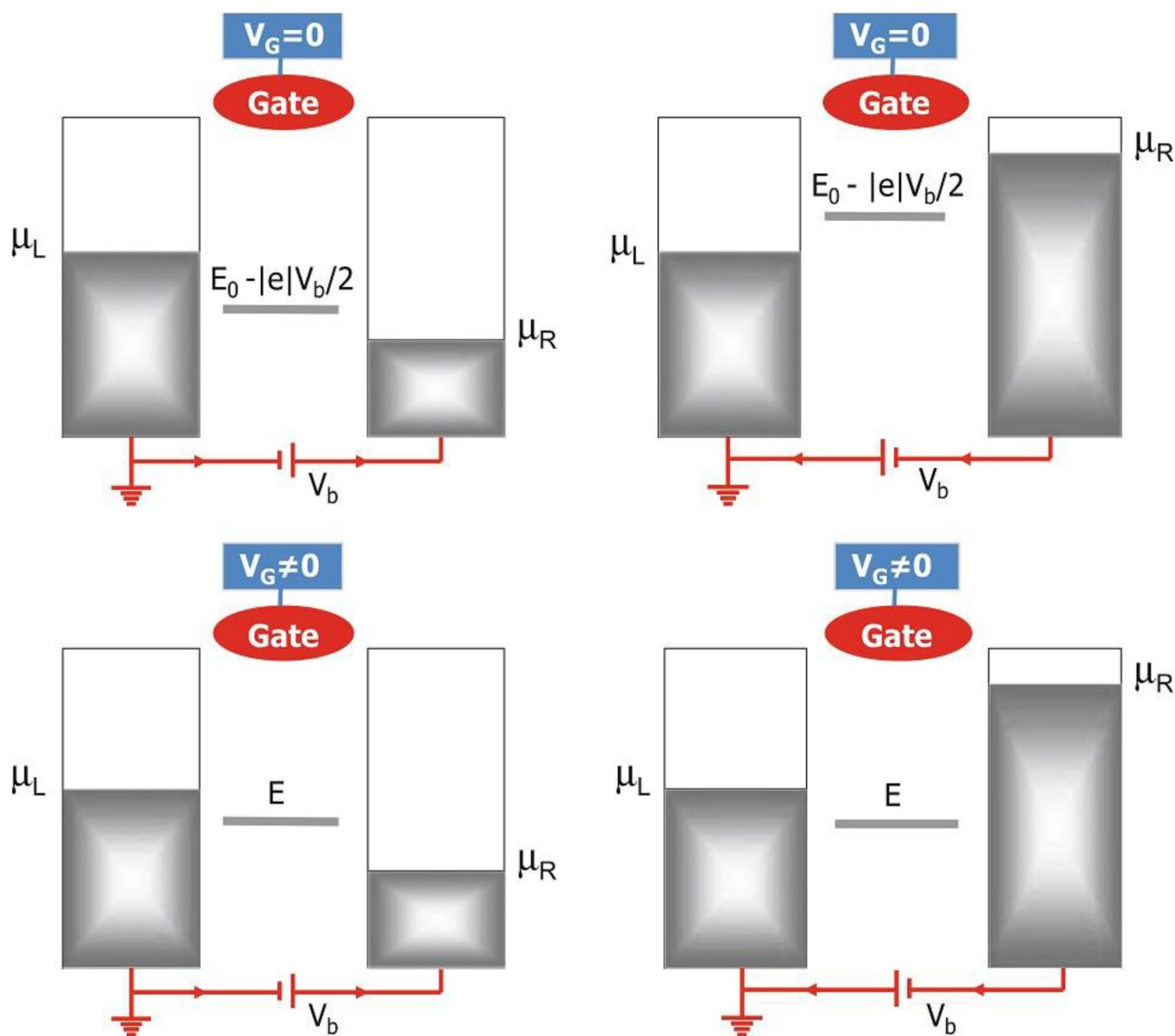


Fig. 21 Schematic of the electronic structure of organic molecular junctions in four modes: a direct bias voltage application, b reverse bias voltage application, c direct bias voltage application simultane-

ously with gate voltage application, and d simultaneous reverse bias voltage application by applying gate voltage [16]

9 Electron Displacement in the Electronic Structure of Organic Molecular Bonds

One of the major challenges in the field of electron transfer in molecular bonds and its relationship to the band structure of molecular units is the answer to the question of whether electrons can only move through the LUMO energy level and higher levels along the molecular component or pass through them. There is also a HOMO level. The answer to this key question requires examining the conditions required for the movement of load carriers between two different strip structures. In general, in order for electrons to be able to move along molecular waves, the following two conditions must be met simultaneously:

- Existence of an empty or half-filled level that can accept new cargo carriers.
- The ratio of the energy level of an empty or semi-full molecular component to the energy level of the electron under investigation.

As a general rule, any electron balance that can meet these two conditions can act as a conduction channel in organic molecular junctions. For example, Fig. 21 shows the band structure of some molecular junctions that are able to transfer electrons along their lengths. In Fig. 22a, the electron in the metal electrode enters the LUMO plane for displacement, and at the same time, the electron exits the HOMO plane and reaches the Fermi level of the second electrode. Under such conditions, the transfer of each electric charge through the bond causes the simultaneous formation of a pair of electrons and holes in the material. This type of load transfer is called inelastic co-tunneling. In Fig. 22b, the electrons enter the empty LUMO level of the molecular component and through it, move to the Fermi level of the second electrode. In Fig. 22c, the HOMO plane contains only one electron with a specific spin and can accept another electron with the opposite spin. In this case, the electron easily enters the HOMO

level, and thus, the transfer of electrical charge in the junctions takes place [109, 110]. As observed, in some cases, the HOMO level can also act on the conduction channel in the molecule and facilitate the charge transfer process in organic molecular junctions. On the other hand, by increasing the bias voltage, it is possible for energy levels higher than the LUMO level to contribute to the transmission. Therefore, it seems more appropriate to use the term “conduction channel” instead of HOMO and LUMO balances in discussions of charge transfer through molecular junctions [2, 3]

10 Simplification of the Electronic Structure of Organic Molecular Compounds

In describing the electronic structure of molecular connections and how the charge is transferred between energy levels, the general preference is to avoid as much as possible the details of the strip structures and to display these energy levels in the simplest possible way. For example, if the bias voltage between two metal electrodes is very small, the energy levels are often considered to be Extended MOs, and based on this, the integrated electronic structure can be defined as equivalent to the actual band structure of the molecular component. For example, Fig. 23a and b relate to the electronic structure of a junction that, in the presence of a very small bias voltage, has non-positioned molecular orbitals and its band structure is considered to be fully integrated. However, increasing the bias voltage causes the separation of the energy level of these molecular orbitals. Under such conditions, each local orbital will have a completely separate band structure (Fig. 23c). The important point is that in all the discussions that have taken place so far, it has been assumed that there is no interaction between the free electrons and the electrons in the band structure of molecular steps as well as the phonon waves formed in the molecular structures [111–113]. In other words, electrons have only potential energy E and no thermal or phonon energy (kx).

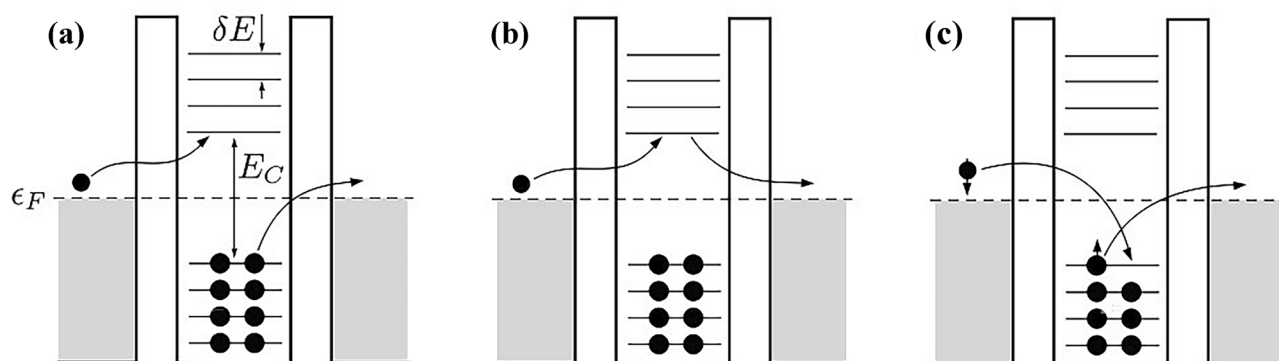
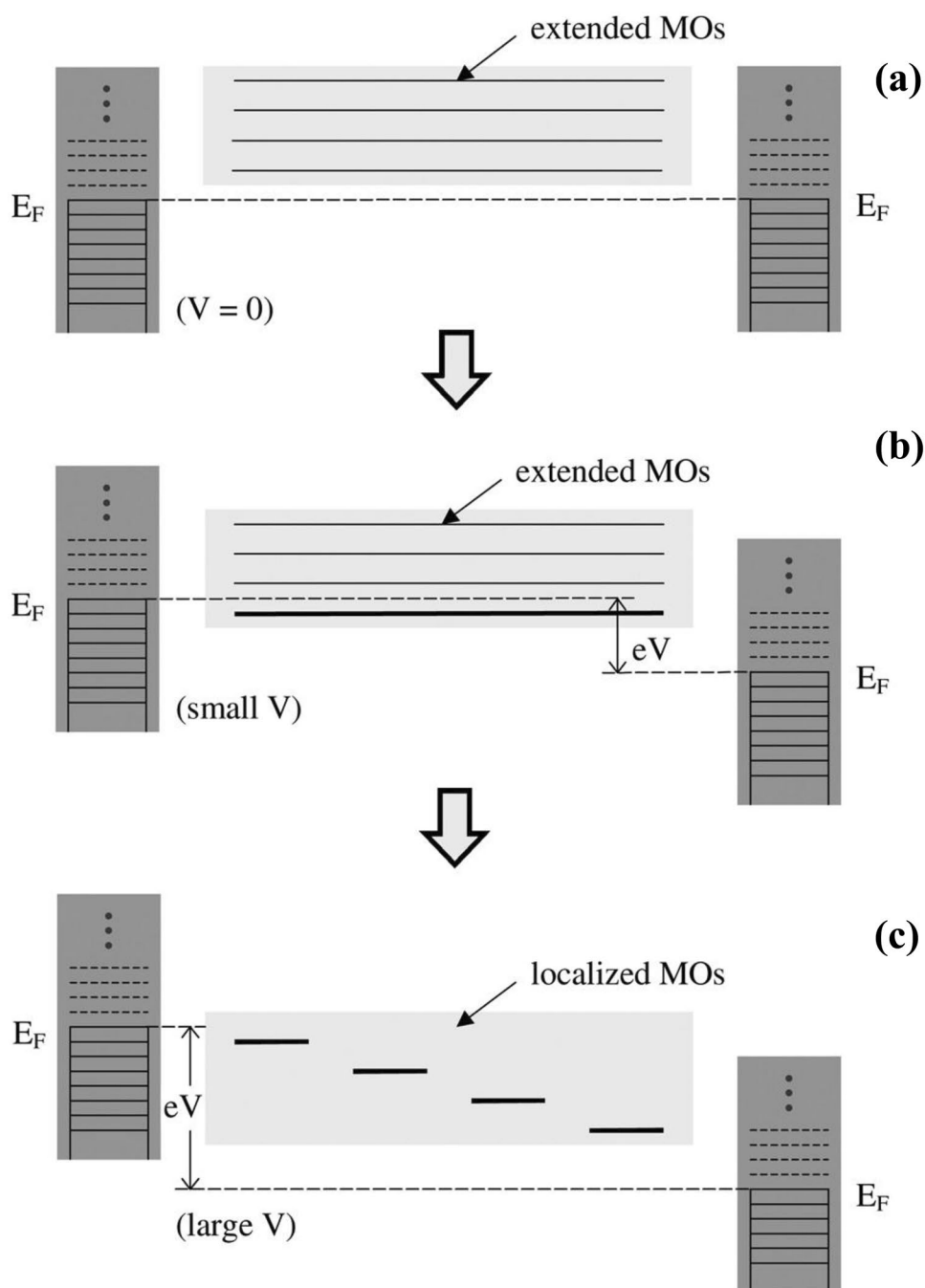


Fig. 22 Examples of electron transfer in organic molecular junctions [2, 3]

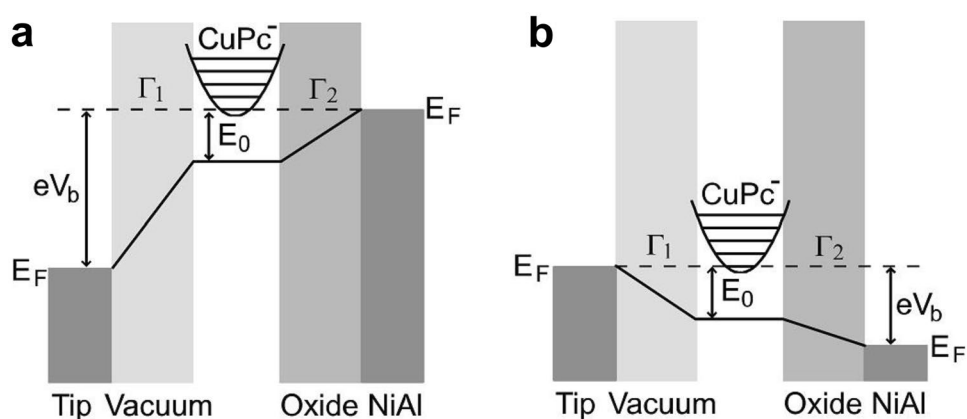
Fig. 23 Conversion of the integrated band structure of organic molecular junctions into completely separate electronic structures in the presence of bias voltage [12]



Under such conditions, the energy levels of the electrons in the electronic structure of the electrodes and molecular units can be considered as continuous bands and the Fermi energy level is quite definite. The reason for this generalization is due to the simplification of the analysis of different stages of charge transfer in organic molecular junctions. However, in order to study the electron transfer process in

more depth, in some cases, it is necessary to abandon the use of some of these assumptions and consider the effect of different interactions. For example, Fig. 24 shows a diagram of the electronic structures of organic molecular bonds without conventional approximations. In this structure, the phonon energy of the local electrons of the molecular component (K_x) is also considered [2, 3, 12, 16, 114].

Fig. 24 Schematic of band structures in junctions in which the conventional energy level approximations of molecular orbitals [11]



11 Conclusion

1. Molecular junctions are of particular importance in the manufacture of electronic devices, because the behavior of electrons in these regions is completely different from bulk material. It has been shown that by controlling various manufacturing factors, junctions with the desired electronic properties can be produced. The most important of these factors are the type and type of molecule used, the working environment, the temperature, the electronic structure of the molecules used, and their spatial conformations. Conventional methods for making molecular junctions were also discussed. It was observed that each of these types of junctions have unique characteristics and they can be used in the design of nanoelectronic equipment.

2. In this paper, the electrical conductivity of molecular junctions and the nature of related phenomena are discussed. It was said that several factors affect the electrical conductivity of these junctions. The most important of these factors are the geometry of the metal/molecule bond, the strip structure of the electrode/molecule bond, the application of external forces, the pH of the study medium and the presence of metal ions in it, doping, and local heating of the joints due to high current density. It was emphasized that by applying the bias voltage, the Fermi energy level of metal electrodes can be changed and by applying the gate voltage, the energy of HOMO and LUMO surfaces can be changed as desired, and through this, the conductivity of molecular junctions can be controlled. What is important about electron transfer in joints is the band structure of the molecular units and the electrodes relative to each other, and any factor that alters them can affect the conductivity of the junctions.

3. In this paper, organic molecular junctions were introduced and the electron transfer behavior in them was investigated. It was shown that the behavior of these junctions strongly depends on the nature of the metal/molecule interface and the band structure of the molecular unit. The most important phenomenon in these systems is the formation of dipoles at the interface, which provide the driving force for

electron transfer. It was said that a concept called “neutral charge surface or CNL” could be used to study the passage current through organic molecular junctions, and by comparing it with the Fermi surface of metal electrodes, the amount and intensity of the passage current could be estimated. What controls the passage of electrons in these junctions is their band structure. This structure can be manipulated by applying bias voltage and gate voltage. The bias voltage shifts the Fermi level surface of the metal electrodes relative to each other, but the gate voltage further shifts the energy levels of the organic molecular unit. Therefore, by optimally controlling these two voltage differences, the current intensity can be controlled with Nano ampere accuracy.

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Availability of Data and Material Not applicable.

Declarations

Ethics Approval and Consent to Participate Saade Abdalkareem Jasim, Mustafa M. Kadhim, Venu KN, Indah Raya: investigation, concept and design, experimental studies, writing—original draft, reviewing and editing. Sarah Jawad Shoja, Wanich Suksatan, Muneam Hussein Ali, Ehsan kianfar: investigation, concept and design, data curation, conceptualization, writing—original draft, reviewing, and editing.

Consent for Publication Not applicable.

Conflict of Interest The authors declare no competing interests.

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