

# Quantum interference effects in molecular electronics

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**Abstract** In order to keep up with the trend of decreasing size of electronics components electronics will have to shrink in size towards the molecular level. Decreasing the length scales will introduce quantum effects in the transport of electrons. When multiple paths are available in the molecule for the electron traverse, quantum interference effects can occur. The nature of this interference depends on the topology of the conjugated  $\pi$  system of the molecule. In crude approximation, cross conjugated molecules or paths through molecules are found to show destructive interference leading to a node in transmission probability.

The quantum interference effects are studied in a variety of systems, from simple conjugated wires to complex logic gates in a single molecules. In conclusion, molecular electronics is a promising field reaching the fundamental size limit of electronics. Quantum interfere can help achieve this since it provides a way to regulate current depending on the topology of the  $\pi$  system of the molecule.

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## 1 Introduction

Moore’s law has dictated the progress in electronics for the last five decades. The law states that the number of components in integrated circuits will double roughly every year. Or, as in the original paper, “the complexity for minimum component costs has increased at a rate of roughly a factor of two per year”.<sup>1</sup> Either way, an exponential increase in components leads to an inescapable decrease in the size of transistors. When Moore’s law is extrapolated it is to be expected that in about 20 years the transistors have reached single-molecule size.

Electronics on a single molecule level means a radical shift from traditional silicon based integrated circuits to electronics based on organic (carbon) molecules. This field of ‘molecular electronics’ has its origin in the 1940s.<sup>2</sup> In this year, the chemistry Nobel prize laureate Robert S. Mulliken worked out the early development of the molecular orbital (MO) theory. It was this theory that allowed conductance to occur in a single molecule, a crucial feat for molecules to be applied in electronics.

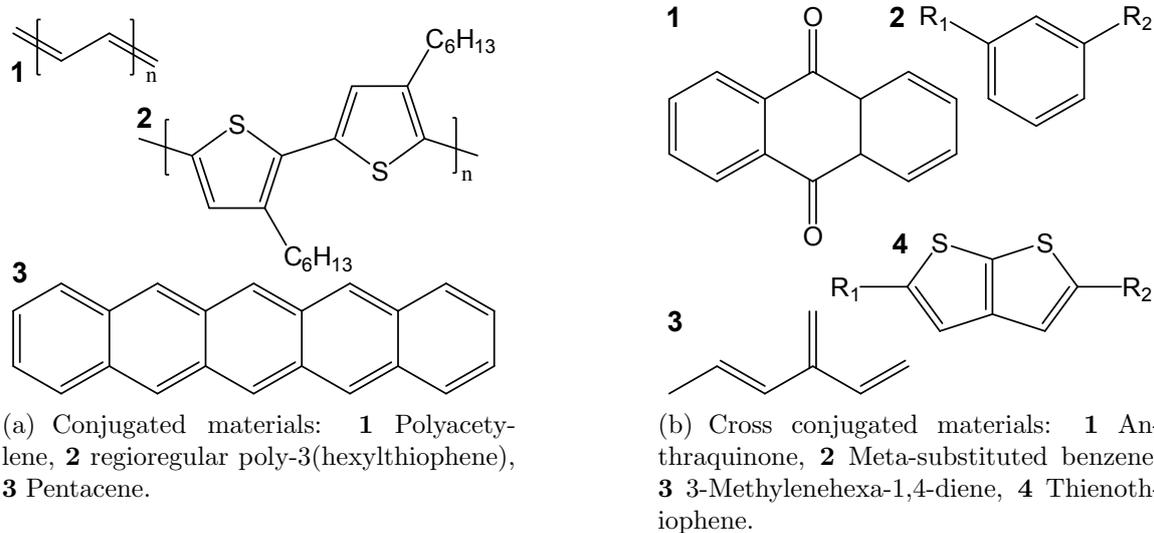
Inspired by electron transfer and storage in biological systems, the first tangible suggestion for molecular electronics came from Aviram and Ratner in 1974.<sup>3</sup> The paper shows the first suggestion of a single molecule exhibiting properties useful for devices, namely a rectifying molecule.

Since the proposal of the first concepts much progress has been made. The molecules applied today in electronics have in common that they possess a conjugated carbon backbone. A conjugated system is defined as a molecular entity whose structure may be represented as a system of al-

ternating single and multiple bonds.<sup>4</sup> The electronic properties arising from the conjugation originates from the molecular orbitals of the molecule. These MOs are formed by combining the  $p_z$  orbital which is responsible for  $\pi$  bonding in  $sp^2$  or  $sp^3$  hybridized molecules. It is the delocalized nature of the molecular orbitals which allows charges to be transported through the molecule.

Another topological possibility for conjugation is cross conjugation. Here, all carbon atoms are involved in double bonding and are  $sp^2$  hybridized. However, in contrast to *linear* conjugation the *cross* conjugated molecules do not have a strictly alternating double-single bonded pathway. (Figure 1).

The class of organic semiconductors has opened up the new field of organic electronics. The materials are already applied in devices like transistors, light-emitting diodes and solar cells and these technologies already found their ways to the commercial market. However, a major step in the miniaturization of electronics would be to reach the single molecule level. Today, the first examples of single molecule devices already exist. Molecular wire conductance has been measured first by Reed and Tour using mechanically controllable break junctions<sup>5</sup> and also working single molecule transistors have been demonstrated, a single fullerene molecule ( $C_{60}$ ) has been utilized an electromechanical amplifier<sup>6</sup> and single carbon nanotube transistors<sup>7</sup> are realized.



**Figure 1:** A few examples of conjugated (a) and cross conjugated compounds 1(b).

## 2 Quantum Interference effects in molecules

Quantum interference (QI) is a well known effect occurring in cyclic systems, however it is not always clear that the observed effect is of quantum mechanical nature. An example is the effect of donor/acceptor groups in electrophilic aromatic substitution. An electron donating group is known to direct the substitution towards the ortho and para positions, virtually no meta product is formed. This is explained by drawing *resonance structures* of the transition state involved. Drawing resonance structures is a model to describe the way in which electrons can delocalize in a conjugated molecule and by doing this it is found that the ortho and para substituted transition states have more stabilization through resonance.

Another way of looking at this is stating that the meta position is cross conjugated with respect to the acceptor group, and

the ortho and para positions linearly conjugated. This results in a reduced electronic coupling between meta and the acceptor group. We will find that this reduced coupling is a result of a destructive quantum interference effect occurring in molecules depending on their topology.

In general, interference effects occur when a wave propagates through multiple paths from an origin to another point in space. This principle works for all kinds of waves, be it sound, light or, in the case of quantum interference in molecules, electron waves. The waves will travel through all available paths and upon arrival at the point of interest, they are superimposed. When both paths are of equal length both waves will arrive with the same phase, thus interfering constructively. On the other hand, when one wave has a phase shift of  $\pi$  destructive interference will occur resulting in zero transmission.

The difference in electronic coupling between ortho meta and para positions in ben-

zene has been studied in detail, using different theoretical methods.<sup>8-10</sup> The general conclusion is that meta substituted benzene indeed shows lower conductance in comparison to ortho and para.

To explain the origin of the zero transmission node we need to consider the Feynmann path integral formulation of quantum mechanics. This approach generalized Hamilton's principle of least action to be applicable in the quantum regime. The principle states that the action of classical trajectory between the points  $x_1(t_1)$  and  $x_2(t_2)$  is given by:

$$S = \int_{t_1}^{t_2} L[x(t), \dot{x}(t)] dt \quad (1)$$

With the Lagrangian L:

$$L(x, \dot{x}) \equiv T(x, \dot{x}) - V(x) \quad (2)$$

Where  $T$  represents kinetic energy and  $V$  potential energy. Hamilton's principle says that of all possible paths the actual physical path followed is the path which minimized the integral in equation (1). Feynmann presented a new formulation of quantum mechanics<sup>11</sup> based on this classical principle. In this quantum mechanical approach instead of one path with least action the electron follows all possible paths and the final path taken is given by summation over all possible paths. When this is applied to the original transmission problem we see that in the benzene ring multiple paths can be taken. Electrons entering the ring at the Fermi level will have a wave vector of  $k_d = \pi/2d$ , where  $d$  is the C-C spacing in the benzene ring. With the electrodes in the meta position the two shortest paths have lengths  $2d$  and  $4d$  resulting in a phase

difference of  $k_F 2d = \pi$ , giving destructive interference. All paths which make an extra loop through the ring will destructively interfere pairwise, resulting in zero transmission.

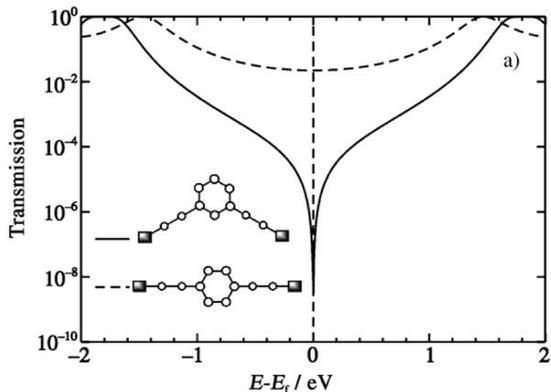
This simple approach considers only the occurrence of destructive or constructive interference by looking at the topology of the system. A more detailed insight is provided by calculating the transmission curve of the system. These curves are obtained by theoretical calculations on the system. The methods used differ however a general approach is through a non-equilibrium Green function. The transmission is the probability of an electron entering the system at a given energy to be transmitted to the other terminal. By using the Landauer-Buttiker formalism the current can be found from these transmission curves by integration:

$$I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} (f_L(E, V) - f_R(E, V)) T(E, V) dE \quad (3)$$

Where  $2e/h$  is the conductance quantum,  $f_L(E, V)$  and  $f_R(E, V)$  are the Fermi functions for the left and right electrodes and  $T(E, V)$  is the transmission. This relation makes transmission curves a valuable tool to investigate conductance in molecules.

In figure 2 the transmission curve for meta and para substituted benzene is presented. The calculation has been done using the Hückel method. In this relatively simple approach the atomic orbitals are combined to form linear combinations of atomic orbitals (LCAO) to give molecular orbitals (MO). In this approach only  $\pi$  orbitals are considered, leaving out any effects

from the  $\sigma$  bonds. In this  $\pi$  orbital approach there is a clear node in the transmission curve for meta substituted benzene.



**Figure 2:** Transmission curves for para and meta substituted benzene rings. The meta topology clearly shows a node in the transmission.<sup>12</sup>

Of course there are many more molecular wires conceivable which may show quantum interference effects than just wires with meta substituted benzene ring. A simple graphical method has been developed<sup>13</sup> which predicts occurrence of quantum interference. First, a path is drawn through the conjugated molecule (Figure 3) from one lead to the other. Then the remaining atoms are paired up with the neighbours where possible (blue ellipses). Now, if there are any remaining isolated atoms in the conjugated system, the system is expected to show destructive interference effects.

In Figure 3 the molecules **1**, **2** and **3** have isolated atoms and will show quantum interference. In molecule **4** all atoms are paired up and no quantum interference is expected. The molecules **1** - **3** are all cross conjugated. When considering a cross conjugated molecule, it is impossible to add a single atom to the structure without introducing charges or radicals. Atoms can then

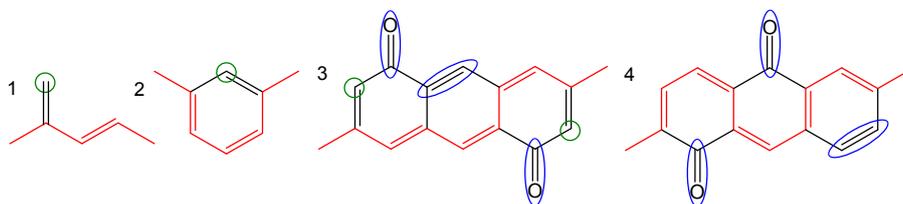
only be added in pair which will not remove quantum interference effects. Therefore we can conclude that all neutral closed-shell cross conjugated molecules will show quantum interference. It is clear that the quantum interference is a direct consequence of the topology of the  $\pi$  conjugated system.

However, it must be noted that this method is derived from Hückel calculations, considering only the  $\pi$  electrons. When  $\sigma$  electrons contribute significantly to charge transport they can severely suppress quantum interference effects.

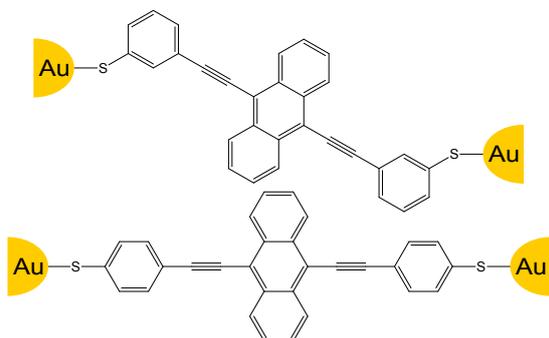
## 2.1 Quantum interference in molecular wires

Over the last years different methods have been employed to measure the conductance in molecular wires, as to find experimental evidence for quantum interference. There are several methods for the measurement of conductance along few or large amounts of molecules, namely large area molecular junctions<sup>14</sup> or EGaIn droplets against self-assembled monolayers (SAMs).<sup>15</sup> Also single-molecule methods are now possible, these methods include STM based break junctions,<sup>16,17</sup> mechanically controlled break junctions (MBJ)<sup>18,19</sup> and time-resolved electron transfer measurements in donor-bridge-acceptor molecules.<sup>20-22</sup>

The conductance of meta and para substituted wires has been investigated experimentally by MBJ<sup>23</sup> (Figure 4). In these studies it was indeed found that the conductance for meta substituted wires is two orders of magnitudes lower. This is in agreement with theoretical studies.<sup>8,9</sup>



**Figure 3:** A simple graphical method to predict if molecules will show destructive quantum interference. A path is drawn through the backbone of the molecule (red), then all remaining atoms are paired up with neighbours (blue). If any isolated atoms (green) are present, the molecule will show QI.



**Figure 4:** Mechanically controlled break junction measurements on meta and para substituted molecular rods.<sup>23</sup>

More experimental evidence is obtained by comparing the current density through SAMs of molecular wires based on different anthracene derivatives.<sup>15</sup> The wires have approximately the same length but the anthracene cores are linear conjugated (anthracene), cross conjugated (9,10-anthraquinone) or broken conjugated (9,10-dihydroanthracene). The conductance through a SAM of these molecules is measured by making a top-contact with the non-Newtonian liquid metal alloy EGaIn (Eutectic Gallium Indium).

The observed current across the SAM was found not to differ by much for the cross conjugated and broken conjugated species, the current for linear conjugated anthracene was around one or two order of magnitude higher. The values found are in good agree-

ment with theoretical studies for these systems, where the lower conductance of the cross conjugated anthracene is explained by destructive quantum interference.

Another way to study quantum interference in wires is through donor-bridge-acceptor systems.<sup>20-22</sup> These system consist of a donor and acceptor with the wire of interest in between. This eliminates the need for attaching electrodes to get electrons through the wire. Photoinitiated charge separation and recombination is investigated by time-resolved spectroscopy.<sup>22</sup> The charge transfer for a linear conjugated bridge was found to be 30 times faster than for a cross conjugated bridge of similar length. DFT calculations on this cross conjugated bridge gave the expected node originating from destructive interference, suppressing transport through the  $\pi$  system. The charge transport relies then on the slower  $\sigma$  system transport, and indeed the charge transfer dynamics of a  $\sigma$  system bridge is comparable to the cross conjugated bridge. Again, these results support the theory of quantum interference.

## 2.2 On/off switching in molecular wires

A large collection of switching mechanisms has been proposed for the switching of conductance in molecular wires. Apart from mechanisms which not depend on QI effects occurring there are mechanisms proposed which operate by switching between destructive and constructive interference.

Among these switching mechanisms are electrochemical<sup>24-27</sup> or light-induced<sup>28-30</sup> methods. They both rely on an structural change of the molecule, going from linear to cross conjugated. Due to the introduction of QI effects the difference in conductance can be several orders of magnitude.

These switches can be integrated into larger molecular electronic circuits. A computing device fully based on molecular electronics will also need memory, this can be provided by molecular switches. The existing wires can already be read out non-destructively simply by probing their resistance. For full implementation in molecular circuitry switches will need to be designed which can be switched (write) by the molecular circuit itself. Since the energy required to introduce structural changes in molecules this is still a challenge for the field of molecular electronics.

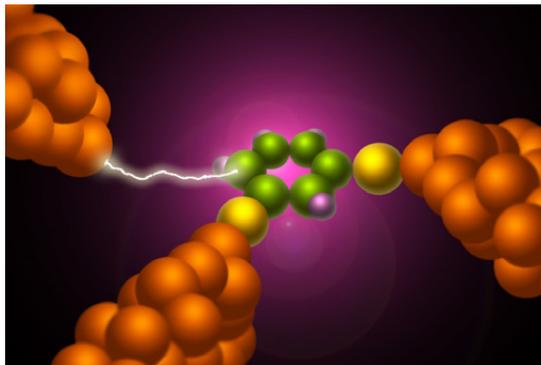
## 3 The Quantum Interference effect Transistor

The suggestion of a transistor based on quantum interference dates back from late 1980s.<sup>31</sup> In this paper a T-shaped three terminal waveguide system is described. To introduce quantum effects the length scale of the gate side arm needs to be below 1

$\mu\text{m}$  in size. With these dimensions this is a mesoscopic system, however their results are generally applicable if the de Broglie wavelength scales with the dimensions of the system.

### 3.1 Quantum interference in benzene ring systems

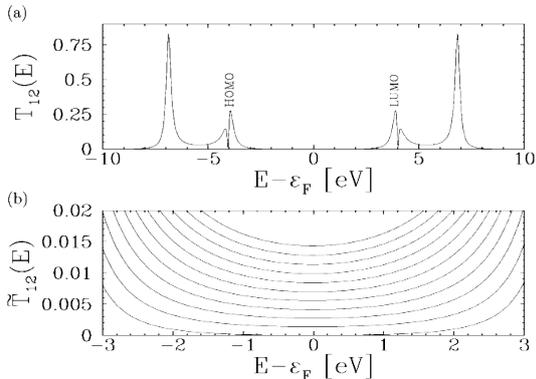
A design of a transistor at the single molecule level has been proposed recently.<sup>32,33</sup> This quantum interference effect transistor (QuIET) exploits the wave nature of the electron leading to interference effects to control the current.



**Figure 5:** Artist's impression of the QuIET. In this figure carbon atoms are green, sulfur yellow and gold atoms are orange. The two contacts are connected in the meta position, resulting in destructive interference and no current between the source (bottom) and drain (right) electrodes. The device is switched on by introducing decoherence with the third electrode.

The transmission from source to drain electrodes through the molecule can be calculated using a nonequilibrium Green function approach,<sup>32</sup> the resulting transmission curve is shown in Figure 6.

The figure shows a zero transmission node midway between the HOMO and LUMO energy levels. The presence of this



**Figure 6:** Transmission probability  $T_{12}$  at room temperature.<sup>32</sup> (a) Transmission with zero bias on the gate electrode. (b) Transmission with increasing decoherence introduced by the gate. Bottom curve at zero, increasing by 0.24 eV in each successive one.

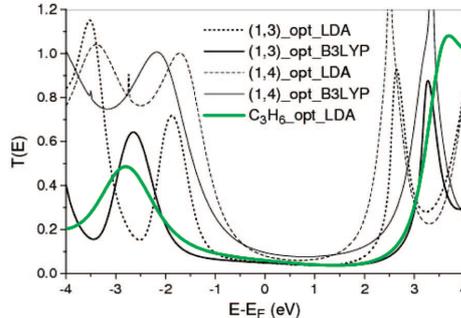
node originates from destructive interference, a crucial prerequisite for QuIET operation.

For transistor operation, there needs to be control over the current with a third electrode. This is done through a STM tip which introduces decoherence or elastic scattering, affecting the phase of the electron waves. In part b of Figure 6 the effect of the third lead on the transmission is shown. The transmission goes up when the voltage applied to the third lead increases, giving transistor action.

There are several advantages which these QuIETs have over traditional transistors. First of all, they are one molecule in size pushing electronics towards the fundamental size limit of one atom. Second, all field-effect devices rely on the raising and lowering of an energy barrier of at least  $k_B T$ . Every device then dissipates energy of this order of magnitude and the heat dissipation will be enormous when the devices are downscaled any further. The QuIET is insensitive to molecular vibrations. The

vibrational modes that destroy the 6-fold symmetry of the benzene ring are only active above about 500 K, thus it can operate at room temperature.

One phenomena that can interfere with the operation of QuIETs is the influence of charge transport through the  $\sigma$  system. The calculations presented above only take  $\pi$  electrons into account. More realistic calculations on the benzene system have been done by Ke and Yang.<sup>34</sup> In contrast to previous work these calculations did not only consider  $\pi$  molecular states but also the influence from contact  $\sigma$  states. The resulting transmission curves for meta (1,3) and para (1,4) connected leads is shown in Figure 7. Two theoretical methods are used: LDA, local density approximation and B3LYP, hybrid density functional theory (DFT).

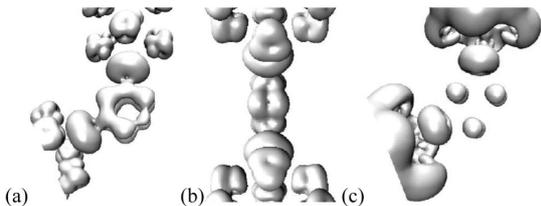


**Figure 7:** Transmission curves of the Au-S-benzene-S-Au system in the (1,4) and (1,3) configuration calculated by B3LYP and LDA (black lines). A 3 carbon alkane system is shown in comparison.

In comparison to Figure 6 it is striking that the node around the Fermi level has disappeared. The authors of the above mentioned paper ascribe this difference to the influence of  $\sigma$  states. Considering the (1,3) configuration, the first indication for  $\sigma$  tunnelling effects comes from the fact that the calculated HOMO-LUMO gap in

the transmission curve (Figure 7) calculated does not correspond to the HOMO-LUMO gap of the free benzene molecule. This mismatch suggests that the HOMO and LUMO resonances may not be dominated by  $\pi$  orbitals.

To illustrate this, the local density of states (LDOS) for the HOMO resonance ( $-2.5 - 1.0$  eV) are plotted in Figure 8. Figures 8a and 8b show that the HOMO resonance has a strong contribution from contact  $\sigma$  states. In Figure 8 the LDOS around the Fermi energy is shown, and this plot suggests that the current in this energy range is largely carried by tunnelling through  $\sigma$  states, reducing the quantum interference effect.



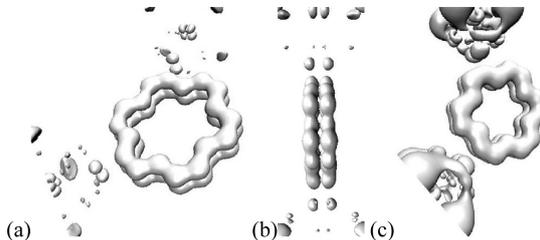
**Figure 8:** The local density of states (LDOS) for the benzene QuIET with gold electrodes in the meta positions.<sup>34</sup> (a) Top view in the energy range  $-2.5 - -1.0$  eV (HOMO resonance). (b) Side view. (c) Top view in the energy range  $-0.2 - 0.2$  eV

### 3.2 Larger ring systems

In an attempt to get around these  $\sigma$  tunnelling problems we move to a larger ring system, [18] annulene. Several configurations are considered: the (1,7) and (1,9), which, by symmetry, should give destructive interference and the symmetrical constructive configuration (1,10). Again, the transmission is calculated. The conductance for the (1,7) and (1,9) is found to be approximately two orders of magnitude

lower than that of the (1,10) configuration, suggesting that in this case quantum interference effects are preserved. When looking at the LDOS (Figure 9) we find that the HOMO resonance is dominated by  $\pi$  states and transport around the Fermi energy is through the  $\pi$  ring.

This difference in  $\sigma$  character is explained by considering the energy levels involved. When a conjugated system is extended, the HOMO rises in energy. In the case of benzene the HOMO level lies in the range of the Au-S bonding at the contact. The HOMO level of the annulene ring lies above the energy range of the Au-S bonding. The result of this is that in benzene,  $\sigma$  orbitals are involved in the frontier orbital, whereas for the annulene system the frontier orbital is the  $\pi$  orbital, preserving the quantum interference effect.



**Figure 9:** The local density of states (LDOS) for the (1,7) annulene system. (a) Top view in the energy range  $-1.0 - 0.2$  eV (HOMO resonance). (b) side view. (c) Top view in the energy range  $-0.2 - 0.2$  eV<sup>34</sup>

## 4 Binary logic functions in single molecules

The applications of QI goes further than just transistors. By careful design of molecular structure quantum interference effects can be exploited to make single molecules perform binary logic functions, such as

NOR, AND, XOR operations or even more complex digital circuits can be made such as half adders. When traditional CMOS electronics are used the fabrication of one NOR gate requires already 4 transistors and to make a half-adder one would need a XOR and an AND gate. This means that by making a logic circuit in one molecule the size can be further reduced. By investigating single molecule logic gates the size limit of calculating devices can be explored.

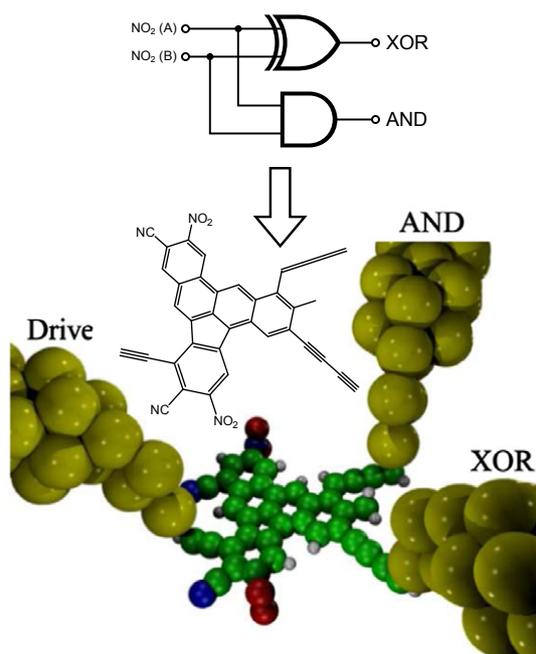
A ‘classical’ approach has been presented earlier.<sup>35,36</sup> These systems are based on donor-acceptor rectifying moieties covalently connected by Tour wires<sup>37</sup> to form logic AND or XOR gates. However, these molecules are bulky and overly complex which makes it impossible to measure any current through the device since this will decrease exponentially as a function of the distance.

A design of a half-adder binary device is shown in Figure 10.<sup>38</sup> The operation of this device depends on quantum interference effect occurring depending on the orientation of two NO<sub>2</sub> input groups. The calculating molecule has a large conjugated system giving a small HOMO-LUMO gap to give a large current when a driving current is passed through. Small wires of butadiyne and butatriene are added to separate the calculating MOs from the large *s* orbitals of the gold electrodes and prevent tunnelling between electrodes.

The nitro groups can now influence the position of nodes in the molecular orbitals. The output is now defined as the resistance from the drive electrode and the output, a large resistance corresponds to ‘0’ and a small resistance corresponds to ‘1’.

The input is given by the NO<sub>2</sub> groups, in

parallel orientation the input of the groups is defined as ‘1’ where the perpendicular to the molecule plane orientation is defined as ‘0’ input. The calculations is then done by only five molecular orbitals, and the orientations of NO<sub>2</sub> groups will introduce or remove destructive interference features.



**Figure 10:** Molecular structure and artist impression of a molecular half adder whose operation depends on quantum interference effects.<sup>38</sup>

Although this system provides an interesting display of the possibilities of using quantum interference effects in molecular electronics, this theoretical system is very far from practical realization. Assuming synthesis of the molecule is no obstacle, the attaching of three electrodes on a single molecule and keeping it stable is very challenging at least, so far only two electrodes have been attached to molecules. The manipulation of the NO<sub>2</sub> groups is suggested to be done by STM tips. Although the manipulation of chemical groups can be done

by STM,<sup>39</sup> however it has only been done on surfaces with large chemical groups. For this half adder to work one would need to have two STM tips manipulating the small NO<sub>2</sub> groups - in close proximity to three gold electrodes.

## 5 Molecular spintronics

So far only neutral closed shell molecules were considered. The application of QI can be expanded by including radicals. Since radicals have a net spin they allow molecular electronics to be used in spintronics. In contrast to regular electronics in spintronics the information is carried by the spin of the electrons, and not its charge. There are several advantages to spintronics. The spin can interact differently with magnetic materials, spin information storage can be non-volatile and can be written using low energies.<sup>40</sup>

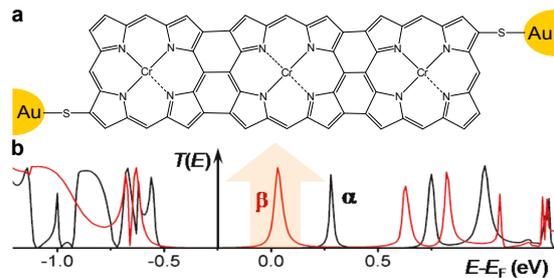
Molecular spintronics combines the fields of molecular electronics and spintronics. Organic molecules are especially suitable for spintronics because of the low spin-orbit coupling making long spin coherence times and lengths possible.

An efficient spin filter requires the transmission for both spin species to be considerably different over a broad energy range around  $E_F$  to give experimentally observable spin filtering. This means we are looking for dips or peaks in the transmission curve for one spin type, and as we have seen these features can be caused by destructive quantum interference. Calculations on organic radicals have indeed shown to have dips or peaks in their transmission curves, depending on spin, meta/para configuration and substituents.<sup>41</sup> In actual de-

vices these types of molecules can act as bridges controlling electronic coupling between components for electrons with different spin.

In ‘classical’ molecular spintronics (no QI effects considered) the molecules of interest are single molecule magnets. These molecules are usually a organometallic complex where the metal center has a net spin.<sup>42–44</sup> These structures have been proposed to be used in spin valves or spin transistors.

Now, the introduction of quantum interference effects allows the fabrication of molecular spintronics components. An example of this is chromium porphyrin array (Figure 11a).<sup>45</sup> This array of porphyrines moieties forms a large extended  $\pi$  system giving the molecule a very small bandgap and therefore a large conductance is expected. The electrons can take multiple pathways and destructive interference effects will occur for both spin polarizations without the metal centres.

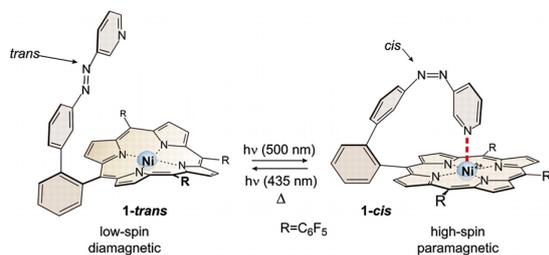


**Figure 11:** Chromium porphyrin array acting as a spin filter. **a** The structure of the chromium porphyrin array connected to gold electrodes. **b** Spin-dependent transmission curves.

The spin filtering properties of the system are investigated by theoretical methods. It was found that there is a bandgap of 0.30 eV for the major spin, and zero band gap for minor spin electrons. This results in sep-

arated peaks in the transmission curve for both spin species (Figure 11b). By applying an infinitesimal small voltage the spin peak near the Fermi energy can be used to give a spin-filtering effect.

The spin dependent transport depends on the asymmetry of the electronics structure caused by the paramagnetic ion in the porphyrins. It has been shown that the magnetic state of metal ions in porphyrins can be switched by photo isomerization of azopyridine. The conformational changes allows another nitrogen atom to coordinate with the nickel centre switching it to a high spin paramagnetic state<sup>46</sup> (Figure 12). With this idea combined with the spin filter array a photoswitchable spin filter can be realized.



**Figure 12:** A magnetic bistable photoswitchable porphyrin complex.<sup>46</sup> The switching to and from a paramagnetic state can be used in molecular spintronics.

## 6 Conclusions and prospects

In this paper quantum interference effects have shown to be of great importance in molecular electronics, from the most simple systems as wires up to more complex electronics such as rectifiers, transistors and logic gates and even in molecular spintronics. The first steps towards the realization of fully organic electronics have been made

by the successful demonstration of quantum interference effects in conjugated wires. There are still obstacles to be overcome, but the field over molecular electronics is moving ahead a fast pace. Recently, a method called ‘chemical soldering’ was presented to overcome to the problem of connecting individual components.<sup>47</sup> In this process a STM tip is used to stimulate a chain polymerization, forming a conjugated wire to connect all components.

Although it has been shown that this method can indeed be used to connect individual molecules with a conjugated wire, the method is not suitable to be scaled to rapidly make a large amount of defect free connections, as would be required to make molecular electronics which can compete with traditional methods. Another possible method to connect components would be using the unique self-recognition property of DNA. This property allows DNA molecules to find each other in solution based on their sequence. Components like transistors and wires can be synthesized and then connected through a DNA molecule with a carefully chosen sequence. When these components are brought together in solution the hybridization of DNA will ensure the electronic circuit is put together as designed. The last step would be to connect the components covalently through a chemical reaction forming the desired conjugation pattern between components.

The large scale of possibilities in molecular electronics allow it to revolutionize electronics and approach the fundamental size limit. Quantum interference effects can help achieve this goal by giving a direct relation between the structure of the molecule

and the electronic coupling of components in a molecular electronics device.

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