Electron Transport Properties in Molecule Transistors

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Abstract In this paper, we have discussed transistors made from single molecules in which one silver ion is connected to gold electrodes by organic barriers. By tuning the length of the organic barrier we are able to control the coupling between the ion and the electrodes. For relatively long linker molecules, giving weak coupling, the molecule functions as a quantum dot. This work shows that the properties of a molecular transistor can be controlled by the physical properties of the molecule .The ability to design the electronic states of a molecular device using (SIESTA and Smeagol), together with the ability to measure individual molecules, will play an important role in molecular electronics and in the physics of nanometer-scale systems. This paper is also to study electron transport in nanoscale objects, especially the devices made from single molecules. We show that the qualitative features of this interference effect arecaptured by the Smeagol COD described above through an appropriate choice of parameters. Finally, we note that quantum interference in such multibranch structures leads tothe appearance of large, internal countercurrents, which exceedthe external current carried by the electrodes, these calculations presented in this work were processing in Centre for Nanoscale Dynamics and Mathematical Modeling in the Lancaster universe uk .

1. Introduction

The field of molecular electronics[1] is a rapidly expanding research area ,which bridges the gap between physics and chemistry. Recently there has been much interest in developing strategies to control the current through a single molecule.[2,3]Of the various effects that can be exploited, quantum interferenceis expected to play a fundamental role in long phase coherent molecules, [4] where multiple reflections can occur, and in molecules made of rings, where electrons can follow multiple paths between the electrodes.[5,6] The modification of the electronic properties of such systems has application such as the quantum interference effect transistor (QuIET) [7] and can potentially be used for implementing data storage,[8] information processing, [9] and the development of molecular switches[10].

In this paper, we study quantum interference effects in molecules between metallic leads *ab initio* simulations.We calculation the electrical conductance of molecular structures of electron transmission through an oligoyne molecular wire connecting gold electrodes. We also present results of an*ab initio* numerical simulation on an electrostatically gatedbenzene-1,2-dithiolate (BDT) molecule, attached to gold electrodes, which is an example of a QuIET. In this calculation, gating is achieved through the presence of a Nitrogen ion, which induces quantum interference as the position of the ion and the molecular orientation are varied. We show that the qualitative features of this interference effect are captured by the Smeagol COD described above throughan appropriate choice of parameters. Finally, we note that quantum interference in such multibranch structures leads tothe appearance of large, internal countercurrents, which exceedthe external current carried by the electrodes.

2 -Smeagol

We set out to develop Smeagol [14-15], a computer software which uses DFT-NEGF to accurately predict the electronic transport properties of molecular devices [16], heterostructures and tunnelling junctions [17-18] to name but a few. In many cases we are interested in the magneto transport properties, therefore one must also be able to treat spin-polarised systems satisfactorily. This is also one of the main goals of Smeagol. One of its features is the calculation of the surface Green function using a semi-analytic approach and the solution of the problem While SIESTA provides the Kohn-Sham Hamiltonian, Smeagol has been made to interface with it and to calculate the non-equilibrium charge density of an open system via Green's function.

3- Results and Discussion

a calculation based on the ab initio transport code, SMEAGOL. This code uses a combination of density functional theory (DFT) [19] and the nonequilibrium Green's function (NEGF)Formalism [20] to calculate the transport characteristics of atomic scale devices. The DFT Hamiltonian is obtained from the SIESTA code[21] and is used by SMEAGOL to calculate the electronic density and the transmission. Within the NEGF,the system is divided into three parts: the left lead, the rightlead, and the extended molecule (EM). The EM contains the molecule plus some layers of gold, whose electronic structure. is modified due to the presence of the molecule and the surfaces, and differs from the bulk electronic structure. The molecular structure consists of oligoynes capped with phenylrings and attached to the electrodes by thiolate groups. TheSMEAGOL results, shown in Fig(E), clearly possess a critical energy, Ec≈ 0.5 eV, at which all curves (at least for the longerchains) intersect.

We now turn to the quantum interference effect transistor (QuIET) discussed in Ref[7], reproduces the key features of a QuIET, we compare it withthe results of a detailed simulation using SMEAGOL[20] .The atomic arrangements for the SIESTA/SMEAGOL calculationsare shown in Fig. A,B,C,D. The first arrangement (A,B,D) corresponds to the point charge located along a line perpendicular to the plane of the molecule, which passes through the molecule's center. In this configuration, the point charge produces a symmetric voltage which affects the two branches to the same extent. The second arrangement (C)corresponds to the point charge located in the plane of themolecule, closer to one branch of the BDT. In this case, the two branches are subject to different electrostatic potentials, which induces quantum interference in the electron transmission through the molecule. Both configurations are simulated usinga point charge of either Nitrogen (N) , giving a total of four cases. N are alkali and alkaline-earth atoms, with one- and two-valence electrons in the last shell, respectively. Due to their high electropositivity, The atomslose their valence electrons when they are inserted in the unit. The complete removal of the valence electrons from these atoms can be ensured by reducing the cutoff radii of their orbitals to 3.5 bohr, which confine the electrons inthe atom more closely and therefore increase their energy, making sure they move to lower energy states in the extended molecule. The basis sets used in the simulationwere single zeta(SZ) for the point charge and double-zeta polarized (DZP) forall other elements. The exchange and correlation potential was calculated with the generalized gradient approximation (GGA)and the Perdew-Burke-Ernzerh of parametrization[22] .The gold leads were grown along the (111) direction, and each side of the extended molecule had three and eight layers, respectively, with 9 atoms (9×8 atoms) per layer. The molecule wascontacted in a hollow configuration to three additional gold atoms on each side. The results are shown in Figs A,B,C and D.

We observe that when the charge moves toward themolecule, the peaks shift in energy in the negative direction due to the

positive potential. However, the effect is different depending on where the charge is located relative to the ring. This supports the observation of the previously suggested QuIET. The essential features of the ab initio simulations, we now show how this calculated can be employed to examine the internal currents within different branches of the molecule clearly demonstrate that the current in a single branch can greatly exceed the total current through the molecule when a countercurrent of opposite sign occurs in the other branch of the molecule and can clearly exceed the upper bound of ITOT = I1 + I2 = T (E) show fig(1). The appearance of such unbounded counter currentsis yet another manifestation of quantum interference within single molecules[22].

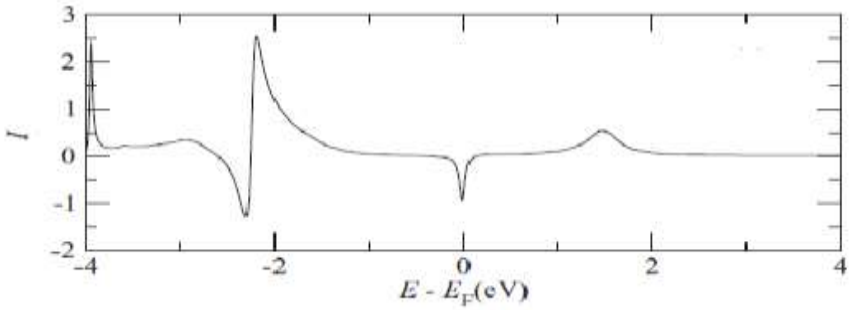


FIG. (1): Total current through the molecule

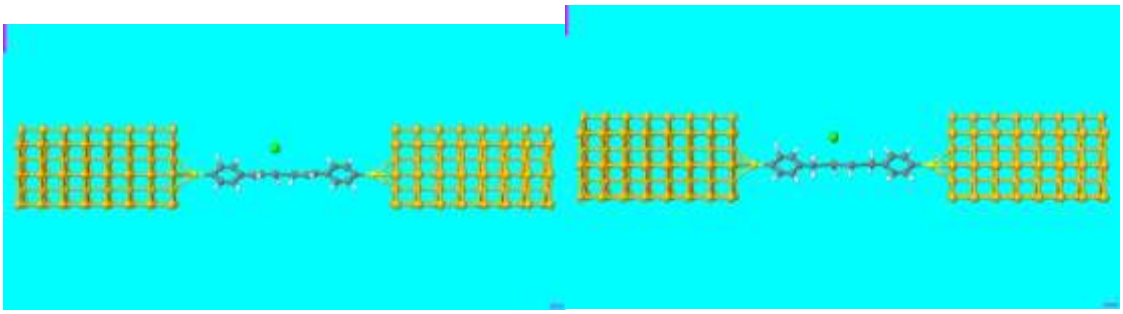
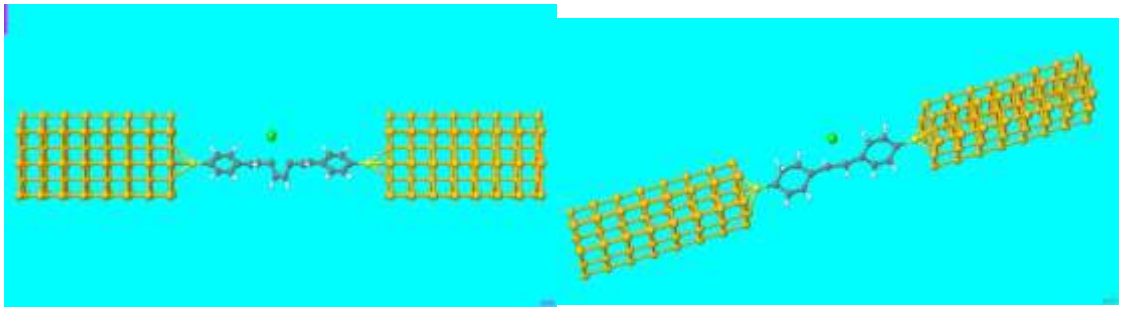


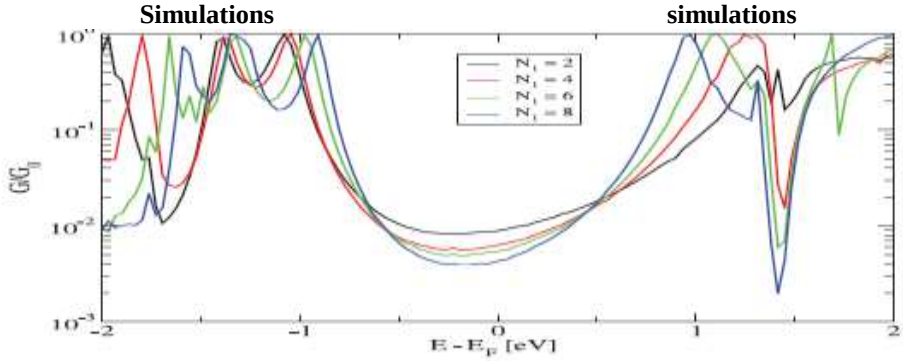
Fig (A)Molecular structure used in the transport Simulations

fig(B))Molecular structure used in the transport simulations



Fig(C)Molecular structure usein the transport Simulations

fig(D) Molecular structure used in the transport simulations



Fig(E) Transmission curvesfrom the SMEAGOL Simulations

4. Conclusions

Ab initio simulations, based on density functional theory, demonstrate the presence of quantum interference in BDT, due to electrostatic interactions associated with a scanning point charge positioned close to the molecule. We have shown that a scanning charge located within the plane of a BDT molecule produces a sizable quantum interference, whereas charge approaching the molecule along a line perpendicular to the plane produces a much smaller effect, in agreement with the analytical. In spite of the consistency between the tight-binding result and the ab initio result for the BDT system, there are, of course, quantitative differences between them. In part this arises because the tight-binding model includes only a single ("π") orbital per atom, whereas the abinitio description includes both π transport and σ tunneling .In addition, the tight-binding model includes only a single scattering channel in each lead, whereas the ab initio model contains multiple channels.

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