IBM Research Report

Understanding the Molecular Transistor

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Abstract

The molecular transistor is treated as an FET and electrostatic screening length, mechanisms of current modulation, and space charge contribution due to the current flow are evaluated semi-quantitatively, in order to compare the potential of the molecular transistor, as a logic element, with more familiar semiconductor-based field-effect transistors. It will be shown that a single resonant level is inadequate for achieving a large on-off ratio concomitant with high performance, leading to the concept of using molecules to design an electronic filter.

1. Introduction

The molecular transistor (MT) holds out the prospect of being the smallest, and perhaps also the fastest logic device, capable of pushing densities, if power permits [1], well beyond those of present day, or even future CMOS. Are not molecules the smallest, organized, unit of condensed matter? By extension are not molecular transistors the smallest possible transistor? The possibility of making transistors, computational circuits, or even entire systems from molecular building blocks is tantalizing, and is predicated on the fact that complex molecular structures can be assembled, tinker-toy-like, from basic molecular units, where the position of each unit is determined with 'digital' precision, dictated by the chemical bonding. This is the promise of molecular electronics [2,3]. This is, however, a very difficult technological challenge which, as yet, has not met with success.

Now many of the proponents of the MT [3-6] say that maybe a three-terminal switch is the wrong element to make, maybe computation can be done with, non-linear, two terminal elements. This seems to be a very difficult and rather far-fetched position. It is very difficult to carry such schemes beyond very few levels of logic (~2) without the need for amplification and isolation i.e. good switches. This paper will therefore concern itself with the switching properties of individual molecular transistors and how they compare with more conventional FET switches.

A by no means obvious question is what the size of the molecular transistor should be to attain useful device characteristics. Like conventional transistors, the on-off switching ratio of a molecular FET is a function of its size [7], and this is an important topic of consideration. The size of a 'molecule' is arbitrary, since chemical bonding, as in polymers, may extend to any scale, within certain thermodynamic requirements, so that the

question to be addressed is how does the quality of the molecular switch depend on the size of the molecule and what is the minimum acceptable size.

2. Simple Model for the Molecular Transistor

Attempts to understand conduction in molecules by numerical modeling techniques have been undertaken in the past to interpret STM measurements [8], but recently this work has focused on molecular devices. Two approaches to modeling of molecular conduction, and the MT are exemplified by the Lang-Avouris approach [9-14] and that of the Datta group [14-18] (This list is by no means comprehensive.). Overall the Datta group takes a more 'electrical engineering' approach, and is the inspiration for our present model, however many elements of our approach are reminiscent of the early Lang [8] paper.

   Our motivation, in creating a simple transistor model, in contrast to the much more sophisticated approaches in [9-17], is to test whether tried and true concepts used to analyze micro-scale and nano-scale FETs can be extended into the molecular domain. If so, this model will give us insight into which parameters are important, and which constraints must be obeyed in making useful MTs. At this point our model is untested, but future tests against numerical models are anticipated.

   In our model we assume that the MT has the following characteristics:
1. The molecule can be represented by a spectrum of internal states which, apart from a rigid shift, is independent of the terminal voltages or currents. This spectrum is derived from the states of the free molecule and modifications caused by the contacts.
2. The model is assumed to be symmetric i.e. equal coupling of the states to the source and drain electrodes.
3. The state spectrum is fixed relative to the electrostatic potential in the central region of the molecule and therefore can be shifted by the electrode potentials.
4. The electrochemical potentials are represented by the source and drain Fermi levels (ballistic transport).
5. State occupancy is unity above (consistent with our use below of positive potentials for negative electron energies) the more positive Fermi level, zero below the more negative Fermi level and half in-between (zero temperature approximation).
6. The total charge in the filled states is equal to the number of electrons in the molecular orbitals represented by the states.
7. The internal charge increases the electrostatic potential by its value divided by the capacitance between the central region and the outer electrodes
8. Any rearrangement of charge (polarization) in states not participating in the transport can be represented as a fixed dielectric permittivity.

Our model is predicated on the second-order Stark effect, where an approximately parabolic potential is developed between the center of the molecule and the edges, which are at the potential of the contacts. Under these conditions this becomes first order in the gate voltage.

Now none of these assumptions is strictly true, as is evident from close examination of references [9-18]. For instance, Lang [14] shows that when a strong first-order Stark effect exists the state spectrum is significantly altered by the gate field. Our assumption of symmetry is arbitrary, and departures from symmetry will modify the occupancy of the states between Fermi-levels [16,18]. Our model assumes a lack of screening caused by the free electrons, yet this is clearly important in long molecules [11,18]. Also, the spatial distribution of the charge in a given orbital is complex, and can be very different for different orbitals, giving different degrees of coupling to the gate. Our model ignores these effects so it should be regarded merely as a first-order approach toward understanding the MT which, we believe, preserves enough of the essential character of molecular conduction to be useful. Like transistor design, to the extent that these 'non-idealities' such as lack of symmetry, both physical and electrostatic, excessive charge sharing with the contacts etc. are detrimental to the performance of the transistor they can perhaps be engineered away, by designing a suitable molecule.

Our model is described in Fig. 1, where the molecular levels can be translated in potential by the gate voltage with respect to the Fermi levels, V_N and V_P, at the contacts. Each state is occupied by two electrons when full, and the peak conductivity of each state (assuming a symmetric configuration) being the quantum of conductance [19], $g_0 = 2e^2/h$. The width of each state represents the degree of coupling to the reservoirs. The states form a density spectrum, $\rho(V)$ and a conductivity spectrum $g(V)$. We choose to represent the state density as a summation of Lorentzian lineshapes, and the conductivity spectrum as the summation of the respective conductivities, such that

$$\rho = \frac{1}{n}\sum_k \mathbf{L}(V - V_C - V_k, \Delta_k),$$
(1)

and

$$g = g_0 \frac{\pi}{2}\sum_k \Delta_k \mathbf{L}(V - V_C - V_k, \Delta_k),$$
(2)

where $\mathbf{L}$ is a Lorentzian of Δ_k full width half maximum, and peaked at potential V_k above the center potential, V_C, of the molecule, and n is the number of states participating in the transport.. This potential is a function of the potentials on the terminals of the molecule, and the internal space charge:

$$V_C = V_{C0} + (1-\eta)\frac{V_N + V_P}{2} + \eta V_G + \frac{Q_{SC}}{C_\Sigma},$$
(3)

where V_{C0} is the zero-bias offset (includes the intrinsic molecular energies and shifts, at zero bias, due to exchange of charge with electrodes), η the gate coupling factor, Q_{sc} is the space-charge caused by the current flow, C_Σ is the capacitance from the center of the molecule to all of the electrodes and V_{sc} is the change in potential caused by the

space-charge potential. In this treatment the potential, V, is the negative of the electron energy in electron volts, so that the potentials are the same sign as ordinary voltages. While in general η and C_Σ may vary with the terminal voltages, they are assumed to be constants in our model.

With these assumptions the terminal characteristics of the MT are easily derived. Care must be taken in designating the FET as P-type or N-type, and therefore these electrodes as the source or drain, since the FET may behave at times like a P-FET and at others like an N-FET, so they are simply called N or P for 'more negative' or 'more positive' respectively. Assuming a low temperature approximation, the current through the FET is the integral of the conductance spectrum between the Fermi levels,

$$I_{NP} = \int_{V_N - V_C}^{V_P - V_C} g(u)du, \qquad (4)$$

where the substitution, $u = V - V_C$, removes the V_C dependent terms to the boundaries of the integral. Similarly, the internal space charge, Q_{sc}, is found by integrating the state density assuming an occupancy of 1/2 between the Fermi-levels and an occupancy of 1 above V_P, consistent with our convention for the potentials:,

$$Q_{SC} = -2en\left[\frac{1}{2}\int_{V_N - V_C}^{V_P - V_C} \rho(u)du + \int_{V_P - V_C}^{\infty} \rho(u)du\right], \qquad (5)$$

counting two electrons per state. The transconductance, g_m, is found by differentiating the boundaries of (4) with respect to V_G, making use of (3) and (5):

$$g_m = \frac{-\eta(g_P - g_N)}{1 + \dfrac{en}{C_\Sigma}(\rho_P - \rho_N)}, \qquad (6)$$

where the shorthand , $g_P \equiv g(V_P - V_C)$, etc. is used. Therefore, for our low temperature approximation, the transconductance depends on the conductance-state density at the 'N' and 'P' Fermi levels. In a similar manner, the output conductance, $g_{0P} = \partial I_{NP}/\partial V_P$, is

$$g_{0P} = \frac{g_P(1+\eta) + g_N(1-\eta) + \dfrac{en}{C_\Sigma}(g_P\rho_N + g_N\rho_P)}{2\left[1 + \dfrac{2en}{C_\Sigma}(\rho_P + \rho_N)\right]}. \qquad (7)$$

The voltage gain is, $A_N = g_m/g_{oP}$, where 'N' is the common electrode (e.g. for an FET when the input is applied to the gate, the output measured on the drain and the source is common).

The intrinsic speed of the MT may be evaluated from the differential charge to current ratio, at constant $V_P - V_C$:

$$\tau_N = -\frac{\partial Q_{sc}}{\partial I_{PN}} = -\frac{en(\rho_p + \rho_N)}{(g_P - g_N)}. \tag{8}$$

The above equations are for the common 'N' case, the equivalent common 'P' equations can be deduced by symmetry.

We see from the above equations that the small-signal (differential) properties of the MT such as gain, transconductance and output conductance are governed by the state densities, g and ρ, at the Fermi levels, V_N and V_P. A positive/negative transconductance indicates N-FET/ P-FET like behavior, e.g. for an N-FET, $g_N > g_P$. Small signal properties are consistent with the transistor type. One can see from (7), for instance, that for a closely coupled gate $(\eta \to 1)$ the voltage gain in common 'N' mode approaches $\eta/(1-\eta)$ for a pure N-FET (g_P, $\rho_P = 0$), and unity for a pure P-FET consistent with common source and common drain modes of operation respectively. Transistor characteristics are shown for a single Lorentzian spectrum, in Fig. 2a and b, where space-charge effects have been included in Fig. 2b only. Note that the transistor changes smoothly from N-FET to P-FET like behavior as the gate voltage is increased from -1 to 1. The maximum conductance, at $V_P = 0$, is g_0. The FET does not turn off very sharply because of the long tails of the Lorentzian distribution.

Inclusion of acceptor-like space charge (system is neutral when states are empty), with a maximum space-charge voltage, $V_{sc0}=2e/C_\Sigma$, of 1, is shown in Fig. 2b (Adding an electron is equivalent to 'reduction' in chemical parlance.). The space charge does not change the drain current or output conductance markedly, but greatly reduces the transconductance of the FET. For the single Lorentzian the importance of the space-charge is given by the ratio of the space-charge voltage to the width of the distribution, V_{sc0}/Δ. For instance, modeling C_Σ as a 0.5nm radius sphere inside a 1nm radius envelope, and a medium with relative permittivity of 4 gives Vsc0=0.7V.

The permittivity used depends on the polarizability of the molecule i.e. the extent that the charge inside the molecule can rearrange itself to minimize the total potential energy. Determination of this important quantity, for a molecule between contacts, is the subject of ongoing investigations [11,13,17,18]. We note that for the MT space charge effects can be very important. This is in contrast to the results of two-terminal simulations where, in some cases, negligible space charge was found [12]. By applying our model to analyze the space-charge we find

$$\frac{\partial V_{sc}}{\partial V_P} = \frac{en}{C_\Sigma} \frac{[(\rho_P - \rho_N) + \eta(\rho_P + \rho_N)]}{2\left[1 + \frac{en}{C_\Sigma}(\rho_P + \rho_N)\right]}, \tag{9}$$

and we see that the space-charge contribution vanishes for a symmetric distribution and for no gate coupling!

The intrinsic delay, for a single Lorentzian, from (8), is just $2\eta/e\Delta$, which is very small, 1.2 fs for $\Delta = 1$V. The time constant, $C_\Sigma/g_0 = h/ eV_{sc0}$, which is larger than the intrinsic delay by Δ/V_{sc0}. This time constant does not directly control the speed of the MT because the quantum capacitance of the molecule (density of states) acts to reduce the effective gate capacitance. Nevertheless, reducing space charge effects does come at the expense of

increased delay, but these delays are so small that it is still worthwhile to increase C_Σ in order to increase transconductance toward its limit of g_0. A much larger penalty is paid by the parasitic (fringing) capacitance between the gate and the other electrodes which depends critically on the transistor design, and an even larger effect is due to wiring capacitance. For instance a 1μm long wire, corresponding to a medium length interconnect, having a capacitance, $C_w = 0.1fF$, will result in a charging time, $Cw/g_0 = 1ps$.

A more detailed examination of the turnoff characteristics of the MT, for a single Lorentzian at finite temperature, is shown in Fig. 3, where the 'Q' factor is $2\ kT/e\Delta$. This characteristic is just the convolution of the Lorentzian with the Fermi distribution. It is seen that an exponential falloff over several decades, characteristic of conventional transistors, is possible only for very narrow resonances, such as were simulated for the alkali-halide molecule [14], however; such narrow peaks (small Δ) would result in very low currents and slow speeds. Thus the single Lorentzian line shape is not very useful for applications involving large scale integration of MTs.

3. Modulation Methods

The difficulty of placing the gate close enough, and the unsatisfactory turn-off characteristics for the direct field-modulated transistor leads one to consider other modulation methods. Ghosh et al. [17] have argued that a transistor based on conformal change (reversible displacement of some internal element, see Fig. 4), can circum-vent conventional size limits by allowing the gate to be more distant for the same degree of discrimination of the modulation with respect to gate vs. drain voltages. This is because the displacement responds to the electric field, a vector, rather than to a scalar potential. While this argument has merit, the geometry of the transistor has to be considered carefully lest this advantage be lost. For instance, in the differential gating scheme of Fig. 5 the electric field, F, which causes the rotation is controlled by the difference in gate voltages, $V_{G1} - V_{G2}$, and only to second order by the source and drain potentials, V_S, V_D. This is important because the voltage gain of a transistor is given by the relative ratio of control of the current by gate and drain terminals respectively. Thus the differential approach, together with directionally sensitive modulation, should enable a thicker gate insulator to be used.

However, if the bottom gate were to be removed, F would be influenced equally by V_S and V_D, so that the discrimination against the drain voltage is almost as poor as for scalar modulation. It is not necessary though, to apply a true differential voltage to the gates, since the differential effect is still the same if one gate is grounded to the source and twice the voltage applied to the other. This approach is shown in Fig.5b, and was in fact used by Di Ventra *et al.* [12] in their simulations.

The problem of remote access to the gate may perhaps be solved using other techniques. A polarization-front may be propagated into the molecule using a molecular Quantum Cellular Automaton (QCA) [20], as shown in Fig. 6. Another method, by analogue with a bipolar transistor, might, for instance make contact to the HOMO (highest occupied molecular orbital) level via a metal contact of suitable work-function, but have the source and drain contact the LUMO (lowest unoccupied molecular orbital) level. This way the modulation path and the

current carrying path are separated in energy, so they need not be separated in space [22]. The recombination strength, between holes in the HOMO and electrons in the LUMO levels is obviously an issue here, which would have to be investigated further.

4. MT as an Electronic Filter

It was shown above that the transfer function of a simple molecular orbital, a Lorentzian, is unsuitable for large-scale circuit applications because of the poor on-off ratio achievable. In electronic circuit techniques a Lorentzian transfer curve (for power) is obtained by a simple *LC* tuned circuit. Such a simple filter is not very useful for achieving a large degree of discrimination, for instance, against nearby communication channels, yet have sufficient bandwidth for required information transfer. In practice more complex filters, or cascaded filters are used to achieve the required goal. An example of a 4th order Chebyshev filter is shown in Fig 7. Notice that with the addition of relatively few elements a much better transfer curve is obtained. The interesting question is whether molecular elements may be combined to form the analog of such a filter. If so the possibilities for molecular transistors may indeed be exciting.

A simple molecular example of a more complex structure is the multi-element biphenyldithiol chain of Rochefort *et al*., [10] where an on-off resonance conductance ratio of 10^8 was obtained.

While the community studying molecular charge transport is presently investigating simple molecules, the flexibility of synthetic chemistry enables more complex and functional molecular systems to be prepared. The fields of organic and organo-metallic chemistry are in the business of designing and synthesizing molecules with desired molecular structures and with a diverse range of properties. Molecular segments that act as single elements may be linked linearly or at other angles, branched into bigger structures, and may be separated by linkages that control the electronic coupling between segments. Examples in nature and in synthesis to tailor the energy levels of individual segments and link them to funnel charge and energy are the basis of energy harvesting systems and research [23]. Arranging molecular segments in series or in parallel to construct systems for molecular electronic devices that are analogs of electronic filters may be envisaged.

Referring to Fig. 2, would it be possible to exceed the logarithmic turn-off rate of eV_G/kT? If so one could realize large power savings in integrated circuits, since the circuits could be run at lower voltages, saving on the component of dynamic power used to charge and discharge capacitors. Such a possibility exists if one could design sharp cut-off filters in tandem, one controlled by the gate voltage and the other fixed. This way the current could be limited by the convolution of the transfer functions, the sharpness depending only on the quality of the filters.

5. Size

Some straight-forward limit may be placed on the transistor's size based on tunneling. As described by us [7], tunneling barriers between source and drain electrodes have to be of the order of 2.5-3nm, or more, for reasonably

low currents, with the gate separation of 1- 2nm, to ensure electrostatic integrity ($\eta \rightarrow 1$). Now these numbers are quite close to the scaling limits of a MOSFET, the main differences being that the larger S/D tunneling barriers, because of the larger bandgap, allowing a smaller S/D spacing for the MT, and a smaller dielectric constant of the organic material, allowing a larger gate separation

As discussed in section 3, other modulation methods might enable one to relax the requirement of gate proximity, allowing the smallest source-drain separations to be approached. On the other hand, end groups will be needed to ensure suitable quantum-mechanical coupling of the molecule to the contacts, while providing electrostatic de-coupling of the central, controlled, region from the contacts.

As we have learned in section 4, the simplest molecular transfer function is not very suitable, and eventually transistors comprising several molecular units might be needed to achieve broad pass-bands with sharp cut-offs. As we see in Fig. 6, the number need not be all that large, approximately four orbitals if each *'LC'* combination in Fig, 6 is represented by 1 orbital. It is possible to fit four benzene rings, including the end groups, into a approximately 3nm space, so that the minimum sized useful MT might indeed be about that size.

The minimum sized experimental silicon CMOS transistor has a ~6nm channel length, which is close to theoretical limits, but the overall size of the transistor is much larger, to allow for contacts and isolation, and to increase the current drive [24]. If the MT were handicapped by similar constraints, then the overall density advantage of the MT over silicon would not be so large, but perhaps the self assembly characteristic of molecules can be used here to advantage.

6. Conclusions

We have examined the electrostatics of the MT with the aid of a simple model. This model is very similar to, and presents many of the same design constraints as a conventional field effect transistor, and the role of space charge in reducing transconductance was elucidated. It was shown that the simple Lorentzian type of transfer function given by a single molecular orbital does not have suitable discrimination to achieve a good on-off ratio concomitant with high current carrying capability, and it was suggested that more complex transfer functions might be synthesized using several orbitals in the current path, by analogue to electronic filters.

7. Acknowledgments

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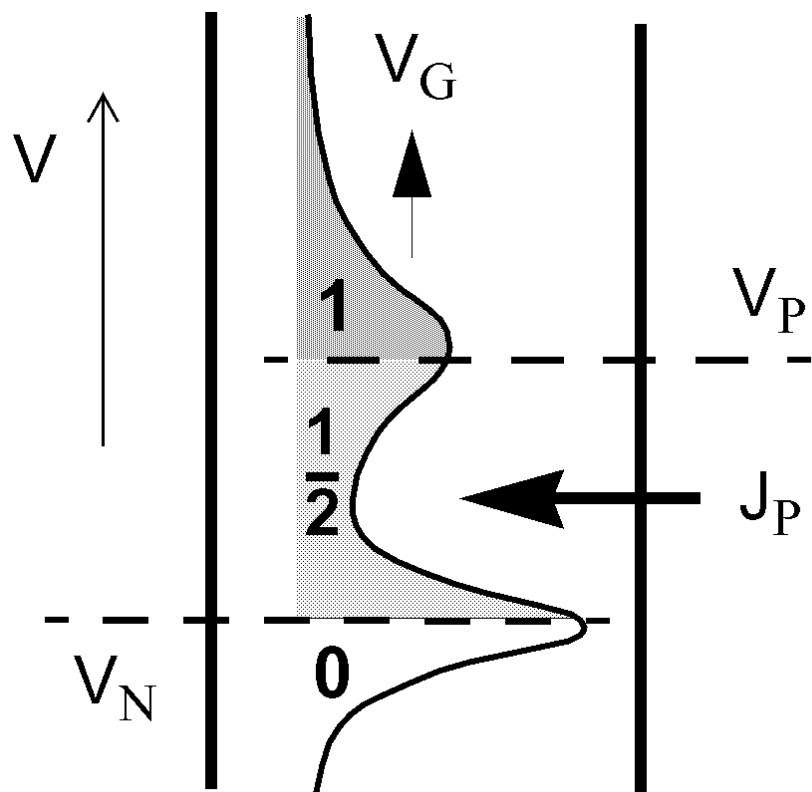
Figure Captions

Fig. 1. Schematic showing principle of operation of a molecular transistor showing the state density spectrum which can be shifting by the gate voltage. Shaded regions and numbers represent energy ranges of 1/2 and full electron occupancy. V = - electron energy (eV).
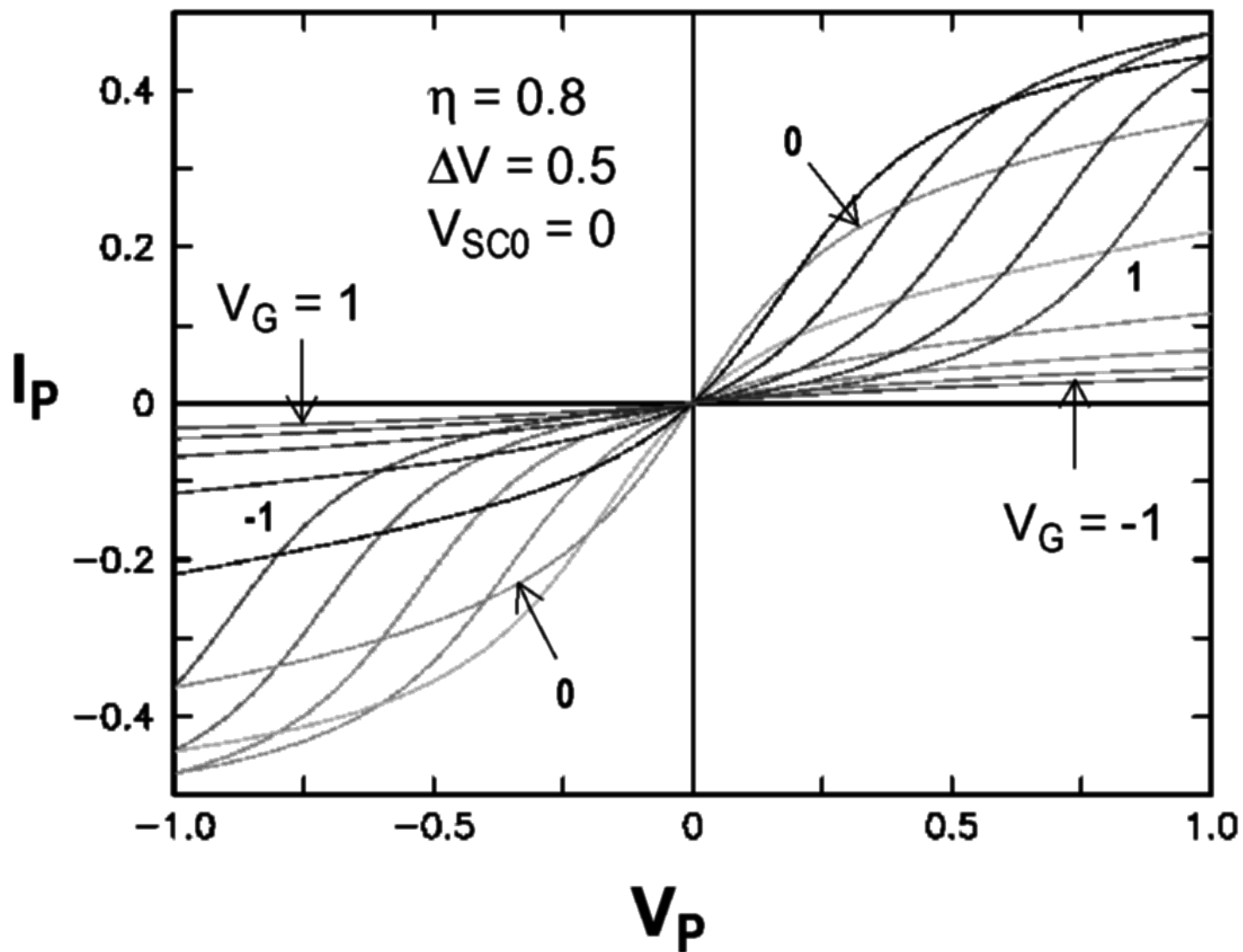
Fig. 2. IV characteristics generated by molecular transistor model having a single Lorentzian state density of width 0.5 and gate coupling factor of 0.8. In (a) there is no space charge contribution, and in (b) a maximum space charge of unity is present when the states are filled with electrons, and zero when empty (acceptor-like).
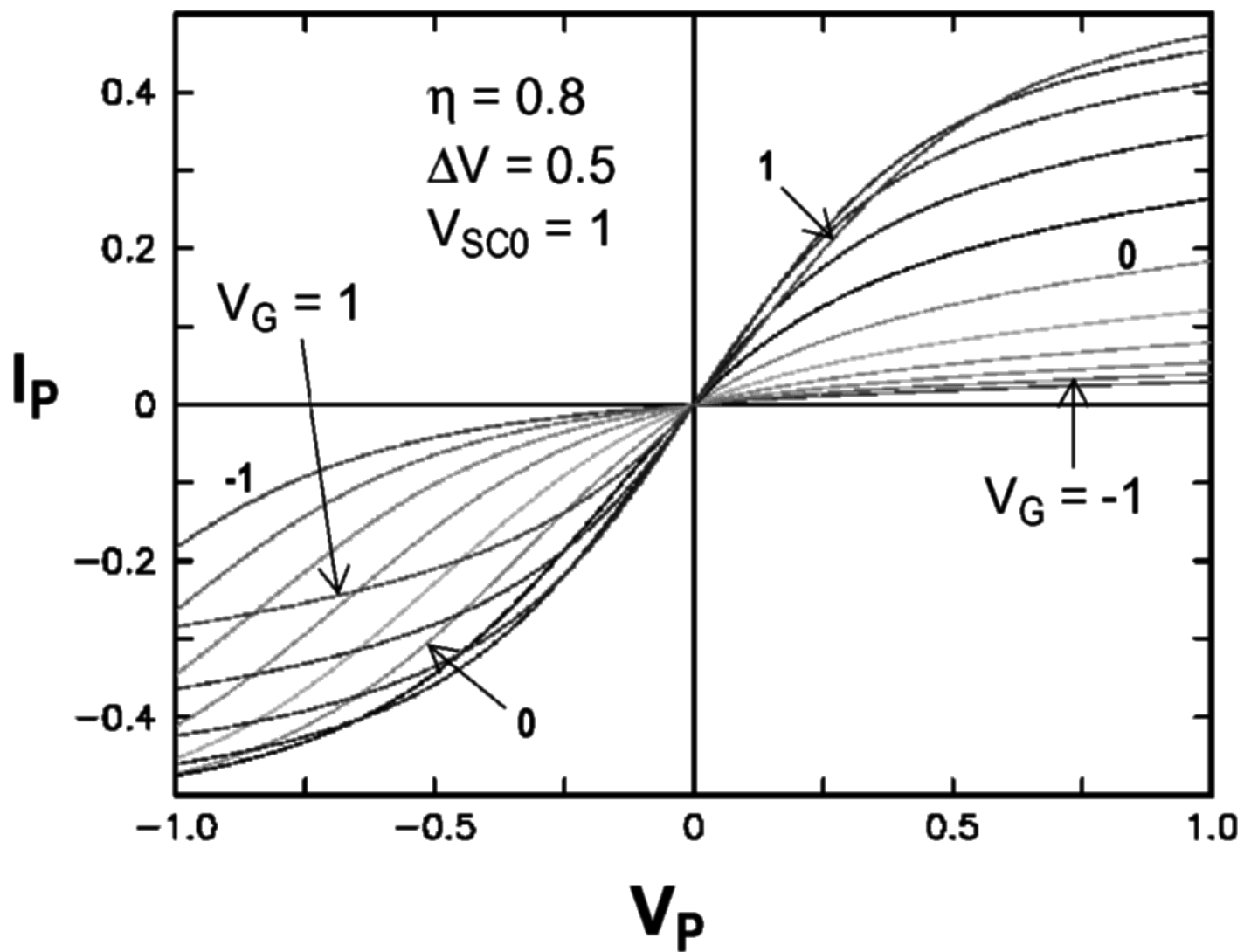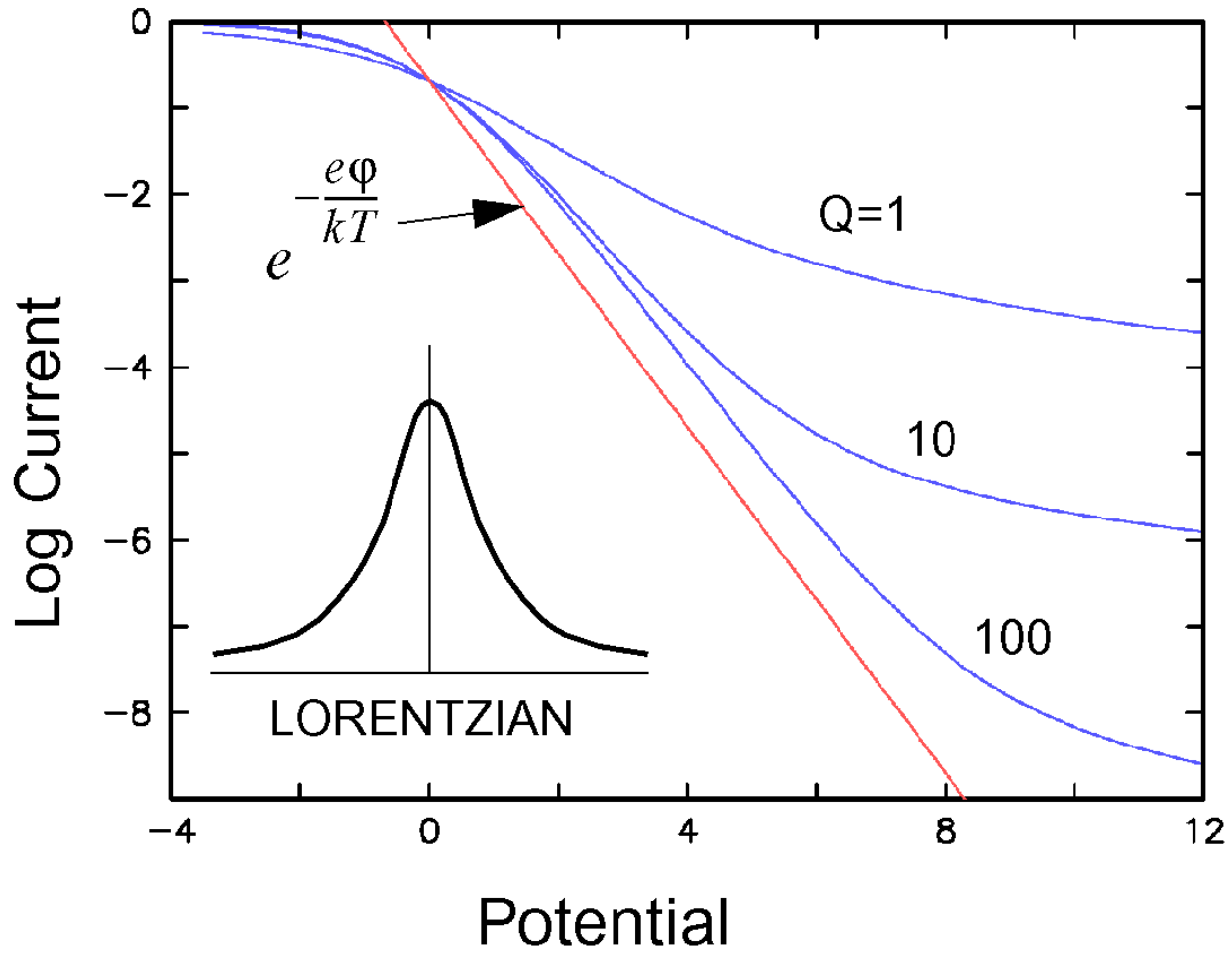
Fig. 3. Current vs. potential of Lorentzian vs. the Fermi level of the injecting electrode, where the Q factor corresponds to the half-width of the Lorentzian.

Fig. 4. Modulation of a current path by rotating a molecule into conjugation.

Fig. 5. Modulation by rotating a molecular element into conjugation with the contacts using a differential gating scheme scheme (a) and single-ended scheme (b). The plane of rotation is actually perpendicular to the current path, but is shown face on in the figure for clarity.

Fig. 6. Chain of QCA cells propagates polarization field into molecule.

Fig. 7. (a) Transfer function and (b) circuit for a 4th order Chebyshev band-pass filter. Courtesy of www-users.cs.york.ac.uk.

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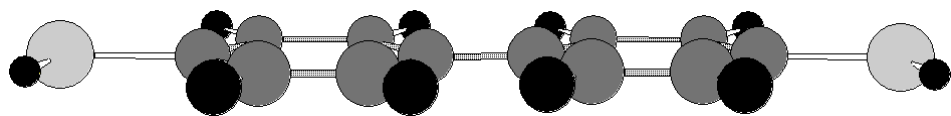Fig. 2b and in (b) a maximum space charge of unity is present when the states are filled with electrons, and zero when empty (acceptor-like).

Fig. 3. Current vs. potential of Lorentzian vs. the Fermi level of the injecting electrode, where the *Q* factor corresponds to the half-width of the Lorentzian.
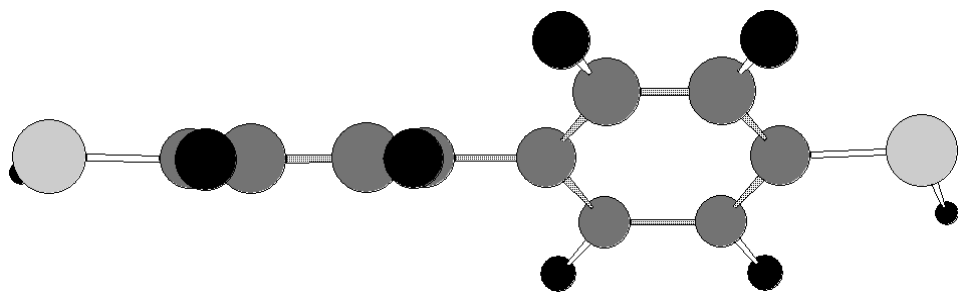
(a)

(b)

Fig. 4. Modulation of a current path by rotating a molecule into conjugation. (a) Minimum Energy of Biphenyl dithiol; rings canted at ~40° = "Off" state." (b) Rings in plane = "On" state.
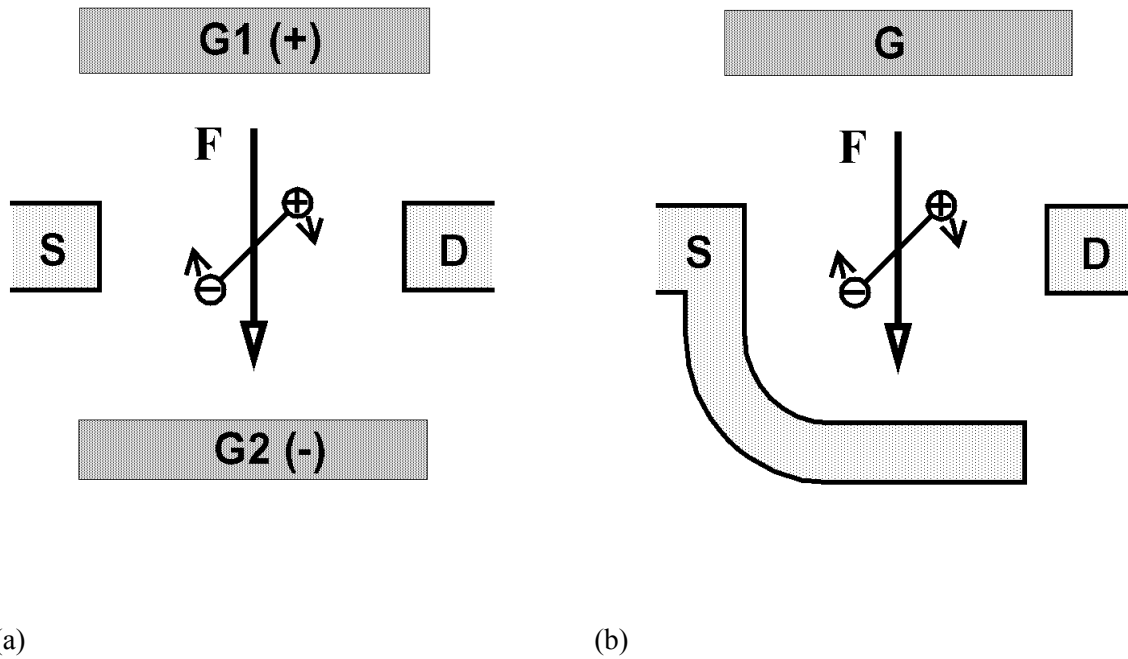
(a)   (b)

Fig. 5. Modulation by rotating a molecular element into conjugation with the contacts using a differential gating scheme (a) and single-ended scheme (b). The plane of rotation is actually perpendicular to the current path, but is shown face on in the figure for clarity.
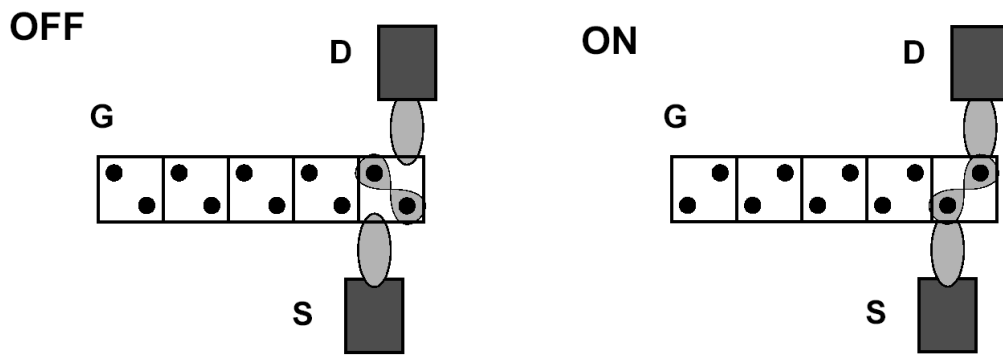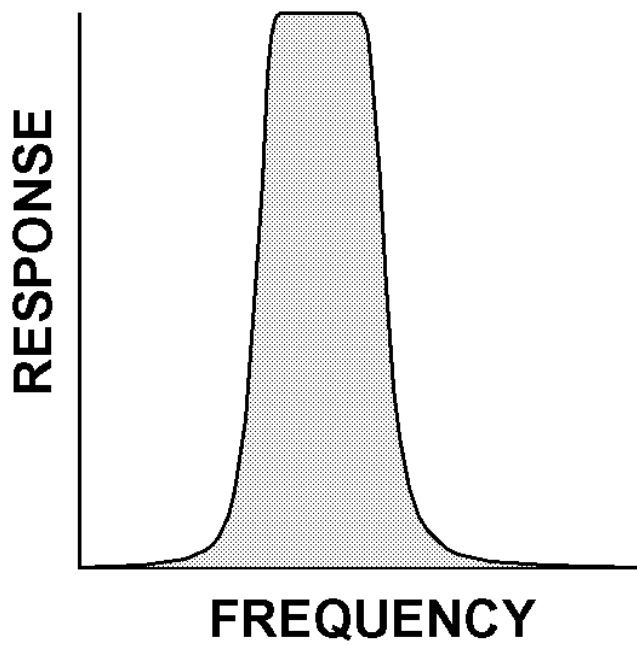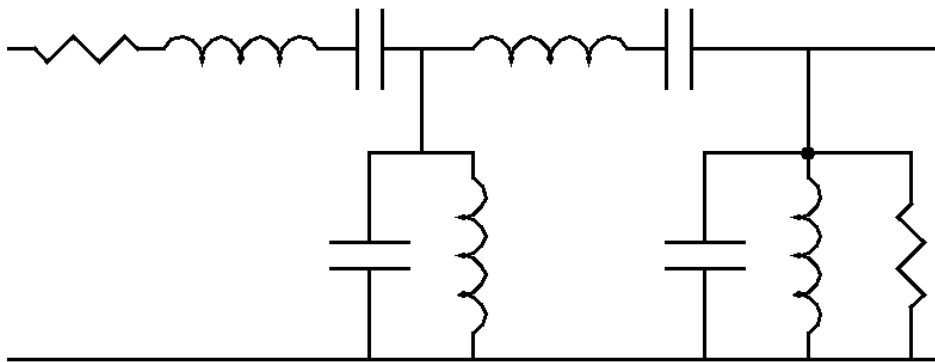
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(a)

(b)

Fig. 7. (a) Transfer function and (b) circuit for a 4th order Chebyshev band-pass filter. Courtesy of www-users.cs.york.ac.uk.