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Quantum-Effect Multi-Terminal
Molecular Electronic Devices
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Abstract – Departing from two-terminal molecular electronic devices (MEE devices), this paper examines multi-terminal MEE devices. These devices are envisioned to be utilized in emerging molecular gates (M-gates) and neuronal hypercels (N-hypercel) for expected molecular integrated circuits (MICs). In addition to molecular-centered processing and memories, MEE devices are of importance in molecular sensing and interfacing applications. We concentrate on the device-level analysis researching transitions and interactions which are due to quantum phenomena and effects exhibited by microscopic (molecular) systems. Our ultimate objective is to analyze the controlled electron transport, study the I–V characteristics, evaluate performance and assess device capabilities. Using three-dimensional Schrödinger and Poisson equations, we study the electron transport by numerically solving the above mentioned equations using the self-consistent conditions. The controlled electron transport, super-fast transitions (switching) and multiple-valued I–V characteristics in MEE devices are observed.

I. INTRODUCTION

One can examine the device physics and apply the basic laws obtaining the steady-state and dynamic characteristics. For various solid-state electronic devices, such as FETs, BJTs and other, this analysis is well-known and the deviations are straightforward [1]. Recently, two-terminal [2–7] and multi-terminal [5] devices have been introduced and studied.

Due to distinct device physics, effects exhibited and phenomena utilized, the foundations of semiconductor devices are not suitable and applicable to MEE devices [5]. For example,

1. Device physics of MEE devices is completely different;
2. Exhibited quantum effects may be utilized resulting in distinct device functionality (in microelectronic devices quantum effects and discrete impurities lead to degraded performance or loss of functionality);
3. Entirely different control, interfacing and fabrication.

In general, MEE devices must be examined using quantum mechanics. For example, the device functionality, capabilities and performance (energetics, electron velocity, transit time, I–V characteristics, etc.) can be found using the wave function \( \psi(t,r) \) which depends on three-dimensional potential as documented in this paper. Under the assumptions reported in [1, 8, 9], with the attempt to apply the well-developed concepts of microelectronics, alternative results in analysis of molecular devices, as scaled solid-state devices, are reported in [10].

For FETs, one may find the total charge in the channel \( Q \) and the transit time \( t \) which gives the time that it takes an electron to pass between source and drain. The drain-to-source current is \( I_{DS} = Q/t \). The electron velocity is \( v = -\mu E_x \), where \( \mu \) is the electron mobility; \( E_x \) is the electric field intensity. One also has \( v = \mu E_x \), where \( \mu \) is the hole mobility. At room temperature, for intrinsic silicon, \( \mu \) and \( \mu_p \) reach ~1400 cm²/V·s and ~450 cm²/V·s. Mobilities \( \mu \) and \( \mu_p \) are functions of the field intensity, voltage, temperature and other quantities, therefore the effective \( \mu_{eff} \) and \( \mu_{eff} \) are used. Using the x component of the electric field, we have \( E_{ox} = -V_{DS}/L \) and \( L \) is the channel length. Thus, \( v = -\mu E_{ox} \), and \( t = L/V_{DS}/\mu_{eff} \).

The channel and the gate form a parallel capacitor with plates separated by an insulator (gate oxide). From \( Q = CV_e \), taking the note that the charge appears when the voltage between the gate and the channel \( V_{GC} \) exceeds the n-channel threshold voltage \( V_t \), one has \( Q = C(V_{GC} - V) \). Using the equation for a parallel-plate capacitors with length \( L \), width \( W \) and plate separation equal to the gate-oxide thickness \( T_{ox} \), the gate capacitance is \( C = \omega L \varepsilon_{ox}/T_{ox} \), where \( \varepsilon_{ox} \) is the gate-oxide dielectric permittivity, and for SiO₂, \( \varepsilon_{ox} \sim 3.9 \times 10^{-11} \) F/m.

These baseline equations in deriving the size-dependant quantities, such as current, capacitance, velocity, \( transit \) time and other quantities are well-known [1]. The analytic equations for the \( I–V \) characteristics for solid-state devices (FETs, BJTs and other) are straightforwardly obtained [1]. The expressions for the so-called Level 1 model of nFETs in the linear and saturation regions are

\[
I_D = \frac{\mu_n \varepsilon_p}{T_{ox}} \frac{W}{L} \left( V_{GS} - V_t \right) \left( 1 + \frac{1}{2} \frac{V_{DS}}{V_t} \right) \left( 1 + \frac{1}{2} \frac{V_{DS}}{V_t} \right)
\]

and

\[
I_D = \frac{\mu_n \varepsilon_p}{T_{ox}} \frac{W}{L} \left( V_{GS} - V_t \right) \left( 1 + \frac{1}{2} \frac{V_{DS}}{V_t} \right) \left( 1 + \frac{1}{2} \frac{V_{DS}}{V_t} \right)
\]

Here, \( I_D \) is the drain current, \( V_{GS} \) and \( V_{DS} \) are the gate source and drain source voltages; \( L \) and \( W \) are the channel length and width; \( L_{sd} \) is the gate-drain overlap; \( L_{sd} \) is the channel length modulation coefficient. For pFETs, one uses \( \mu_p \).

II. QUANTUM-WELL SEMICONDUCTOR DEVICES

Quantum-well resonant tunneling diodes and FETs, Schottky-gated resonant tunneling, heterojunction bipolar, resonant tunneling bipolar and other transistors have been introduced to enhance the microelectronic device performance. The tunneling barriers are formed using AlAs, AlGaAs, AlInAs, AlSb, GaAs, GaSb, GaAsSb, InAlAs, InP, InAs, InGaP and other composites and spacers with the thickness in the range from ~1 nm to tens of nm. The CMOS-technology high-speed double-heterojunction bipolar transistors ensure the cut-off frequency ~300 GHz, breakdown voltage ~5 V and current density ~1 × 10⁶ A/cm². The one-dimensional potential energy profile, shown in Figure 1, schematically depicts the first barrier (L₁L₂), the well region (L₂L₃) and the second barrier (L₃L₄) with the quasi-Fermi levels \( E_{F1}, E_{F2} \) and \( E_{F3} \). The device physics of these transistors is reported [1], and the electron transport in double-barrier single-quantum-well is straightforwardly examined by applying a self-consistent approach and numerically solving the one- or two-dimensional Schrödinger and Poisson equations.
III. MULTI-TERMINAL MOLECULAR ELECTRONIC DEVICES

Departing from planar solid-state microelectronic devices, the idea of multi-terminal ME devices has been extensively studied [2-5]. Various single-molecule two-terminal ME devices were synthesized and experimentally characterized [2-5]. We introduce 3D-topology multi-terminal ME devices which can be formed using cyclic molecules with a carbon interconnecting framework as shown in Figure 2.a [5]. Different Mgates can be implemented using cyclic molecules as multi-terminal ME devices if the electronic characteristics and acceptable performance are achieved. Figure 2.b illustrates the overlapping molecular orbitals for monocyclic molecules to implement ME devices which form MAND, $^a$NAND, $^a$OR and M$^a$NOR gates.

Fig. 1. One-dimensional potential energy profile and quasi-Fermi levels in the double-barrier single-well heterojunction transistors

Fig. 2. (a) Three-terminal ME device comprised from a monocyclic molecule with a carbon interconnecting framework; (b) $^a$AND, $^a$NAND, $^a$OR and M$^a$NOR gates formed by cyclic molecules; (c) Six-terminal ME device

The reported monocyclic molecule can be used as a six-terminal ME device as illustrated in Figure 2.c. The proposed carbon-centered molecular hardware solution, in general,
- Ensures a sound bottom-up synthesis at the device, gate and system levels;
- Guarantees aggregability to form complex MICs;
- Results in the experimentally characterizable $^a$ME devices and Mgates.

The use of side groups $R_x$, shown in Figure 2.c, ensures the variations of the energy barriers and wells potential surfaces $V(x)$. This results in:
1. Controlled quantum transitions due quantum effects and phenomena exhibited;
2. Controllable electron transport, tunneling, scattering, hopping, etc.;
3. Varying quantum interaction ensuring device functionality

IV. QUANTUM-EFFECT MOLECULAR ELECTRONIC DEVICES

We consider a three-terminal ME device with the input, control and output terminals as shown in Figure 2.a. The device physics of this ME device is based on:
- Quantum phenomena, e.g., quantum interactions and quantized energy levels;
- Controlled potential-assisted electron transport.

The applied $V_{control}(t)$ changes the charge distribution $\rho(t,r)$ and $E_d(t,r)$ affecting the electron transport. This ME device operates in the controlled electron-exchangeable environment due to quantum transitions and interactions. The controlled super-fast potential-assisted electron transport is achieved. The electron-exchangeable environment interactions qualitatively and quantitatively modify the device behavior, its characteristics and capabilities.

Consider the electron in the time- and spatial-varying meta-stable potentials $\Pi(t,r)$. The changes in the Hamiltonian result in:
1. Changes of tunneling $T(E)$;
2. Quantum interactions due to variations of $\rho(t,r)$, $E_d(t,r)$ and $\Pi(t,r)$.

One achieves the controlled electron transport between the input and output terminals. The device controllability is ensured by varying $V_{control}(t)$ which affects $\rho(t,r)$, $E_d(t,r)$ and $\Pi(t,r)$ leading to variations of $T(E)$. Hence, the device switching, $I-V$, $G-V$ and other characteristics are controlled.

We conclude that for a molecular device under consideration:
- Device physics is fundamentally sound;
- Device can be tested and characterized because the Heisenberg uncertainty principle, in particular the energy-time limits $\sigma_E \sigma_t > h$, is met;
- Synthesis and interfacing with $^g$hypercell which should be aggregated to MICs is to be examined.

V. MODELING AND ANALYSIS OF A ME DEVICE

We perform high-fidelity modeling for the studied ME device. To ensure data-intensive analysis, heterogeneous simulations must be performed. For heterojunction microelectronic devices, one usually solves one-dimensional Schrödinger and Poisson equations applying statistical thermodynamics (Fermi-Dirac distribution function) and electrostatics [1, 10]. For the studied ME devices, conventional approaches cannot be applied. The distribution functions and statistical mechanics postulates may not be applied.

Quantum mechanics must be applied, and a 3D problem cannot be simplified. We consider 9 atoms with motionless protons with charges $q_i$. The radial Coulomb potentials are $\Pi(r)=-\frac{Z_{eff}}{4\pi \varepsilon_0 r}$.

For example, for carbon $Z_{eff}=3.14$. Using the spherical coordinate system, we solve the Schrödinger equation

$$\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial r^2} + \frac{1}{r^2} \frac{\partial \Psi}{\partial r} - \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Psi}{\partial \phi^2} \right)$$

$$+ \Pi(r,\theta,\phi) \Psi(r,\theta,\phi) = E \Psi(r,\theta,\phi). \quad (1)$$
For the problem under our consideration, it is virtually impractical to find the analytic solution by using the separation of variables concept. We represent the wave function as
\[ \Psi(r, \theta, \phi) = R(r)Y(\theta, \phi) \]
to solve the radial and angular equations.

The Schrödinger and Poisson equations are discretized and numerically solved using the MATLAB environment [5]. The magnitude of the time-varying potential applied to the control terminal is bounded due to the thermal stability and energetics of the molecule. We have \( |V_{\text{control}}| \leq V_{\text{control max}} \) and \( |V_{\text{control}}| \leq 0.25 \) V. The charge distribution is of our particular interest. Figure 3 documents a three-dimensional charge distribution in the molecule if \( V_{\text{control}}=0.1 \) V and \( V_{\text{control}}=0.2 \) V. The total molecular charge distribution is found by summing the individual orbital densities.

![Fig. 3. Charge distribution ρ(r)](image)

The Schrödinger and Poisson equations are solved using a self-consistent algorithm [5]. Our goal is to examine the device physics soundness and derive the baseline performance characteristics. To obtain the current density \( j \) and current in the MEdevice, the velocity and momentum of the electrons are obtained by making use of the observable momentum, e.g.,
\[ \langle p \rangle = \int \Psi^*(t, r) \left( -i \hbar \frac{\partial}{\partial r} \right) \Psi(t, r) dr. \]

The wave function \( \Psi(t, r) \) is numerically derived for distinct values of \( V_{\text{control}} \). The I-V characteristics of the studied MEdevice for two different control currents \( 0.1 \) and \( 0.2 \) nA are reported in Figure 4. The results documented illustrate that the proposed MEdevice may be effectively used as a multiple-valued primitive in order to design enabling multiple-valued logics and memories. The multiple-valued characteristics result due to the quantized energy levels.

![Fig. 4. Multiple-valued I-V characteristics](image)

The traversal time of electron transport is derived from the expression
\[ \tau(E) = \frac{E}{\hbar} \sum_{n} \frac{m}{2|\Pi(r) - E|} \Delta r. \]
It is found that \( \tau \) varies from \( 2.4 \times 10^{-15} \) to \( 5 \times 10^{-15} \) sec. Hence, the proposed MEdevice ensures super-fast switching.

VI. PHYSICAL LIMITS AND ENERGETICS OF MOLECULAR DEVICES

For MEdevices and MEdevices, the analysis of physical limits and performance estimates, applied to microelectronic and solid-state devices, cannot be applied. The term \( k_B T \) has been used to solve distinct problems. Here, \( k_B \) is the Boltzmann constant, \( k_B=1.38 \times 10^{-23} \) J/K; \( T \) is the absolute temperature. The expression \( k_B T (\gamma > 0) \) was used to assess the energy, and \( k_B T \) (\( \gamma = 0 \)) was used to assess the energy dissipation. The expression \( k_B T \) (\( \gamma = 0 \)) was applied with the attempt to assess the lowest energy bound for a binary switching. The applicability of distinct equations must be examined applying sound concepts. Statistical mechanics and entropy analysis coherently utilize the minimal energy required to ensure the transition (switching) between two \( \gamma > 0 \) or to erase a bit of information (energy dissipation) is \( k_B T \), which for \( T=300K \) gives \( k_B T \approx 2.87 \times 10^{-21} \) J. Indeed, under this reasoning, one assumes the validity of the averaging kinetic-molecular Newtonian model and applies the assumptions of distribution statistics, at the same time allowing only two distinct \( \gamma > 0 \) system’s states.

**Example.** The Boltzmann distribution \( f(E) = \frac{e^{-E/k_B T}}{\int_0^\infty e^{-E/k_B T} dE} \) describes the distribution of energy among distinguishable particles. One can obtain the average energy per particle if there is no energy-dependent density of states to distort the distribution. Using the probability for a given energy, we perform normalization \( \int_0^\infty e^{-E/k_B T} dE = k_B T \) when the energy is randomly distributed among the available energy states.

The energy estimates must be performed applying quantum mechanics. Examining the discrete energy levels of an electron in the outermost populated shell, one yields
\[ E_n = -\frac{m Z_{\text{eff}}^2 e^4}{32 \pi^2 \hbar^2 n^2}, \text{ and } E_n = -2.17 \times 10^{-18} \frac{Z_{\text{eff}}^2}{n^2} \text{ J}. \]

From \( Z_{\text{eff}}=1 \), we conclude that \( AE = 1 \times 10^{-19} \) to \( 1 \times 10^{-18} \) J. If one supplies the energy greater than \( E_n \) to the electron, the energy excess will appear as kinetic energy of the free electron. The transition energy must be adequate to excite electrons. For different atoms and molecules, as the prospective solid MEdevices, the transition (switching) energy is estimated to be \( 1 \times 10^{-19} \) to \( 1 \times 10^{-18} \) J. This estimate is in agreement with biomolecular devices.

Considering an electron as a non-relativistic particle. From \( E = \frac{1}{2} m v^2 \), we obtain the particle velocity as a function of energy.
\[ v = \sqrt{\frac{2E}{m}}. \]
For \( E = 1.6 \times 10^{-20} \) J, one obtains \( v=1.9 \times 10^5 \) m/sec. Letting 1 nm path length, the traversal (transit) time is \( \tau = \frac{L}{v} = 5.3 \times 10^{-15} \) sec. Hence, MEdevices can operate at a high switching frequency. One may not conclude that the device switching frequency to be utilized is \( f=1/(2\pi\tau) \) due to device physics features (number of electrons, heating, interference, potential, energy, noise, etc.), system-level functionality, circuit specifications, etc.
We studied the microscopic system energetics applying quantum mechanics. The derived qualitative estimates must be observed to characterized devices. The exhibited changes and transitions must be measured because the device and system testing, characterization and evaluation are critical. In general, ICs cannot be designed without these tasks. The Heisenberg uncertainty principle provides the fundamental limits on the measurements implying constraints on the testability, characterization, etc. The Heisenberg uncertainty principle provides the position-momentum and energy-time limits on the measurements as $\sigma_\alpha \geq \frac{1}{\hbar}$ and $\sigma_\beta \geq \frac{1}{\hbar}$.

Using the energetic estimates, letting $\sigma_\alpha$ be $1 \times 10^{-18}$ J, one obtains the standard deviation $\sigma_\beta \geq 5 \times 10^{-15}$ sec, which implies that at least $5 \times 10^{-15}$ sec are required to measure the changes of $E$. The resulting $\sigma_\alpha$ is not associated with the derived transit time $t = 5.3 \times 10^{-15}$ sec. It should be emphasized, that the Heisenberg uncertainty principle does not define the device functionality and/or physical limits on energy, transit time, momentum, velocity, device dimensionality, etc.

Fig. 5 reports some performance estimates [5].

VII. MODELING AND ANALYSIS OF MOLECULAR DEVICES

Molecular devices ($M$-devices) can be utilized in combinational and memory modules and systems. These devices can be also used as routers to achieve a reconfigurable networking-processing-and-memory. Molecular devices, used as a switch or transmission devices, allow one to design the neuromorphological reconfigurable processing platforms.

The interconnected $M$-devices are well defined in the sense of their time-varying variables, e.g., input $r(t)$, control $u(t)$, output $y(t)$, state $x(t)$, disturbance $d(t)$ and noise $\xi(t)$ vectors. The potential and electric or magnetic field intensities can be considered as $u(t)$, while wave function, momentum, velocity, displacement, current and voltage can be related to the state and/or observable variables or quantities. For example, for a controllable solid $M$-devices examined, the voltage (potential) at any terminal is well defined with respect to a common datum node (ground). Figure 6 documents a multi-terminal $M$-device with input, control and output terminals reporting time-varying variables. The disturbances and noise vectors are also documented. The phenomena exhibited and effects utilized are defined by the devices physics. As illustrated, the proposed $M$-device is modeled by using the Schrödinger and Poisson equations. The $M$-devices for admissible inputs and disturbances must be coherently characterized (described) by the governing differential equations and constitutive relations. Neglecting disturbances, unmodeled phenomena and noise, the transient dynamics and steady-state behavior of $M$-devices is described by the behavioral quadruple $(r, x, y, u)$, where $r \in \mathbb{R}^n, x \in \mathbb{R}^n, y \in \mathbb{R}^k$ and $u \in \mathbb{R}^m$. We denote by $R, X, Y$ and $U$ the universal sets of achievable values for each vector. In general, the $M$-device response (behavioral) sextuple is

$$(r, x, y, u, d, \xi) \in R \times X \times Y \times U \times D \times \Xi, d \in \mathbb{R}^d \text{ and } \xi \in \mathbb{R}^k.$$ 

To perform the device testing, characterization and evaluation, one uses the measurement set which is given as

$$M = \{ (r, x, y, u, d, \xi) \in R \times X \times Y \times U \times D \times \Xi, \forall t \in T \}.$$ 

The state transitions are controlled by changing $u$ to: (i) guarantee device functionality; (ii) ensure optimal transients; (iii) guarantee the specified steady-state characteristics. The measurement set can be found for the gates, $M$-hypercells and systems. For example, for the $M$-hypercells one has

$$M = \{ (r, x, y, u, d, \xi) \in R \times X \times Y \times U \times D \times \Xi, \forall t \in T \}.$$ 

Control $u$

Fig. 6. Molecular device with time-varying variables which characterize dynamic and steady-state device performance in the behavioral sextuple

VIII. CONCLUSIONS

We reported results on devising and analysis quantum-effect multi-terminal $M$-devices. The device physics of these devices was described proving the overall soundness and feasibility. The analytic and numerical results on high-fidelity modeling and data-intensive analysis are reported.

References