Characterisation of a bis-ferrocene molecular QCA wire on a non-ideal gold surface

Mariagrazia Graziano ✉*, Ruiyu Wang, Massimo Ruo Roch, Yuri Ardesi, Fabrizio Riente,*
Gianluca Piccinini

Department of Electronics and Telecommunications, Politecnico di Torino, Torino 10129, Italy
✉ *E-mail: mariagrazia.graziano@polito.it*

Field-coupled nanocomputing represents one of the possible proposals for the post-Complementary Metal Oxide Semiconductor (CMOS) scenario. Contrarily to standard technology, the information is not propagated using electron transport, but via field interactions among single elements. The molecular quantum-dot cellular automata (QCA) is one of the most promising implementations; redox centres of oxidised molecules are used to concentrate charges. Coulomb interaction between redox centres enables the information propagation. The necessity for charge transport is overcome, entailing very low power consumption notwithstanding the nanometric size and the very high expected operating frequency. Nevertheless, as the Coulomb interaction strongly depends on the distance between charges, the position of each molecule plays a relevant role in the interaction. This work investigates the information propagation of a possible molecular wire thiolated on a non-ideal gold surface, where the intermolecular distance may vary due to the surface roughness and possible defects introduced in the formation of the molecular wire. The efficiency of the information transfer is analysed with the aim of providing significant constrains and suggestions for future fabrication steps.

1. Introduction and background: Unlike traditional CMOS technology, field-coupled nanocomputing (FCN) paradigm uses local field interaction to forward digital information between nanoscale dimension building blocks, eliminating the need for electric current. In particular, quantum-dot cellular automata (QCA) provides a feasible solution for the FCN paradigm. Coulombic interactions among basic elements, i.e. QCA cells, determine the logic information propagation without the need for electronic transport, therefore, evidently decreasing the power dissipation.

According to the QCA theory, the fundamental cell is square shaped and it is composed of six quantum dots. Two free charges are inserted in the cell and can occupy two of the available quantum dots [1]. In Fig. 1*b*, a basic representation of the ideal QCA is shown; four dots are distributed along the two diagonals of the cell and are used to encode the logic states of the devices; the remaining two dots in the middle are used for the 'NULL' state configuration. Based on the position of those two mobile charges, three different states can be encoded: two conventional logic states, '0' and '1', are determined if the two mobile charges localise along one of the two diagonals of the square cell; the 'NULL' state is encoded if these mobile charges are forced to occupy the two central dots by means of an external electric field (i.e. the clock). Even though the 'NULL' state is not needed for defining logic states, it is important for realising adiabatic switching among QCA devices [2].

Since QCA cells communicate with each other via electrostatic interaction among free charges, basic logic gates could be realised by properly arranging the cells. The QCA wire in Fig. 1*c* is recognised as the basic block for building logic circuits. It could be constructed by aligning a group of QCA cells with a cell-to-cell distance, measured between cell centres that equals the width of the single cell. Other devices such as the majority voter, shown in Fig. 1*d*, and other fundamental logic gates, like the inverter [3], can be realised and used to design more complex digital systems (e.g. the arithmetic circuits).

Regarding the physical implementations of QCA technology, the molecular approach examined in this work is expected to be the most performing among all the proposals [3, 4]. Indeed, many molecules have been synthesised following the urgent need of

suitable candidates for realising QCA computation, the *bis-ferrocene* molecule is one of those [5]. The structure of the bis-ferrocene molecule is illustrated in Fig. 1*e*: two ferrocene groups constitute the dots used to encode the logic states; a carbazole connects the two ferrocene groups and acts as central dot for the 'NULL' state. An alkyl chain with the ending thiol (–SH) group is added to anchor the bis-ferrocene to the gold substrate by means of self-assembled-monolayer (SAM) formation [5].

The single bis-ferrocene molecule, having three dots, is considered as a QCA half-cell. A complete molecular QCA (MQCA) cell can be built by aligning two molecules (Fig. 1*f*). The oxidised form of the molecule is typically exploited to achieve optimum QCA performance [2]: considerations on the counterion of the molecule are presented in [6].

Concerning the analysis of MQCA logic blocks from an electronic point of view, Pulimeno *et al.* [7] have evaluated the charge interaction along a bis-ferrocene based MQCA wire. Results in terms of charge distribution on the wire are obtained by means of iterative steps of ab initio simulations and post-processing of data. Specifically, during simulation, molecules are ideally aligned on a smooth nanowire. In the reality, the realisation of MQCA devices may bring several problems related to the position of molecules; the substrate might be rough and the procedure used for the formation of the SAM may introduce some misalignments due to technological issues (e.g. problems caused by steric hindrance) [8]. Since the propagation of the information between molecules is based on Coulomb interaction, strongly dependent on the distance, the possible misalignment between molecules might impinge on the quality of the molecular interaction.

In this Letter, we make use of the profile of a real gold surface proposed in [8], to study the behaviour of a MQCA wire. We analyse the device capability of continuing to propagate properly the binary information, even in presence of misalignments between molecules.

The defects of the gold surface are modelled into variables or parameters which could be externally applied to ab initio simulations for the analysis of molecular performance [8]. The molecular interactions allowing the information to propagate have been evaluated adopting an iterative method based on ab initio simulations and post-processing of data. This method is similar to the one
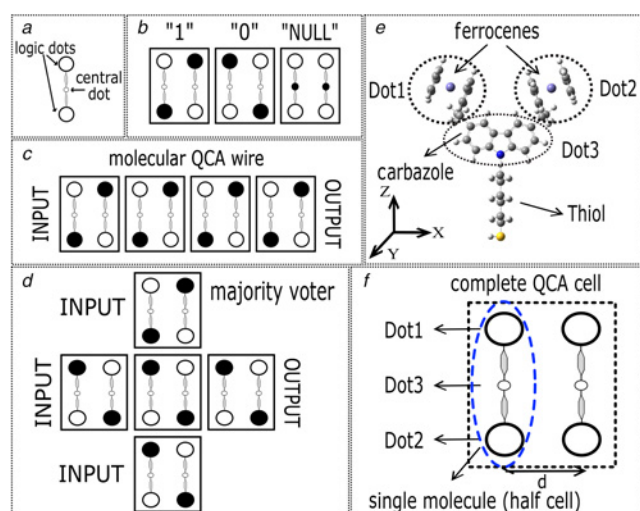
Fig. 1 *QCA cells and fundamental QCA functional logic blocks*
a Logic and central dots of the ideal QCA half-cell
b Six dots of the ideal QCA cell: two mobile charges (represented by filled black circles) are localised on the antipodal sites of the square cell encoding logic states '0' and '1'; the 'NULL' state is encoded with the free charges forced in the central dots
c QCA wire: an external input forces a logic state on the first cell on the left (as INPUT), then each cell along the line arranges its logic state according to its neighbouring cells due to electrostatic repulsion, thus allowing the binary information to propagate until reaching the OUTPUT in a domino-like style
d Three-input majority voter: the logic state of the output cell depends on the majority of the three input cells
e Structure of bis-ferrocene molecule
f Top view of a complete QCA square cell

Fig. 2 *MQCA wire and molecules interaction modelling*
a Schematic view of a MQCA wire built with bis-ferrocene molecules and of the electrodes used for providing the switching field. Concerning molecular interaction, two random bis-ferrocene molecules *Molecule i* and *Molecule j* on the wire are highlighted in bold
b One of the two molecules, e.g. *Molecule i*, is replaced by its aggregated charges $Q1$, $Q2$ and $Q3$ becoming a driver for *Molecule j*
c Output voltage V_{out} is generated by the aggregated charges of *Molecule i*
d *Molecule i* becomes driver and stimulates the other molecule generating the input voltage V_{in}

proposed in [7], but it models charge interactions not only between two nearby molecules but considering interactions among all the molecules along the wire [9], by calculating the so-called *forward* and *feedback* effects. This method is briefly discussed in Section 2.1.

Finally, the method will output figures of merits as *aggregated charge* distributed along the wire [10], illustrating the propagation of binary information along the MQCA wire. The influence of possible fabrication defects to the QCA wire behaviour is examined. The analysis is intended to facilitate the possible set-up of MQCA devices.

2. Methodology: In this part, the methodology developed to study the behaviour of the MQCA wire in presence of defects is discussed. The methodology is mainly composed of three parts: design suite 'MoSQuiTo'; modelling of molecular interactions along MQCA wire; gold substrate preparation and possible defect modelling.

2.1. 'MoSQuiTo' suite: The *molecular simulator quantum-dot cellular automata Torino* suite ('MoSQuiTo') is implemented to model MQCA as electronic devices [11, 12]. It introduces figures of merits to demonstrate the ability of MQCA devices to perform the computation. In particular, 'MoSQuiTo' consists of three stages – stage I: ab initio simulation, stage II: definition of figures of merit, stage III: molecular interaction.

Stage I: ab initio simulations of the MQCA are performed. Electric fields and point charges can be inserted as biasing conditions to analyse molecule performance [11]. In Fig. 2*a*, the electric field, which is parallel to the axis of the logical dots of the molecule (switching field), is applied to force *Molecule 1* in a specified logic state in order to work as wire *INPUT* [13]. The electrostatic interaction between two general *Molecule i* and *Molecule j* is modelled by representing the former bis-ferrocene molecule with a set of
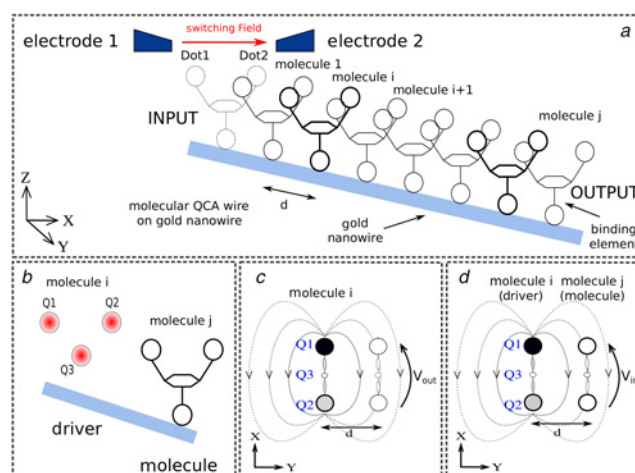
point charges, as shown in Fig. 2*b*. The two molecules are thought as a *Driver-Molecule* system, in which *Molecule* (*Molecule j*) is influenced by the point charges of the *Driver* (*Molecule i*).

Stage II: the electrostatic properties of MQCA systems are analysed defining the *Aggregated Charge* and the *Input-Voltage* V_{in} as figure of merits [12], evaluated with Octave [14] by post-processing simulation data [11]. To be specific, the aggregated charge is calculated based on the obtained atomic charges [15] which are spatially collected in three groups, representing the dots, and summed up to obtain the aggregated charge distribution of the bis-ferrocene molecule.

The charge distribution of a molecule in presence of biasing conditions is represented by the set of aggregated charges $Q1$, $Q2$ and $Q3$. The charges can be used to evaluate the electric field at any point around the molecule with simple electrostatic equations. In order to 'measure' the effects of *Molecule i* on *Molecule j*, the input voltage V_{in} is calculated integrating the value of the electric field on the segment connecting the two logical dots of the latter molecule, as depicted in Fig. 2*c*. In this context, *Molecule i* influences *Molecule j* as a *Driver* (see Fig. 2*d*) and *Molecule j* reacts to V_{in} in terms of re-localising its charge on *Dot1*, *Dot2* and *Dot3*.

Stage III: a MQCA wire could be built by aligning a group of bis-ferrocene molecules together with distance *d* in between, as depicted schematically in Fig. 2*a*. Concerning the modelling of the electrostatic interactions among molecules along the wire, Pulimeno *et al.* [7] adopted a method of iterating steps of ab initio simulation and post-processing of results. During each step, the evaluation of the generic *Molecule i* is performed by replacing *Molecule i*−1 with the aggregated charges obtained at the previous step. These point charges are then considered as a driver that forces the adjacent *Molecule i* to re-arrange its charge configuration. After that, the aggregated charges of *Molecule i* are obtained and the procedure is iterated by considering charge distribution of *Molecule i* as a driver for *Molecule i*+1 in the next step of the simulation. In the end, the aggregated charge distribution of all molecules located on the wire is obtained.

Regarding the modelling of molecular interactions in this Letter, it is reminded that *Molecule i* does not affect only the adjacent

Molecule i + 1, but also all the other molecules of the wire. As a consequence, the molecule which reacts to the driver influence also provides a feedback in reciprocation to the driver molecule. As discussed in stage II of 'MoSQuiTo' suite, two molecules interact with each other in terms of input voltage V_{in} generated by a molecule to the other.

The relation between the charge distribution and the V_{in} is described using the V_{in}-aggregated charge transcharacteristics (VACT), figure of merit which links the input voltage with the value of the aggregated charges [12]. An alternative transcharacteristics to describe the interaction between two molecules was evaluated analytically in [16], in the present work we use the VACT because it is evaluated directly with ab initio simulation and it enables the evaluation of molecule polarisation considering the influence of all the molecules of the wire.

For the evaluation of the information propagation, we adopt a novel iterative method, proposed in [9], which evaluate the distribution of the aggregated charge on the wire using a self-consistent procedure.

In fact, when a generic *Molecule i* is inserted in a system of many molecule, each molecule generates an electric field that depends on the charge distribution of the other molecules and that impacts to the *Molecule i*. *Molecule i* changes its charge distribution according to the value of the electric field generated by all the other molecules. In turn, the electric field which *Molecule i* generates changes as a consequence of the variation of its charge distribution. It is clear that there must be a consistency between the electric fields that impact on all the molecules of the wire and the charge distributions of all the molecules.

The algorithm we use for the simulation of molecular devices bases its evaluation on the concept of the VACT and it holds on a simple self-consistent procedure. A self-consistent procedure has been used also in [17] for the study of wires made with ideal QCA cells. The algorithm used in this work was created ad-hoc for the analysis of MQCA devices.

2.2. Substrate preparation and defect modelling: The bis-ferrocene MQCA wire is schematically thiolated on the surface of a gold surface that has to be prepared to guarantee the lowest level of roughness. For the purpose of this work, possible existing defects have to be modelled for the evaluation of molecular interaction.

Substrate preparation: an experimental scheme for depositing the bis-ferrocene MQCA wire by exploiting self-assembly fabrication has been previously proposed; the exact experiment procedure to prepare a smooth gold substrate for the nanowire and to realise bis-ferrocene MQCA wire deposition has been described in detail in [8].

According to the need for the smooth surface, a low roughness gold substrate was reported by Pulimeno *et al.* [8]. A clean glass microscope slide was smoothed following the procedure described in [18]. Fig. 3*a* depicts the chosen profiles within the same gold grain, of a 500 nm × 500 nm sample highlighting the appearance of the gold substrate surface. After examining their smoothness, the length range from 15 up to 25 nm of the first profile is mapped with the aim of simulating the molecular wire behaviour (Fig. 3*b*, bottom). Fig. 3*c* shows eight bis-ferrocene molecules schematically deposited on the chosen gold substrate segment with an identical distance *d* in between.

Defects modelling: the procedure that enables the formation of the gold SAM and the deposition of bis-ferrocene molecules may lead to several defects, for instance, the misalignment in all possible directions and the non-ideal parallelism between two nearby molecules [8]. Such defects are considered to be harmful to the correct behaviour of molecular electronics circuits in terms of influencing information propagation [19, 20].

The table in Fig. 3*c* indicates the exact positions along the *z*-axis of the eight deposited bis-ferrocene molecules; the first molecule is
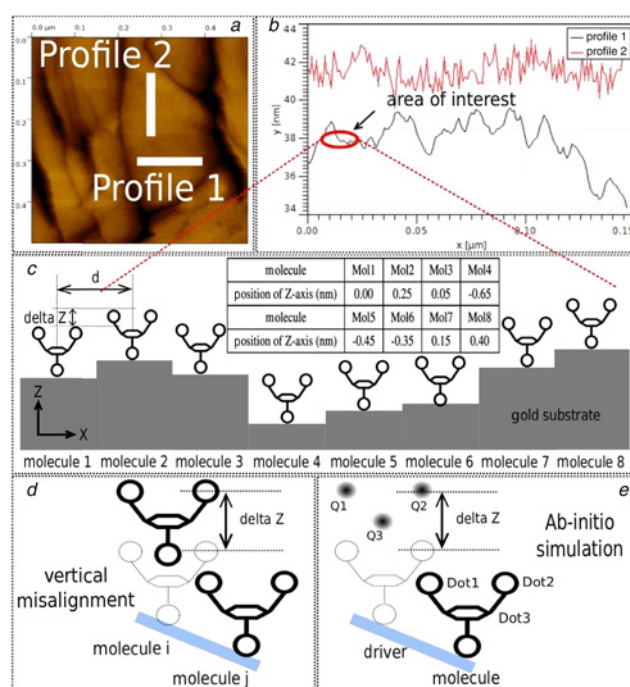

Fig. 3 *Models of vertical defects for molecules anchored on a gold wire*
a Scheme of the gold grain sample
b Smoothness of two proposed gold nanowire profiles
c Eight bis-ferrocene molecules are schematically deposited on the chosen sample
d Vertical misalignment is modelled as *deltaZ* along *Z*-axis between two bis-ferrocene molecules
e In ab initio simulation, *Molecule i* is replaced by its aggregated charges *Q*1, *Q*2 and *Q*3 to compute its interaction with *Molecule j*, as a driver-molecule system, considering the vertical misalignment

assumed to be at the origin of the surface plane and molecules are considered to be equally distributed along the horizontal axis of the gold substrate, with ideal intermolecular distance (i.e. equal to the distance between logic dots). The vertical misalignment along the MQCA wire is constructed following the roughness of the chosen gold profile.

In particular, the vertical misalignment between two molecules *Molecule i* and *Molecule j* along the wire is computed evaluating the difference between their position along the *z*-axis, which is denoted as *deltaZ* (see Fig. 3*d*). In ab initio simulation *Molecule i* can be replaced by its aggregated charges (*Q*1, *Q*2 and *Q*3), as driver molecule, whereas the vertical misalignment can be added to *Molecule j* to calculate the interaction between two molecules when a vertical defect is present, as depicted in Fig. 3*e*.

The procedure applied for the creation of the molecular wire, concerning the molecule deposition, can be subdivided in two parts: thiol deposition and carbazole connection. In the first step, all the thiols are connected to the gold substrate following a precise layout. The layout imposes a specific distance between each molecule with the consequence of a discretisation in terms of molecule positions. The positions of the molecules imposed by the SAM formation are of high importance for the correct Coulomb interaction among molecules [6]. Many efforts have been carried out by the scientific community to study the properties of the sulphur–gold interface [21–24]. The typical scenario is the anchoring of the thiols on the (111) gold substrate, according to profiles $c(4 \times 2)$ and $(\sqrt{3} \times \sqrt{3})$-R30°, where the thiol–thiol distance is around 0.5 nm, as depicted in Fig. 4*a*.

In the second step of the deposition process, bis-ferrocene molecules are connected to the thiols following the layout of the molecular wire.
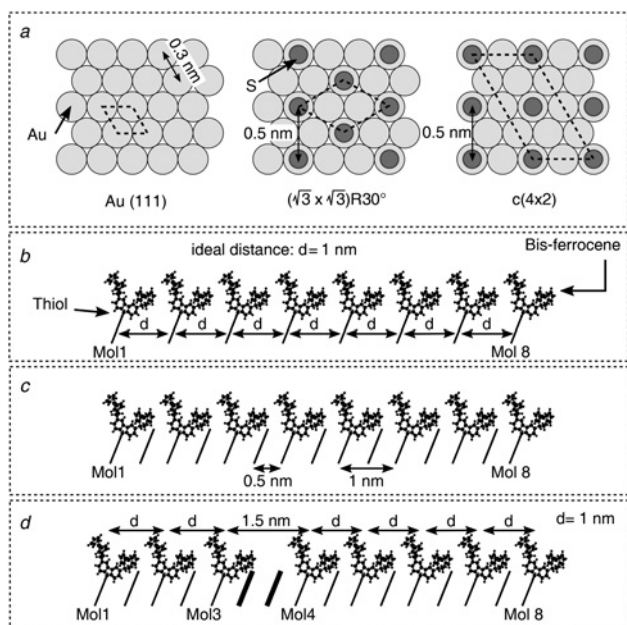
Fig. 4 *Models of horizontal defects for molecules anchored on a gold wire*
a Lattice structures of gold and sulphur on gold
b Ideal MQCA wire
c Possible real configuration of a real MQCA wire considering the steric hindrance effect
d Possible real configuration of a real MQCA with missing connection error

In the ideal case, all thiols should be connected to bis-ferrocene molecules. However, due to the steric hindrance, the size of molecules plays a relevant role in the process; according to bis-ferrocene size reported in [5] it seems reasonable that molecules might connect to half of the available thiols leading to 1 nm as intermolecular distance, as shown in Fig. 4c.

3. Result and discussion: The aggregated charges of molecules are evaluated adopting the iterative method discussed in Section 2. By taking into account the presence of vertical and horizontal defects, several cases are analysed:

• Ideal case: the molecular wire is composed by considering the ideal distance between each molecule (distance between logical dots, 1 nm), as shown in Fig. 4b.

• Distance analysis: the distance between molecules is varied by 20% (i.e. $d = 0.8$ nm and $d = 1.2$ nm) to analyse the effects introduced by the variation of the intermolecular distance. The relation between the disposition of gold atoms and molecule anchoring is not considered.

• Discontinuity analysis: the intermolecular distance is kept fixed to 1 nm. However, the distance between two particular molecules (i.e. *Mol3-Mol4* then *Mol5-Mol6*) is increased to 1.5 nm to simulate a vacancy in the adhesion of the bis-ferrocene molecules to the thiols, as shown in Fig. 4d, thus taking into account the real substrate and possible defects introduced due to the steric hindrance or possible impurities on the substrate [19, 20].

In all the cases, the vertical displacement is varied according to the profile in Fig. 3c. The molecular wire is created as a system of 11 molecules where the first one is used as driver. A segment containing the first eight molecules is shown in the results. Remaining three molecules are used to terminate the wire avoiding parasitic border effects (long wire assumption). Therefore, all the analyses are performed both on the ideal flat substrate and on the rough gold substrate to study the effects of all the possible defects combined. Fig. 5 shows the resulting aggregated charges of two logic dots *Dot1* and *Dot2*, of each molecule.
3.1. Ideal case: Figs. 5a and b show that, with 1.0 nm intermolecular distance, the information propagates as expected.
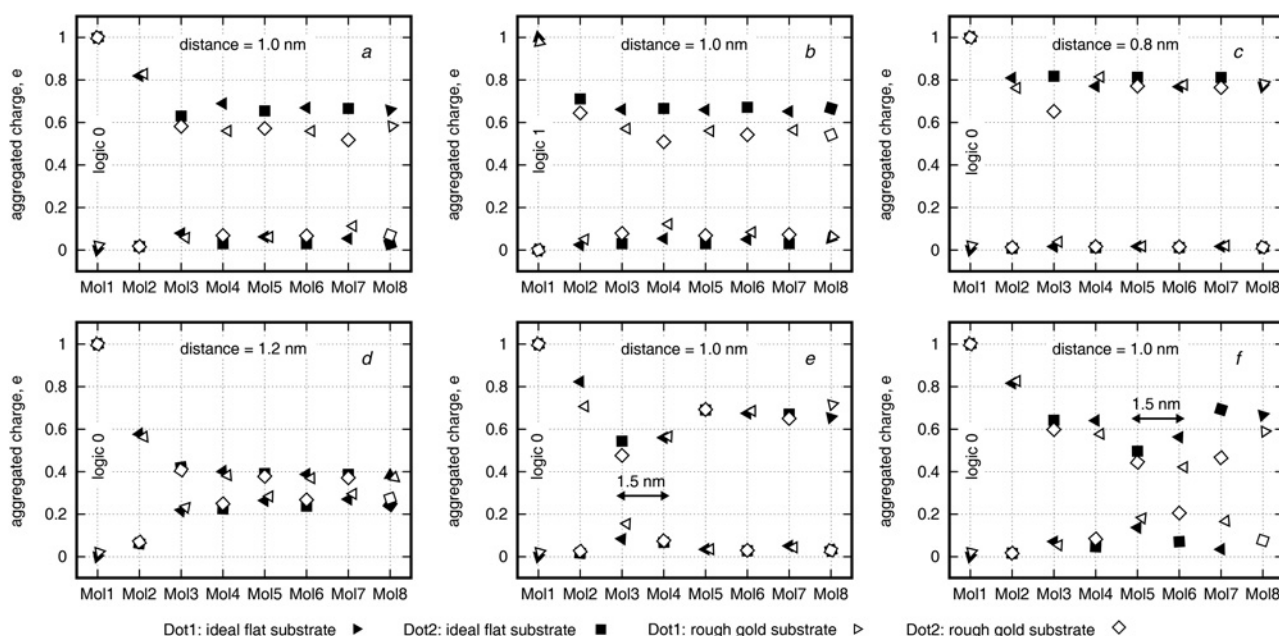

Fig. 5 *Aggregated dot charges along MQCA wire are reported for following cases of study*
a 1.0 nm intermolecular distance and Logic 0 as INPUT
b 1.0 nm intermolecular distance and Logic 1 as INPUT
c 0.8 nm intermolecular distance and Logic 0 as INPUT
d 1.2 nm intermolecular distance and Logic 0 as INPUT
e 1.0 nm intermolecular distance and Logic 0 as INPUT, with 0.5 nm of shift between Mol3 and Mol4
f 1.0 nm intermolecular distance and Logic 0 as INPUT, with 0.5 nm of shift between Mol5 and Mol6

The two figures are related to different input values, Logic 0 and Logic 1, respectively. For the ideal flat substrate (filled marks in the picture), a good charge separation between *Dot1* and *Dot2* is obtained for all the molecules. The introduction of the rough gold substrate (empty marks in the picture), considering the vertical defects, slightly impinges on the quality of information propagation along the molecular wire. The vertical misalignment enlarges intermolecular distances and obstructs Coulomb interaction thus decreasing the charge separation between logic dots. Indeed, the lowest charge separation is obtained for *Mol3* and *Mol4*, with Logic 0 and Logic 1, respectively, which corresponds to the molecules in which *deltaZ* is maximum.

3.2. Distance analysis: Fig. *5c* shows the results for the case Logic 0 with both the flat and rough gold substrate with a 0.8 nm intermolecular distance. Shorter intermolecular distance is expected to lead to stronger electrostatic interaction among molecules. Indeed, the charge separation in this case is higher and it guarantees better quality for the propagation of the information. Moreover, the behaviour of wires on the rough gold substrate and the ideal flat substrate almost coincides. Strong interactions along the wire outweigh the vertical misalignment between nearby molecules that still interact with each other allowing information to move correctly.

On the contrary, Fig. *5d* shows the results obtained for an intermolecular distance equal to 1.2 nm. In this case, the degradation phenomenon is hardly noticeable either using the flat or the rough gold substrate with vertical shifts. The propagation of the information is not possible since the charge separation between *Dot1* and *Dot2* does not ensure detectability of logic state in the single molecule. Cases for logic 1 are not reported for the sake of brevity but shows very similar results.

3.3. Discontinuity analysis: Two cases in which molecules are not correctly thiolated to the substrate are finally analysed. Fig. *4d* shows the presence of two consecutive thiols not connected to bis-ferrocene molecules forcing the intermolecular distance of *Mol3* and *Mol4* to 1.5 nm. Fig. *5e* shows the relative results for this case; the charge separation is reduced almost of the expected values for *Mol3* and *Mol4*. By comparing this scenario with the ideal one (Fig. *5a*), a degradation phenomenon can be observed. It is interesting to note that molecules following the defect tend to reconstruct the information; this effect is also present with the rough gold substrate but it is reduced by the effects of vertical defects. Despite the defects, the charge separation of *Dot1* and *Dot2* for the last molecule is almost equal to the case in which no vertical defect is present. The reconstruction effect compensates the presence of the horizontal defects. The same scenario can be seen (Fig. *5f*) when the defect is moved to another couple of molecules in the wire (*Mol5* and *Mol6*), indeed the reconstruction phenomenon is still able to compensate for the error.

4. Conclusions: In the MQCA technology, propagation is enabled by the electrostatic interaction among molecules. Therefore, the intermolecular distance plays a key role in the information propagation, which is enhanced by a short intermolecular distance whereas worsened with a large distance.

An iterative method, which is based on the post-processing of ab initio simulation data, is used to simulate a QCA wire. The molecules which compose the wire are anchored on a possible non-ideal gold surface. Misalignment among molecules is introduced in the wire layout, considering real measurements, to study the quality of the information propagation.

The vertical disposition of molecules depends on the roughness of the gold substrate, while the horizontal disposition depends on the formation of the self-assembled monolayer thus on the sulphur–gold interface. Vertical and horizontal defects might increase the intermolecular distance, making the information

propagation difficult. In this work, three possible scenarios are investigated.

In the first case, a rough substrate is analysed. The roughness of the substrate introduces vertical misalignments among molecules which increase the intermolecular distance. The effects on the information propagation turn out to be not troubling. Indeed, the information propagation is only slightly worsened and the charge separation among logical dots is kept large.

In the second case, the intermolecular distance is varied by 20% to analyse the effects of horizontal defects. The decrease of the intermolecular distance strengthens the electrostatic interaction, leading to a higher charge separation among logical dots. On the other side, by enlarging the intermolecular distance, the interaction is diminished and the propagation is worsened. The charge separation among logical dots of all the molecules is strongly reduced thus the information on the wire is lost.

In the end, all the molecules are anchored on the substrate with an intermolecular distance equal to the distance between dots. This distance demonstrated the correct propagation of the information. A horizontal shift is added between some molecules to emulate a possible error introduced by the formation of the self-assembled monolayer. The simulations highlight the tendency of the wire to reconstruct the information and to retain the logical value in the molecular wire. The bi-stability of the system compensates for the presence of sparse horizontal defects on the wire.

This work wants to highlight the importance of vertical and horizontal misalignments between molecules, which are introduced by the non-ideal roughness of the substrate and by the nature of the self-assembled monolayer. The obtained quantitative results clearly demonstrate the importance of the intermolecular distance and contribute towards the real fabrication of MQCA devices.

5 References

[1] Lent C.S., Tougaw P.D., Porod W., *ET AL.*: 'Quantum cellular automata', *Nanotechnology*, 1993, **4**, (1), pp. 49–57

[2] Wang R., Pulimeno A., Roch M.R., *ET AL.*: 'Effect of a clock system on bis-ferrocene molecular QCA', *IEEE Trans. Nanotechnol.*, 2016, **15**, (4), pp. 574–582

[3] Lent C.S., Isaksen B., Lieberman M.: 'Molecular quantum-dot cellular automata', *J. Am. Chem. Soc.*, 2003, **125**, (4), pp. 1056–1063

[4] Lu Y., Liu M., Lent C.S.: 'Molecular quantum-dot cellular automata: from molecular structure to circuit dynamics', *J. Appl. Phys.*, 2007, **102**, (3), p. 034311–1/7

[5] Arima V., Iurlo M., Zoli L., *ET AL.*: 'Toward quantum-dot cellular automata units: thiolated-carbazole linked bisferrocenes', *Nanoscale*, 2012, **4**, (3), pp. 813–823

[6] Christie J.A., Forrest R.P., Corcelli S.A., *ET AL.*: 'Synthesis of a neutral mixed-valence diferrocenyl carborane for molecular quantum-dot cellular automata applications', *Angewandte Chemie*, 2015, **54**, (51), pp. 15448–15451

[7] Pulimeno A., Graziano M., Wang R., *ET AL.*: 'Charge distribution in a molecular QCA wire based on bis-ferrocene molecules'. IEEE/ACM Int. Symp. on Nanoscale Architectures (NANOARCH), Brooklyn, NY, USA, July 2013, pp. 42–43

[8] Pulimeno A., Graziano M., Sanginario A., *ET AL.*: 'Bis-ferrocene molecular QCA wire: ab-initio simulations of fabrication driven fault tolerance', *IEEE Trans. Nanotechnol.*, 2013, **12**, (4), pp. 498–507

[9] Wang R., Chilla M., Palucci A., *ET AL.*: 'An effective algorithm for clocked field-coupled nanocomputing paradigm'. Proc. IEEE Nanotechnology Materials and Devices Conf., Toulouse, France, 9–12 October 2016

[10] Pulimeno A., Graziano M., Antidormi A., *ET AL.*: 'Understanding a bisferrocene molecular QCA wire', in Brown S. (Ed.): 'Field-coupled nanocomputing' (Springer, Heidelberg, Germany, 2004), pp. 307–338

[11] Graziano M., Pulimeno A., Wang R., *ET AL.*: 'Process variability and energy optimization of molecular QCA', *ACM J. Emerging Technol.*, 2015, **12**, (2), p. 18

[12] Ardesi Y., Pulimeno A., Graziano M., *ET AL.*: 'Effectiveness of molecules for quantum cellular automata as computing devices', *J. Low Power Electron. Appl.*, 2018, **8**, (3), p. 24

[13] Pulimeno A., Graziano M., Demarchi D., *ET AL.*: 'Towards a molecular QCA wire: simulation of write-in and read-out systems', *Solid State Electron. Elsevier*, 2012, **77**, pp. 101–107

[14] Octave community: 'GNU octave 3.8.1'. Available at www.gnu.org/software/octave/

[15] Singh U.C., Kollman P.A.: 'An approach to computing electrostatic charges for molecules', *J. Comput. Chem.*, 1984, **5**, pp. 129–145

[16] Lu Y., Lent C.S.: 'A metric for characterizing the bistability of molecular quantum-dot cellular automata', *Nanotechnology*, 2008, **19**, (15), p. 155703

[17] Lent C.S., Tougaw P.D.: 'Lines of interacting quantum-dot cells: A binary wire', *J. Appl. Phys.*, 1993, **74**, (10), pp. 6227–6233

[18] Eske L.D., Galipea D.W.: 'Characterization of SiO$_2$ surface treatments using AFM, contact angles and a novel dewpoint technique', *Colloids Surface A: Physicochem. Eng. Aspects*, 1999, **154**, (1), pp. 33–51

[19] Valley D.T., Onstott M., Malyk S., *ET AL.*: 'Steric hindrance of photo-switching in self-assembled monolayers of azobenzene and alkane thiols', *Langmuir*, 2013, **29**, (37), pp. 11623–11631

[20] Love J.C., Estroff L.A., Kriebel J.K., *ET AL.*: 'Self-assembled monolayers of thiolates on metals as a form of nanotechnology', *Chem. Rev.*, 2005, **105**, (4), pp. 1103–1170

[21] Pensa E., Cortés E., Corthey G., *ET AL.*: 'The chemistry of the sulfur-gold interface: in search of a unified model', *Acc. Chem. Res.*, 2012, **45**, (8), pp. 1183–1192

[22] Bürgi T.: 'Properties of the gold-sulphur interface: from self-assembled monolayers to clusters', *Nanoscale*, 2015, **7**, (38), pp. 15553–15567

[23] Häkkinen H.: 'The gold-Sulfur interface at the nanoscale', *Nature Chem.*, 2012, **4**, pp. 443–455

[24] Laibinis P.E., Fox M.A., Folkers J.P., *ET AL.*: 'Comparisons of self-assembled monolayers on silver and gold: mixed monolayers derived from HS(CH2)21X and HS(CH2)10Y (X, Y = CH3, CH2OH) have similar properties', *Langmuir*, 1991, **7**, (12), pp. 3167–3173