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Rotaxane Based Molecular Junctions Have Emerged as Promising Components For Electronic and Optoelectronic Applications

Hiba Abbas Mohammed[*1] , Hussein N. Najeeb[2] , Oday A. Al-Owaedi[3]

1College of science for women University of Babylon, hibaabaas45@gmail.com, Hilla , Iraq .
2College of science for women, University of Babylon, dhifafhussein@yahoo.com, Hilla , Iraq.
3College of science for women, University of Babylon, oday.alowaedi@uobabylon.edu.iq , Hilla , Iraq.

***Corresponding author email:** hibaabaas45@gmail.com ; mobile: +9647601046698

الوصلات الجزيئية القائمة على الروتاكسان كمكونات واعدة للتطبيقات الالكترونية والالكترونات البصرية

هبه عباس محمد[*1]، حسين نعمه نجيب[2]، عدي اركان العويدي[3]

1 كلية العلوم للبنات ، جامعة بابل، hibaabaas45@gmail.com، صندوق بريد4- مدينة الحلة ، الحلة ، العراق

2 كلية العلوم للبنات، جامعة بابل، dhifafhussein@yahoo.com ، الحلة ، العراق

3 كلية العلوم للبنات، جامعة بابل، oday.alowaedi@uobabylon.edu.iq ، الحلة ، العراق

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ABSTRACT

Background: Rotaxane molecule consists of three main parts: wheel, axle, and stoppers. This study was conducted to increase the number of wheels to get the electronic, electrical and thermal properties of Nano molecular junctions based on rotaxane.

Materials and Methods: Calculations were performed to evaluate the transport properties and the geometrically optimization of these molecular junctions using a combination of DFT, SIESTA code, Gollum code and a non-equilibrium Green's function formalism. Each molecule was attached to opposing 35-atom (111) directed pyramidal gold electrodes. DFT and GGA were used to compute the ground state energy of various molecular junctions.

Results: The results of the T(E) showed high values, and this is evidence of that constructive interference that is controlled and reinforced by changing the number of wheels in the rotaxane molecules, which affected the HOMO-LUMO gap and thus contributed to raising or lowering the T(E) values. The relationship between G/G_o and thermopower showed that the highest G/G_o yields to low thermopower. The decay constant is a fundamental property that influences the transmission of electrons, conductance properties, and threshold voltage in the rotaxane molecules.

Conclusion: Molecular junctions based on Rotaxane showed high values of the T(E), which increase the electrical conductivity, making them promising for electronic applications. The smaller value of threshold voltage is a useful property for different applications. The results of power factor bring to us an important conclusion, which is that the impact of G/G_0 is more dominant than that of thermopower in the case of rotaxane molecular junctions.

Key words: Transmission coefficient T(E) ; (DFT) Density Functional Theory ; (HOMO-LUMO) Highest Occupied Molecular Orbital- Lowest Unoccupied Molecular Orbital ; (GGA) Generalized Gradient Approximation ; G/G_o Electrical Conductance.

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INTRODUCTION

The field of molecular electronics aims to harness the unique properties of molecules for electronic functions and computing. It offers a promising avenue for advancing technology beyond the sub-10 nm scale, where traditional approaches face limitations. Molecular electronics involves the synthesis, design, and fabrication of devices using molecular building blocks, providing opportunities for further size reduction in electronic components. Molecular electronics was first proposed in 1974 by Aviram and Ratner, using molecules as substitutes for silicon chips[1].Since then, the electronic behavior of molecules has been understood through a combination of theoretical and experimental efforts . Advancements in computing power and modeling tools have led to results that closely approximate experimental measurements. One of the major challenges in molecular electronics is identifying the appropriate functionalities, materials, and techniques to achieve desired device properties[2]. Rotaxane molecules are promising candidates for molecular electronics with their unique properties. Rotaxane is a mechanically interlocked molecular structure consisting of a linear molecule (the axle) that is linked by hydrogen bonds or coordination bonds via a macrocycle (the wheel). The macrocycle in a rotaxane can act as an electron donor or acceptor, depending on its functional groups and the nature of its interactions with the axle. However, in general , a rotaxane molecule can be described as having three main parts: the wheel, the axle, and the stoppers. The wheel is a cyclic molecule with a cavity that is large enough to accommodate the axle. The wheel is made of a variety of cyclic compounds, such as crown ethers, Cyciodextrins, or Calixarenes, so that it is designed in a size and shape that suits the specific characteristics of the axle. Depending on the particular design of the molecule, rotaxane molecules can have different structural and morphological properties. The system is stable because of this molecule's interlocked design. Furthermore, the limited range of motion of the Stability is increased by interfacial elements in the interlocking structure[3]. Because of their special structural makeup, rotaxane molecules make it possible to see how their individual molecules move, which makes them useful for building molecular machines[4], As we see in Figure 1[5].

The transmission coefficient (T(E)) of rotaxane molecules was examined in this work. Generally speaking, the The GOLLUM algorithm was used to determine the transmission coefficient in this paper after the relevant Hamiltonian and overlap matrices were obtained using SIESTA. The outcomes demonstrated high T(E) value for molecule R-5, , while the lowest value of the transmission is presented by molecule R-1. On the other hand, it can be seen that the transport mechanism for molecules are a LUMO-dominated transport. This trend can be attributed to the increase of the transmission coefficient by increasing the rings in the molecules. the presence of functional groups[6] on the rings can also influence the electronic structure of the rotaxane and its conductivity.

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Overall, the electronic properties of rotaxanes can be influenced by the presence of the macrocycle and the axle, as well as the nature of their interactions[7]. The macrocycle in a rotaxane can act as an electron donor or acceptor, depending on its functional groups and the nature of its interactions with the axle[8].

this work advances The electrical conductance of a rotaxane molecule which be influenced by various factors, such as the degree of delocalization of the electrons, the presence of any defects or impurities, and the external conditions such as the temperature and the presence of any electromagnetic fields.

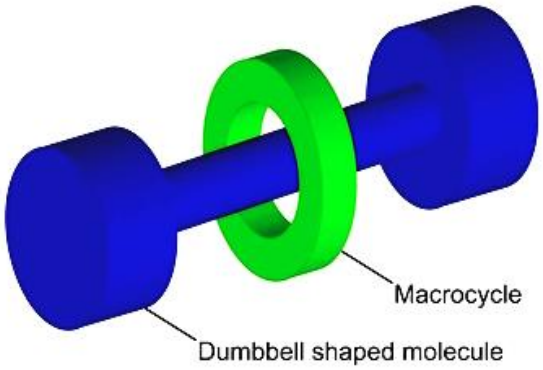

Fig.1: Graphical Representation of a Rotaxane[5].

In this paper we present one possible way to increase the efficiency of electrical conductivity and thermoelectric characteristics for molecular junctions based on Rotaxane molecule by using computational and theoretical methods.

MATERIALS AND METHODS

The Avogadro program[9] was used to draw the rotaxane molecule as a preliminary stage. After that, algorithms pass that rotate the molecule to be on the z axis, which represents the axis of the passage of electrons through the molecule, and then number the atoms of the molecule in the logical order. To obtain the optimized geometries of all systems under investigation in this work, and to compute the electrical conductance , Current-Voltage Characteristics and thermopower, the density functional theory (DFT) methods[10] (the SIESTA code), and a non-equilibrium Green's function formalism , were utilized. For the transmission and Seebeck coefficients calculations, the molecular junction was created by attaching the relaxed molecule to 35-atom pyramidal gold electrodes as shown in Figure 2 with 8 base layers, each layer consisting of 6×6 atoms and a layer spacing of 0.235. From these model junctions the conductance and thermopower, were calculated using the GOLLUM code. All molecules in this study were initially geometrically relaxed in isolation to yield the geometries. To investigate ideal junction

geometries, a small four-atom gold pyramid was attached to the N atoms of the molecules, with Au–N–C angle being 120° and Au–N bond length being 0.23 nm. Geometrically optimization were carried out using the DFT code SIESTA, with a generalized gradient approximation (PBE functional), double ζ polarized basis set, 0.01 eV/A force tolerance, a real space grid with a plane wave cut-off energy of 250 Ry, zero bias voltage and 1 k points.

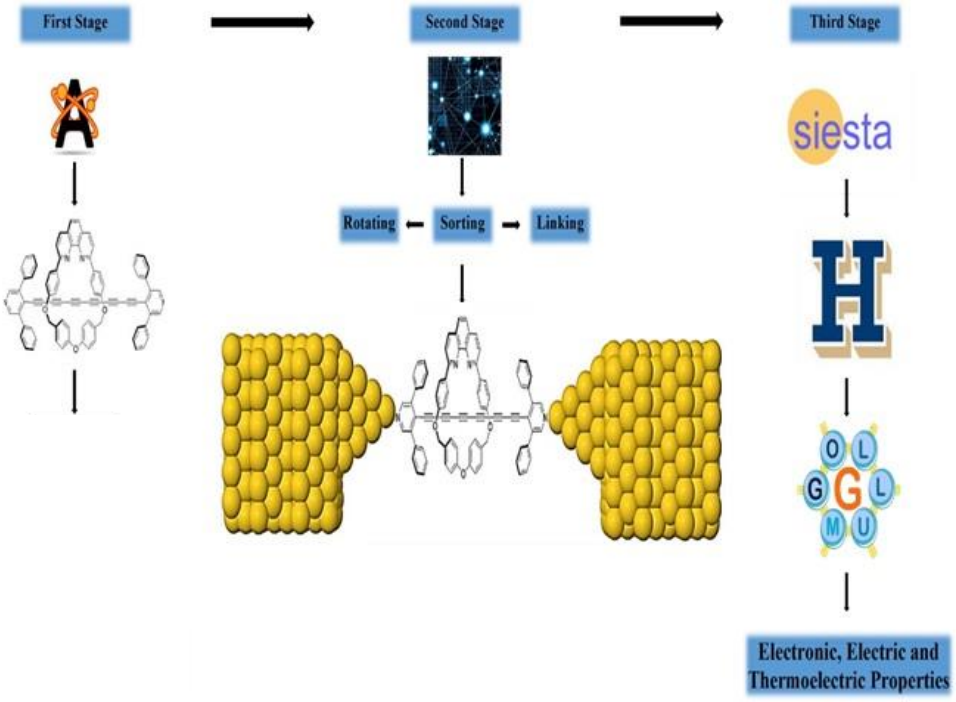

Fig. 2: Theoretical and Computational Methods for Rotaxane junction.

RESULTS AND DISCUSSION

The electronic characteristics of rotaxane molecules depend on the specific design and composition of the molecule. However, the electronic properties of rotaxanes can be influenced by the presence of the macrocycle and the axle, as well as the nature of their interactions [11]. In addition, the electronic properties of the axle can also influence the electronic characteristics of the rotaxane. For example, the axle can have different types of functional groups that can donate or accept electrons, or it can have a specific electronic structure that can defect the interactions with the macrocycle. The nature of the interactions between the macrocycle and the axle in a rotaxane can also affect the electronic characteristics of the molecule. The most basic rotaxane shape consists of a rod-like axle and a ring torus shaped wheel that is threaded on the axle. The wheel part is not covalently bonded to the axle part and is free to move along the axis .This work involves five different rotaxane molecules, which are identical in their backbone (the axle) and differ in the number of rings (macrocycle wheels). The number of rings has been increased from one ring for molecule R-1 to five rings for molecule R-5.

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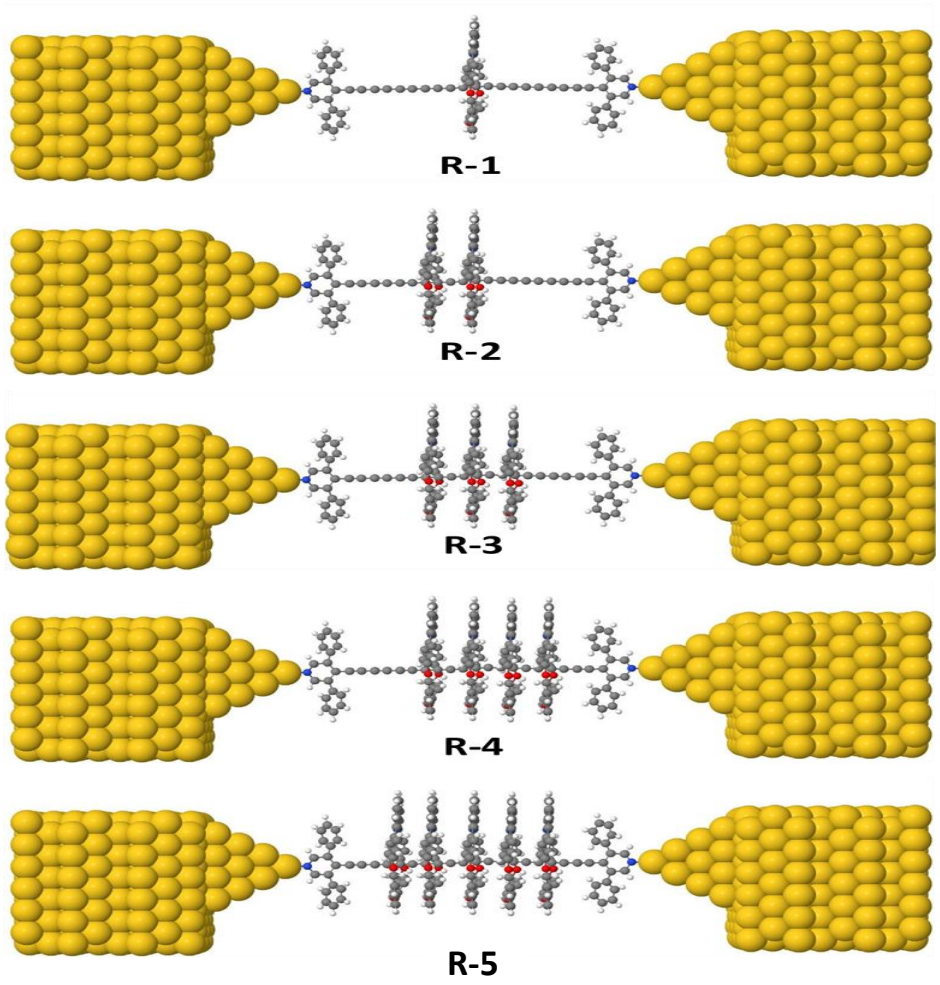

Fig. 3: The optimized geometries at ground state of all molecular junctions.

The transmission coefficient T(E) describing the propagation of electron from the left to the right electrodes. In this thesis, the transmission coefficient have been calculated by obtaining the corresponding Hamiltonian and overlap matrices using SIESTA[12] and then using the GOLLUM code[13]. We note in the Figure 4 that R-5 introduces a high value of transmission coefficient (2.23×10-3), while the lowest value of the transmission (1.61×10-4) is presented by molecule R-1. This result could be explained in terms of the increasing of the donor atoms (oxygen atoms) at the wheels. That means is the raising of oxygen atoms from 3 atoms for R-1 to 15 atoms for R-5, which leads to an increase in the number of transferred electrons Γ as shown in Figure 4. The rings can act as additional pathways for electrons to pass through the molecule, providing more channels for conduction, which leads to increase the value of transmission coefficient and the number of transferred electrons. As a result, the electronic coupling between

the rings and the rest of the molecule can increase, leading to a higher transmission coefficient[14].

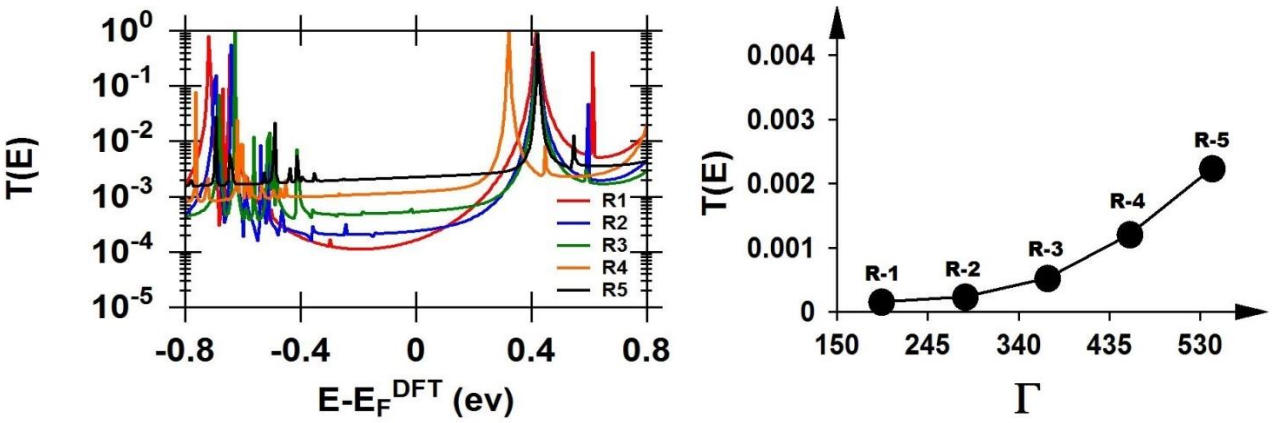

Fig.4: Represents the transmission coefficient T(E) as a function of electrons energy and the transmission coefficient T(E) as a function of the number of electrons transferred from molecule to electrodes of all molecular junctions.

Since Γ equals the number of electrons on the molecule in gas phase (ΓM) minus the number of electrons on the molecule in junction (ΓME),which is the number of electrons transferred from the molecules to the electrodes (Γ=ΓM–ΓME).The bonds that hold the atoms in the rotaxane molecule together act as energy barriers that prevent electrons from moving between atoms. As a result, as the number of wheels increases, so do the atoms. This raises the barriers, which in turn prevents electrons from recombining with holes and increases the amount of free electrons, resulting in a high or low transmission coefficient.

Table 1. Shows the energy levels HOMOs (the highest occupied molecular orbital), and LUMOs (the lowest unoccupied molecular orbital). T(E) is the transmission coefficient. Γ is the number of electrons transferred from molecules to electrodes. H-L gap is the energy gap between the HOMO and LUMO.

Molecule	T(E)	Γ	HOMO (eV)	LUMO (eV)	H–L gap (eV)
R-1	1.6×10^{-4}	196.6	-0.72	0.42	-1.14
R-2	2.4×10^{-4}	283.8	-0.69	0.42	-1.11
R-3	5.2×10^{-4}	369.9	-0.67	0.42	-1.09
R-4	1.2×10^{-3}	455.9	-0.76	0.31	-1.07
R-5	2.3×10^{-3}	542.0	-0.63	0.42	-1.05

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We note in Table1 that the negative sign of the energy gap indicates that the highest occupied molecular orbital (HOMO) energy level is in a lower energy state than the lowest unoccupied molecular orbital (LUMO) energy level.

The molecule is capable of accepting an electron (transition from the HOMO to the LUMO) and participating in electron transfer processes. This explains the negative sign of the energy gap, and the molecule can participate in conducting electrical current, making it important for electronic devices and applications.

The presence of a negative energy gap indicates that the materials or molecules exhibits semiconducting or conducting properties. In these systems, electrons can be easily excited from the filled HOMO to the empty LUMO, allowing for the movement of charge carriers and electrical conductivity.

Defining the concept of the energy gap and its sign is important in the design of electronic devices and provides an insightful study into the electronic properties of molecules, their behavior and performance, which help us in predicting their in various applications, such as molecular electronics and organic semiconductors.

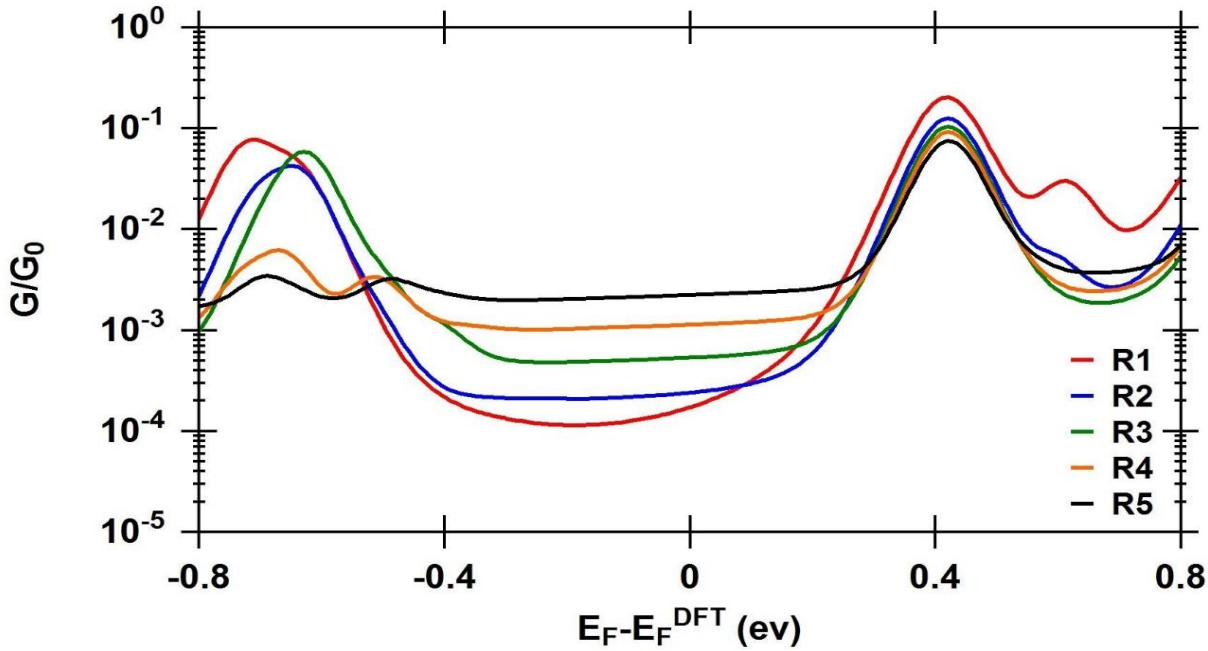

Fig. 5: Represents the electrical conductance (G/G_0) as a function of Fermi energy of all molecular junctions.

An electrical substance's electrical conductance determines its capacity to transfer charges. As seen in Figure 5, the electrical conductance increases with the number of wheels in the rotaxa ne molecule, with R-5 presenting the largest conductance and R-1 introducing the lowest.

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Because of the numerous wheels on the rotaxane molecule, the electric field significantly affects the molecular orbitals' energy levels and charge distribution, increasing conductivity.

Table 2. Shows the electrical conductance (G/G_0). H_{PI} is the HOMO resonance peak intensity. L_{PI} is the LUMO peak resonance intensity. V_{th} is the threshold voltage.

Molecule	(G/G_0)	H_{PI} (eV)	L_{PI} (eV)	V_{th} (eV)
R-1	1.5×10^{-4}	7.6×10^{-2}	2×10^{-1}	0.47
R-2	2.3×10^{-4}	5.9×10^{-2}	1.3×10^{-1}	0.45
R-3	5.1×10^{-4}	4.3×10^{-2}	1×10^{-1}	0.44
R-4	1.1×10^{-3}	6.1×10^{-3}	9.2×10^{-2}	0.43
R-5	2.2×10^{-3}	3.4×10^{-3}	7.5×10^{-2}	0.42

the electrons transport mechanism, since the theoretical Fermi energy (0.0 eV) is located at the middle of the HOMO-LUMO gap[15] close to the LUMO peak resonance.

The current-voltage (I-V) characteristics of a rotaxane molecule describe the relationship between the current flowing through the molecule and the voltage applied across it. The I-V characteristics of a rotaxane molecule can exhibit various behaviors, ranging from ohmic to nonlinear behavior as shown in figure 6. In general, the I-V characteristics can be described by Ohm's law at low voltages, where the current is proportional to the voltage, and the electrical conductance of the molecule is constant. Analyzing the I–V curves in Figure 6 reflects many outcomes. The first one is the value of threshold voltage (V_{th})ranging from 0.47 eV for R-1 to 0.42 eV for R-5. This result means that the increasing of wheels in rotaxane molecules decrease the value of V_{th}. This is an important feature for electronic applications. The second point is exhibited in the framework of the tunneling transport model, it could be identified those contacts are indeed formed by a single molecule. Under these conditions also symmetric coupling situations can be achieved that can be explained by physisorption of the end-groups to the electrodes. Rather high conductance in the range of 1.1×10^{-3} to 2.2×10^{-3} can be adjusted. Further, it has been demonstrated that the change of conductance is mainly achieved by tuning the coupling of the molecular orbital to the metal electrode while the dominant transport level E_0 remains mainly constant. The third point is the molecules favoured physisorption, since both the coupling and the energy of the frontier orbital can be tuned. These findings are important for the further improvement of photochromic molecules in future molecular electronic devices.

Furthermore, these results found rather broad distributions of conductance values in states. The analysis, based on the assumption that the current is carried by a single dominating

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molecular orbital, reveals distinct differences between states. Finally, these results predicated the appearance of light emitting diode-like behavior for the particular species pyridine (PY) that features end-groups, which preferentially couple to the metal electrode by physisorption[16].

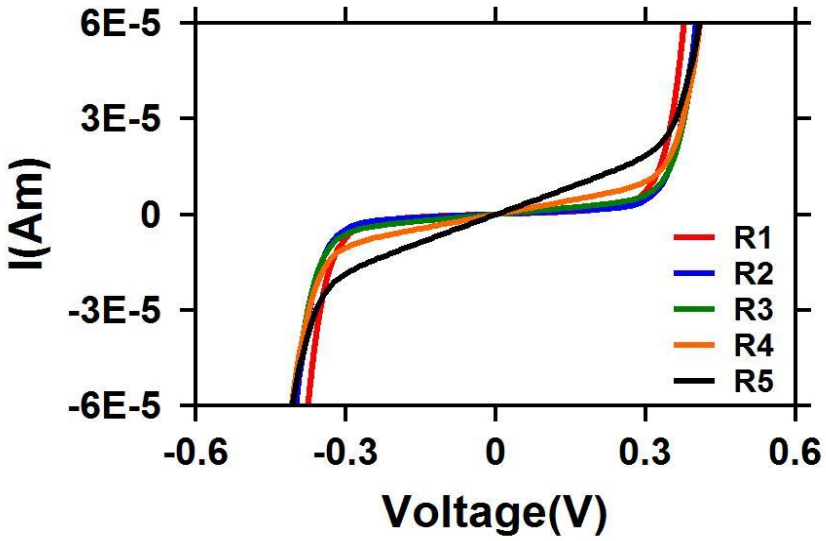

Fig. 6: Represents the current-voltage (I-V) characteristics of all molecular junctions.

The ratio of the perceived power flowing in the circuit to the real power absorbed by the load is known as the power factor of any given system [17].The capacity of a material to extract energy from a thermal differential is represented by the power factor, P, which may also be calculated fr om the single-molecule conductance values, G, and the Seebeck coefficients, S.

$P = GS^2 T$…… (1)

Because molecule R-1 has a considerably greater Seebeck coefficient than molecule R-5, its lower conductance leads to a lower power factor overall. These findings provide significant insight into the relationship between electrical conductance and thermopower: in the context of rotaxane molecular junctions, conductance has a greater impact than thermopower as showed in figure 7.

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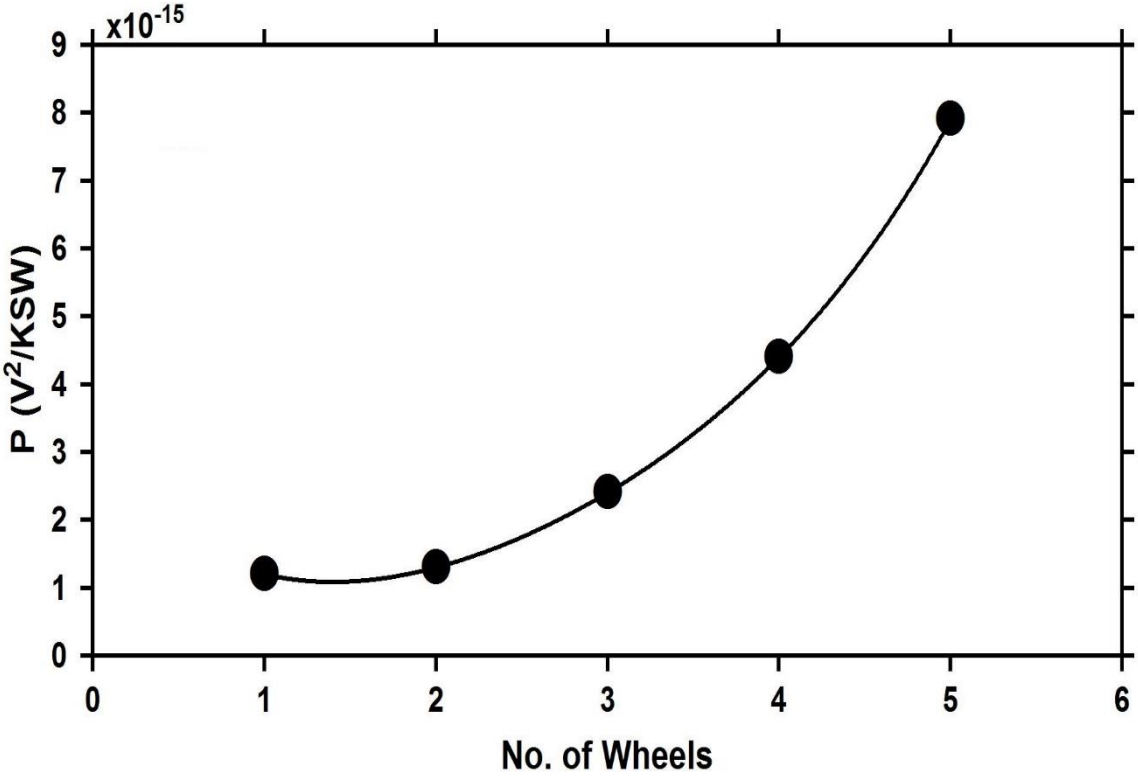

Fig.7:Represents the power factor (P) versus the number of wheels of all molecular junctions.

The decay constant in a rotaxane molecule is a measure of how quickly the electrical or electronic properties of the molecule decay as a function of distance [18]. The decay constant is related to the attenuation length, which is the distance over which the electrical or electronic signal carried by electrons decays as it passes through the molecule. The decay constant can be calculated theoretically or measured experimentally, depending on the specific system and the properties of interest. We notice in Figure 8 that at the beginning of the transfer of electrons and when the Fermi level is close to the Fermi level of the gold electrode, the values increase until the decay reaches its highest possible level at the middle of the Homo-Lumo gap. Then the values decrease until they reach the Homo and Lumo peaks, and this interpretation is completely consistent with Figure 8.Since the lowest T(E) is at the middle of the Homo-Lumo gap in the position where the decay constant value is the lowest possible, we conclude that the calculations of the decay constant are supported by calculations of transmission Coefficient T(E).

For a simple single-channel, rectangular tunnel barrier model, conductance T(E) through the barrier (the molecule) decreases exponentially with the length of the barrier (L) as given equation(2)

$$T(E) = e^{-\beta L} \quad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

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Where β is the decay constant, L is the molecule length. This relationship has formed the basis of many explanations of transmission coefficient within families of similarly structured molecules, with the decay parameter, β, often serving as a proxy measure for the efficacy of wire like behavior.

In the context of rotaxane molecules, the decay constant depends on various factors, such as the length and composition of the molecular wire, the nature of the linker groups between the rings and the axle, and the presence of functional groups on the rings or the axle. The decay constant can also impact other electronic properties such as the threshold voltage (Vth). The threshold voltage represents the minimum voltage required to initiate a significant current flow through the molecule. The given information states that the value of the threshold voltage varies among the different rotaxane molecules, ranging from 0.47 eV for R-1 to 0.42 eV for R-5. This variation in threshold voltage suggests that the decay constant affects the energy barrier for electron transport and influences the onset of current conduction, which shows the behavior between Figure 6 and 8.

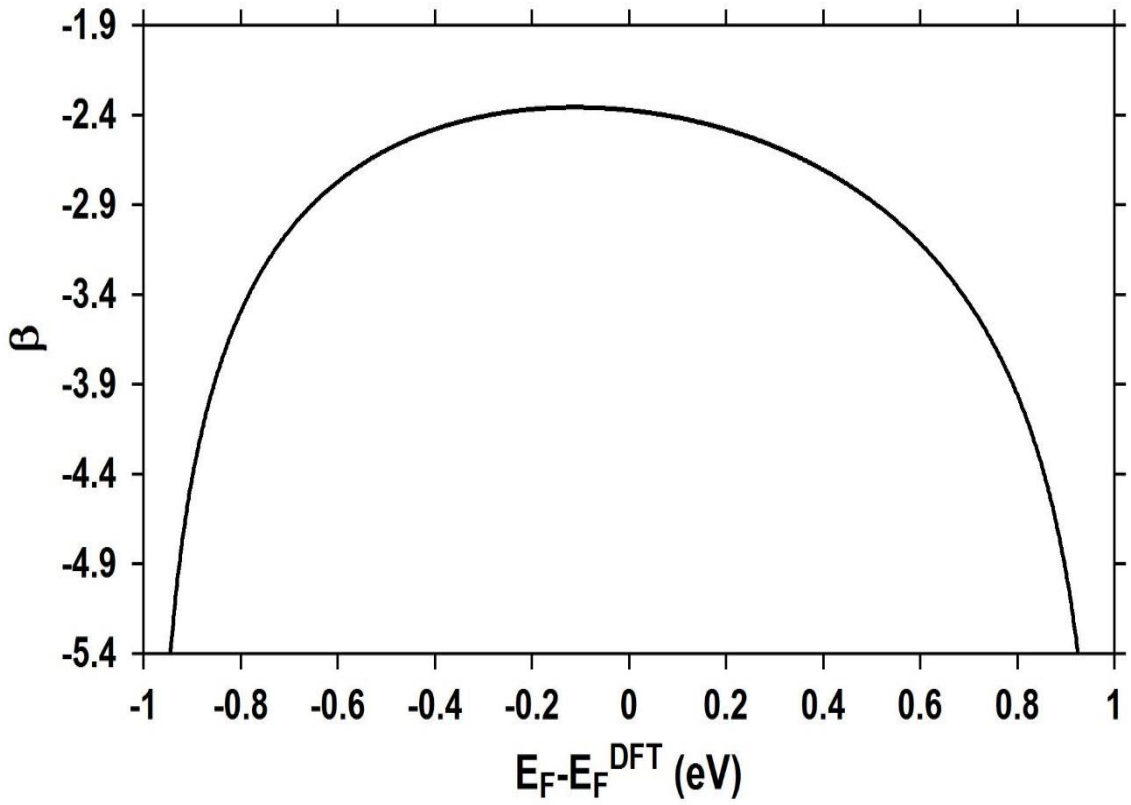

Fig. 8: Represents the electrical decay constant (β) as a function of Fermi energy of all molecular junctions.

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CONCLUSIONS

The findings indicated that the number of wheels in rotaxane molecules can be changed to manage and increase constructive interference, along with the transmission coefficient values. A remarkable conclusion is that the strong relationship between electrical conductance, power factor and threshold voltage potentially leading to a more efficient and high-quality electronic and thermoelectric devices.

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Conflict of interests.

There is no conflict interest

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الخلاصة

المقدمة. يتكون جزيء الروتاكسان من ثلاثة أجزاء رئيسية: العجلة، المحور، والسدادات. أجريت هذه الدراسة لزيادة عدد العجلات للحصول على الخواص الإلكترونية والكهربائية والحرارية لوصلات النانو الجزيئية المعتمدة على الروتاكسان.

طرق العمل: تم إجراء الحسابات لتقييم خصائص النقل والتحسين الهندسي لهذه الوصلات الجزيئية باستخدام مزيج من DFT ورمز SIESTA ورمز Gollum وشكليات وظيفة Green غير المتوازنة. تم ربط كل جزيء بأقطاب ذهبية هرمية موجهة مكونة من 35 ذرة (111). يسمح استخدام DFT وتقريب التدرج المعمم GGA لحساب طاقة الحالة الأرضية لمختلف الوصلات الجزيئية.

النتائج: أظهرت نتائج معامل النقل T(E) قيم عالية، وهذا دليل على ذلك التداخل البناء الذي يتم التحكم فيه وتعزيزه من خلال تغيير عدد العجلات في جزيئات الروتاكسان، مما أثر على فجوة HOMO–LUMO وبالتالي ساهمت في رفع أو خفض قيم معامل النقل. أظهرت العلاقة بين التوصيل الكهربائي والطاقة الحرارية أن أعلى توصيل ينتج طاقة حرارية منخفضة. ثابت الانحلال هو خاصية اساسية تؤثر على نقل الالكترونات، وخصائص التوصيل، وجهد العتبة في جزيئات الروتاكسان.

الخلاصة: أظهرت الوصلات الجزيئية المعتمدة على الروتاكسان قيما عالية لمعامل النقل الإلكتروني، مما يزيد من التوصيل الكهربائي، مما يجعلها واعدة للتطبيقات الإلكترونية. تعد القيمة الأصغر لجهد العتبة خاصية مفيدة لمختلف التطبيقات. نتائج عامل القدرة توصلنا إلى استنتاج مهم، وهو أن تأثير التوصيل يكون أكثر هيمنة من تأثير الطاقة الحرارية في حالة الوصلات الجزيئية الروتاكسان.

الكلمات المفتاحية: معامل الانتقال الالكتروني، نظرية كثافة الحالات، اعلى مدار جزيئي مشغول، ادنى مدار جزيئي غير مشغول، تقريب التدرج المعمم، التوصيل الكهربائي.

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