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## Research Article

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# Spin transport properties in 1D DNA and electrically doped Iron quantum dot organo-metallic junction: A first principle paradigm

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**Abstract:** The DNA sensor has emerged as strong candidates for next generation ultra low power application due to its self assemble technique. Non-Equilibrium Green's Function (NEGF) along with Density Functional Theory (DFT) based First Principle approach is used in investigation of spin transport properties along with quantum scattering transmission characteristics of DNA sensor via Iron (Fe) quantum dots (QD) electrodes at room temperature. Electrically doped Fe QD plays an important role in spin transport mechanism. This electrical doping concentration and weak coupling strength between DNA and Fe QD organo-metallic junction effect into the tunneling contact resistance (TCR) along with quantum-ballistic transmission and junction conductivity of parallel and anti-parallel configuration of this analytical model representation. It has been observed that higher current has been achieved for parallel configuration when compare with anti-parallel configuration at same bias voltage. This voltage-current characteristic is significantly modulated due to the electrical doping effect. This spin transport property shows that this system can well perform for anti parallel configuration. High tunnel organo-metallic resistance approximately 99.9% is observed even at 0V bias voltage. TOMCR remains large at upper bias voltage .

## Keywords:

Nanomaterials, Nanotechnology, Simulation, Spintronics

## Introduction

Spintronics which unlike of electronics uses spin plays a crucial role in the era of nanotechnology. Intrinsic spin of the electron along with its magnetic moment in addition to its fundamental electronic charge is the basics of Spintronics. It is considered to be as one of the most significant rising research arenas with enormous possibilities to provide low power consumption, high speed, and high density logic

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which is applicable for memory electronic devices. This is also useful for lower threshold current and high-power lasers which are applicable for optoelectronic devices as a basis for circularly polarized light. It is not likely that always applicable for magnetic tunnel junction but also applicable for semi-conductor tunnel junction [1, 2]. The effective spin diffusion length is directly proportional to the decay rate of spin current, along with the spin accumulation and the spin chemical potential along the spin current flow direction. In the case of semiconductors the effective spin diffusion length depends on the charge current flowing parallel to the spin current. Spin current is the key concept for Spintronics. There are two significant configurations are described considering spin transport phenomenon. Parallel configuration (PC) and anti-parallel configuration (APC) are the two major configurations which are associated with this spin transmission. These tunnel junctions can be made either for magnetic tunnel or semi-conductor tunnel junction. [1-5]. For the fabrication of Magneto-Tunnel Junctions (MTJ), generally very thin metal oxide layers are used for example SiO<sub>2</sub>, MgO, HfO<sub>2</sub>, ZrO<sub>2</sub> etc. These materials are used as tunnel junctions. Due to limited performance of these materials, inter-diffusion and metal oxide defects affect into these fabrication of tunnel junction devices [6-7]. In some articles, it is illustrated that, Fe doped carbon nano tube (CNT) is used as tunnel junction device. Boron nitride nanotube is also used for this type of spin transport study [3, 4]. Some of the researchers are also advised that SiCNT can be a substitute to CNT due to their improved performance for its large strength, high density, excellent thermal shock resistance property, high operating frequency performance, against harsh environment etc. These properties make this material useful for further studies [8]. Protonation controlled spin transport properties are also conducted for magnetic single molecule junctions. Protonation plays catalytic role in this type of spin transport phenomenon [9]. Multiple molecular effect for example quantum transport, spin-filtering etc. can be investigated for single molecule magnet like Mn(dmit)<sub>2</sub> and phosphorene electrodes using first principle approach [10]. This spin transport phenomenon can be well explained using first principle approach both for organic and in-organic tunnel junctions [11-13].

In this paper, we investigate spin transport properties for DNA and Fe QD organo-metallic junction at room temperature. Two configurations PC and APC for this type of junction are investigated using DFT and NEGF based first principle formalisms. Spin dependent quantum ballistic transmission is investigated in this paper. A comparative study shows the novelty of this tunnel junction in Table 1

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**Table 1. Comparative analysis of existing tunnel junctions along with proposed organo-metallic tunnel junction**

Features	[9]	[10]	[11]	[12]	This work
Approach	DFT+NEGF	DFT+NEGF	DFT+NEGF	DFT+NEGF	DFT+NEGF
Materials	4,40-vinylenedipyridine	Mn(dmit) <sub>2</sub>	benzene ligand	VSe <sub>2</sub>	DNA-Fe QD
Resistance(TMR/90% TCR)		High	High	Very high 1.095×10 <sup>3</sup> %	100%
Current	14×10 <sup>3</sup> nA (approx.)	Satisfactory	20nA (approx)	14nA(approx.)	1.4μA
Force	0.04 eV/Å	0.03 eV/Å.	0.01 eV/Å	0.01 eV/Å	0.01eV/Å

## Materials and Method

This paper presents organo-metallic junction which is formed using DNA and Fe-QD. This Fe-QDs are also used as electrodes. Though weak coupling exists between DNA and two electrodes but it does not affect spin transport phenomenon. This quantum-ballistic model is analytically simulated using Atomistix Tool kit-Virtual Nano Laboratory (ATK-VNL) software simulation package version 13.8.0[14]. This software simulation is used for self-consistent calculations along with Spin polarized Generalized Gradient Approximation (SGGA) exchange correlation procedure. The relaxed geometrical structure with minimum stress is obtained using Quasi-Newton geometry relaxation method. The inter-atomic force and stress is kept minimum. The inter-atomic force is 0.01eV/Å and stress is also 0.01eV/Å<sup>3</sup>. These reduced force and stress are considered to be optimized to get maximum spin transport current flow. This simulation method comprises with single zeta polarization method. The cut-off energy is kept 75Ry with 1×1×100 k-point sampling along x, y, z direction respectively. Electrode temperature is kept 300k to get faster convergence. For PC, the relative spin is to be set at 1/0/1 and for APC it is set to be 1/0/-1 [1]. The gap between electrode and DNA is kept minimal to achieve maximum transport current. The various simulation parameters are shown in Table 2.

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**Table 2: simulation parameters**

Sl. No.	Parameters	Values
1.	Configuration	(x, y, z)
2.	Optical range	Mid-UV (UV-B)
3.	Atomic Force	0.01eV/Å
4.	Poisson Solver	FFT2D
5.	Mesh cut-off density	75Ry
6.	Device algorithm	Krylov
7.	Maximum nos. of steps	200
8.	K-points	1×1×100
9.	Exchange correlation function	Local Density Approximation-Generalized Gradual Approximation (LDA-GGA)
10.	Basis set	Single Zeta Polarization
11.	Hückel Basis set	Hoffmann
12.	Fermi level	0 eV
13.	Atomic Stress	0.01eV/Å <sup>3</sup>
14.	Wavelength	300nm
15.	Input voltage	0V-±0.02V
16.	Time period	1fs

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17. Hybridization	MONO
18. Generic wighting Scheme	Wolfsberg
19. Step size	0.02nm
20. Close neighbour distance	0.01nm
21. Basis sets	Hoffmann

## **Result and Discussion**

This paper shows an organo-metallic junction which is created using DNA and Fe QD. The two ends of this atomistic model are two QDs. The weak coulomb interaction is held between DNA and electrodes. These electrodes are electrically doped to provide faster and highly impressive spin transport quantum-ballistic current flow through the central molecular region. The front view of this organo-metallic junction is shown in Fig. 1. In this device configuration, a single strand DNA is attached with two Fe QDs. The extended parts of these two QDs are considered as two electrodes. DNA is bio-molecule whereas Fe is metallic in nature. Therefore, this organo-metallic junction is to be considered for spin transport activities. The central molecular region is thus considered as a single DNA molecule along with the extended portion of Fe QDs portion.

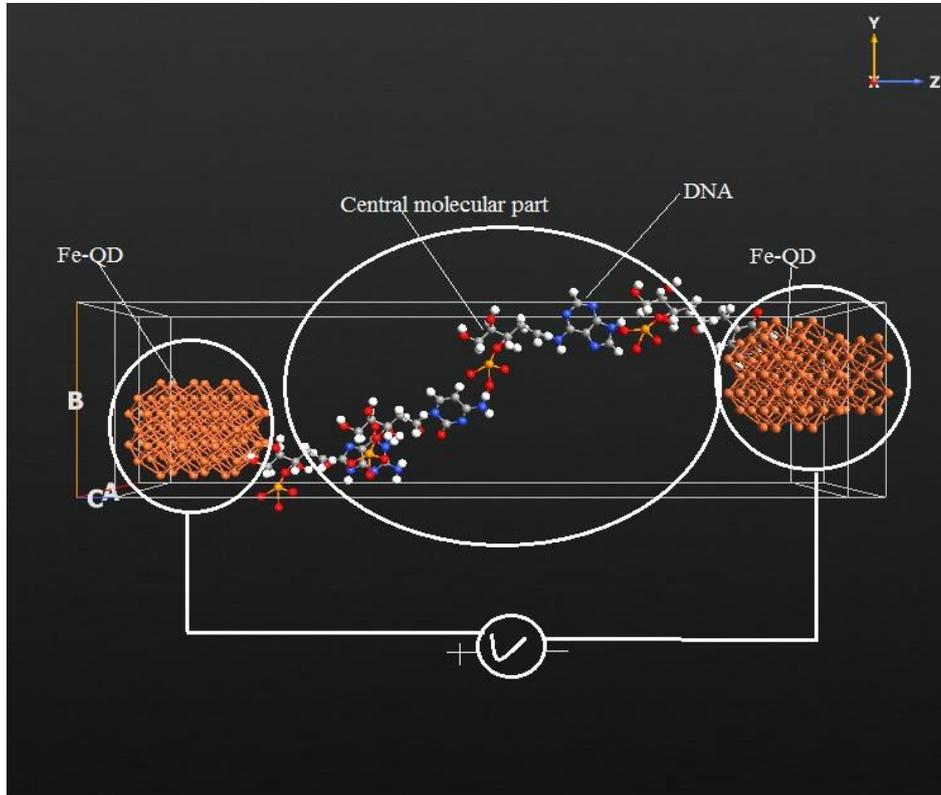


Fig 1. Atomistic model of DNA and Fe QD based organo-metallic junction.

Electrical doping is applied at the two terminals of the electrodes. The amount of doping concentration is changed according to the applied voltage at the two ends of the electrodes. Electrical doping for this device is schematically represented in Fig.2. In this diagram, left electrode and right electrode Fermi level are considered as  $f_L(E)$  and  $f_R(E)$  respectively. A potential drop is generated when an equal and opposite bias voltage ( $V_{DNA}$ ) applied at the two ends of the electrodes. The amount of potential drop into the central molecular region is calculated using Eq.1. This change in electrical doping concentration also makes changes into spin transport current transmission both for PC and APC configuration. The spin resolved current is therefore calculated using Landauer-Büttiker formula which is shown in Eq. (2) [15].

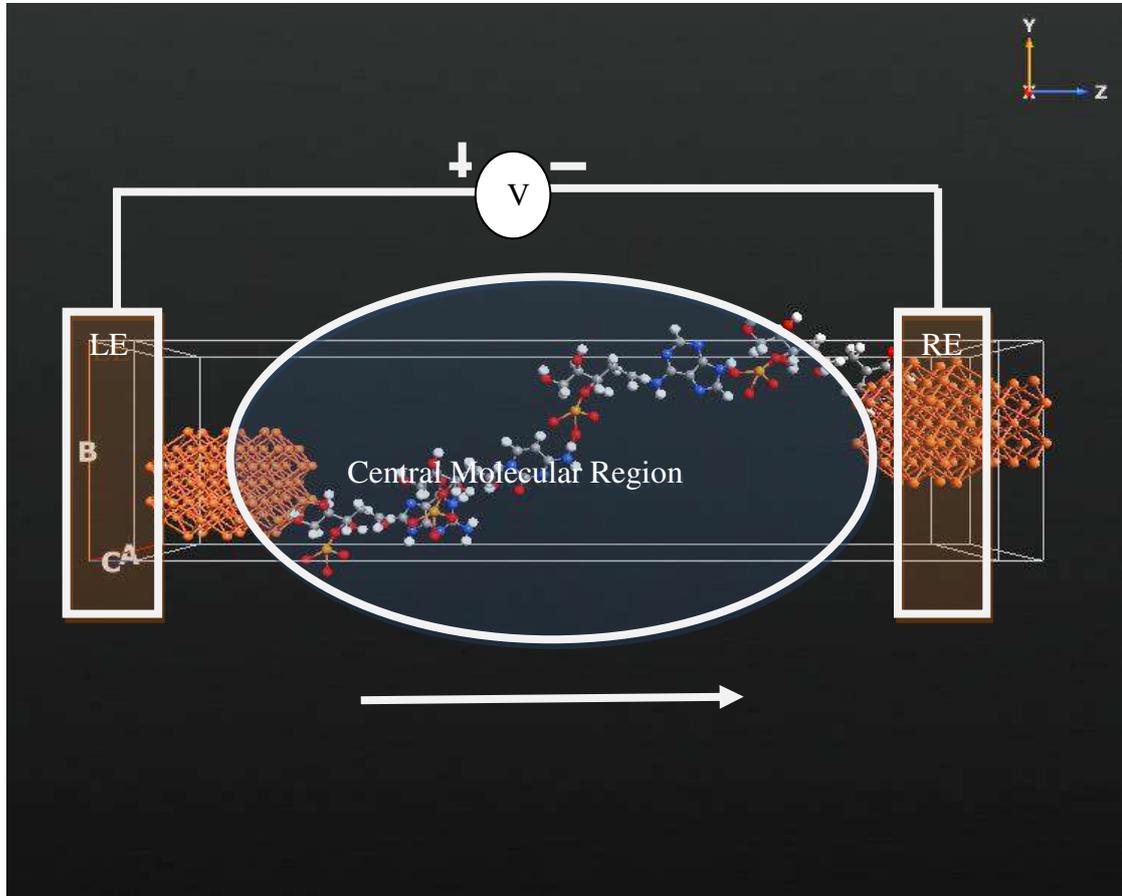
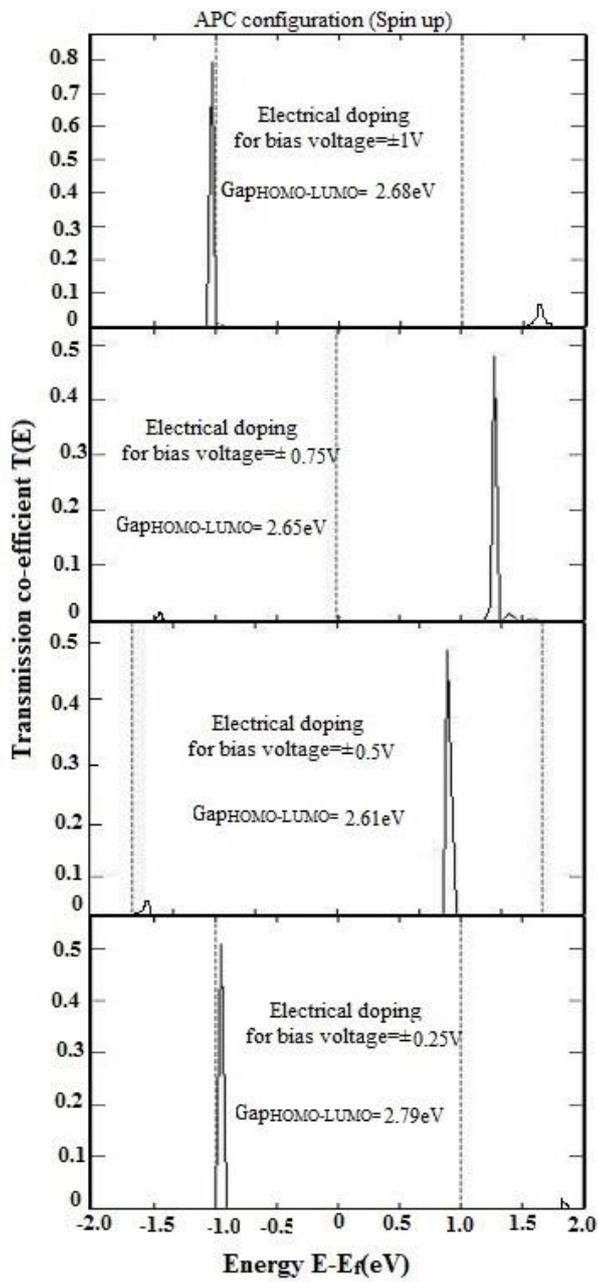


Fig 2: Schematic diagram of the conceptual electrical doping process

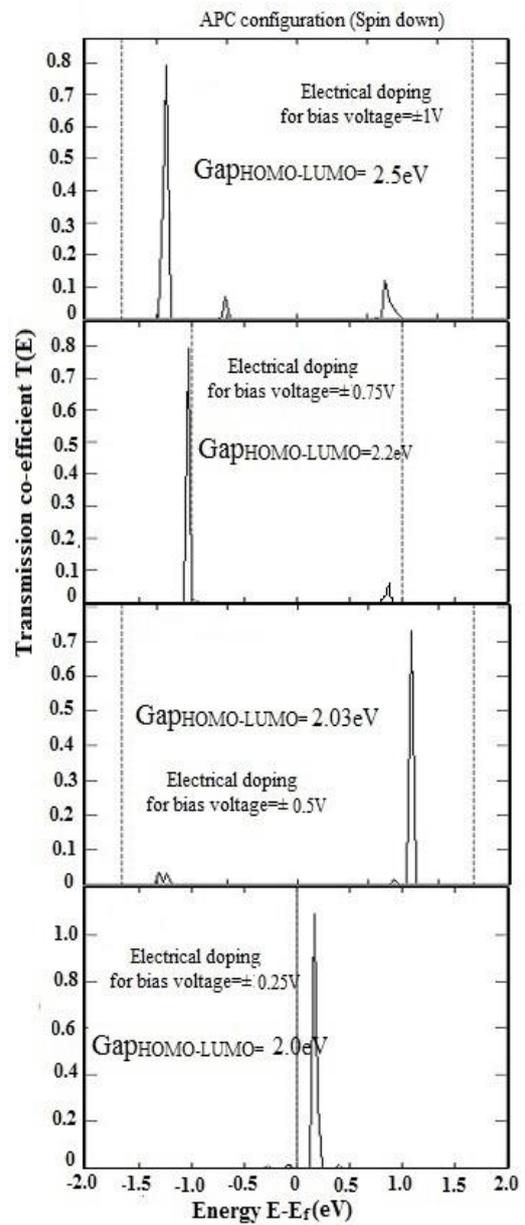
$$f_L(E) - f_R(E) = qV_{DNA} \dots \dots \dots (1)$$

$$I = \frac{2q}{h} \int T(E, V_{DNA}) \uparrow \downarrow [f(E - f_L(E)) - f(E - f_R(E))] dE \dots \dots \dots (2)$$

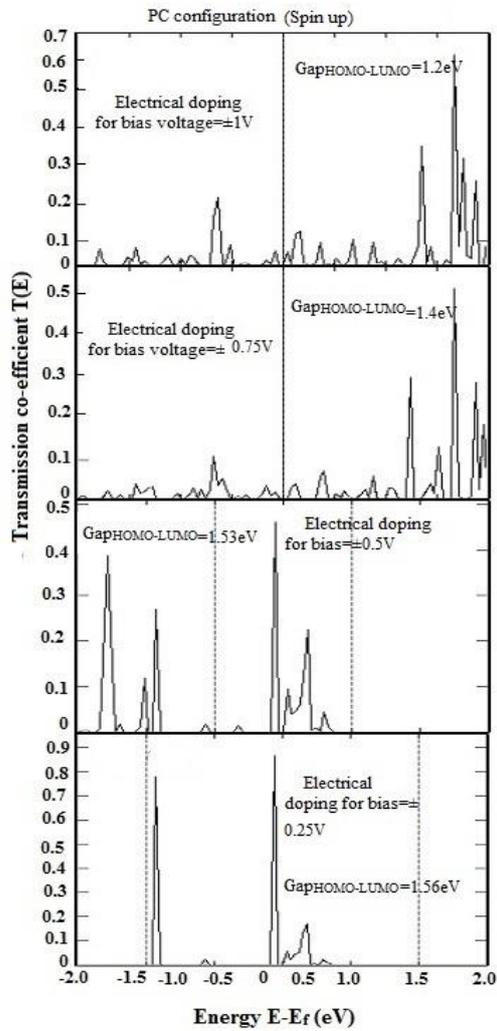
In Eq. (2),  $T(E, V_{DNA}) \uparrow \downarrow$  symbolizes the transport coefficient for spin-up and spin-down channel respectively with energy (E) at bias  $V_{DNA}$ . The transmission spectrum of his device changes for APC and PC configuration. These figures are represented in Fig. 3 both for spin up and down conditions



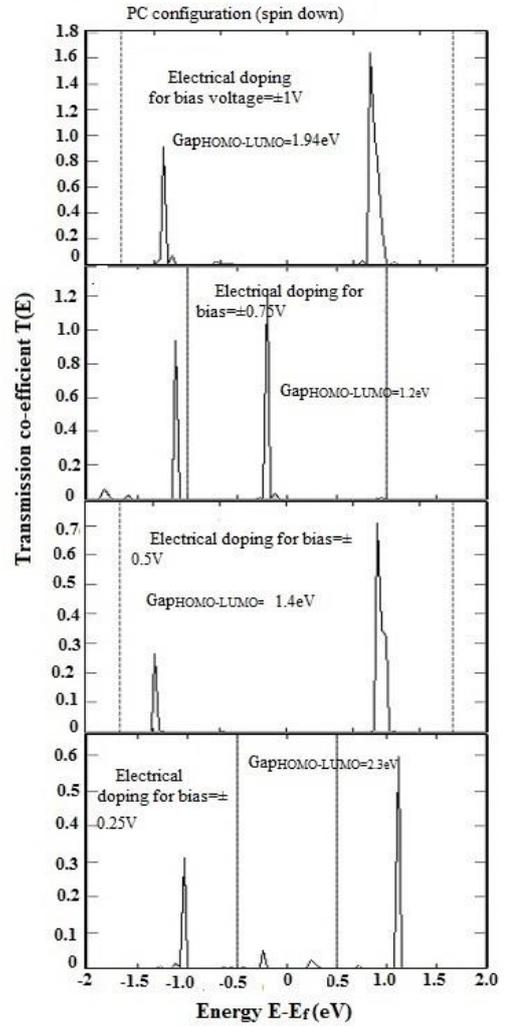
(a)



(b)



(c)



(d)

Fig 3: Transmission spectrum  $T(E, V_{DNA})$  for parallel and anti parallel organo metallic junction configuration for electrical doping concentration ranging from  $\pm 1V$  to  $\pm 0.25V$ .

These figures show that due to the quantum back scattering effect the device has been affected, hence the transmission peaks are slightly displaced from the bias window ( $-2.0V$  to  $+2.0V$ ) for some of the cases which is shown in Fig. 3. It has been observed that transmission peaks as well as Highest Occupied Molecular Orbital –Lowest Un-occupied Molecular Orbital (HOMO-LUMO) gap significantly depends on electrical doping concentration. For APC configuration, we observed maximum gap between HOMO-LUMO during spin up and spin down transport conditions. If the HOMO-LUMO gap is maximum, it signifies high thermodynamic stability which was explained by Jahn –Teller effect [16, 17]. But in the same time, it will reduce channel conductivity as the barrier height is more. Thus spin transport current

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for this APC is lower. Whereas for PC HOMO-LUMO gap is much lower when compared to APC. Thus it provides both thermo dynamic stability as well as higher channel conductivity due to lower barrier height. Therefore, more spin transport current can be observed for PC. High transmission peaks depict higher number of available quantum scattering channels. Therefore, it is also observed that for PC, large number of scattering channels is available. If the electrical doping concentration is increased then barrier height will be lower ,hence large amount of current flows through the central molecular region. Though this transmission is slightly depressed due to back scattering effect which is shown in Eq. (3).Transport co-efficients ( $T[E]$ ) are related with scattering co-efficient. In Eq. (3),  $r$  is the quantum back scattering co-efficient. Due to back scattering effect, quasi-ballistic transport is hampered and the available energy states are less dense within bias window. The dark current is low due to this quantum scattering phenomenon.

$$T[E] = \frac{1-r}{1+r} \dots \dots \dots (3).$$

V-I characteristics for PC and APC are shown in Fig.4 and Fig. 5 respectively. It has been observed that due to lower barrier transmission height, channel conductivity is high, hence large amount of current flows through the central molecular region for PC. High current is observed both for spin up and spin down configuration for PC. Whereas due to large barrier height, low channel current is observed for APC both for spin up and spin down configuration. In case of PC, spin up current is much more compared to spin down current. It can be observed from transmission spectra plot and spin current graphs, that though higher transmission peaks are available for spin down condition but due to smaller barrier height large current is available for spin up condition for PC.

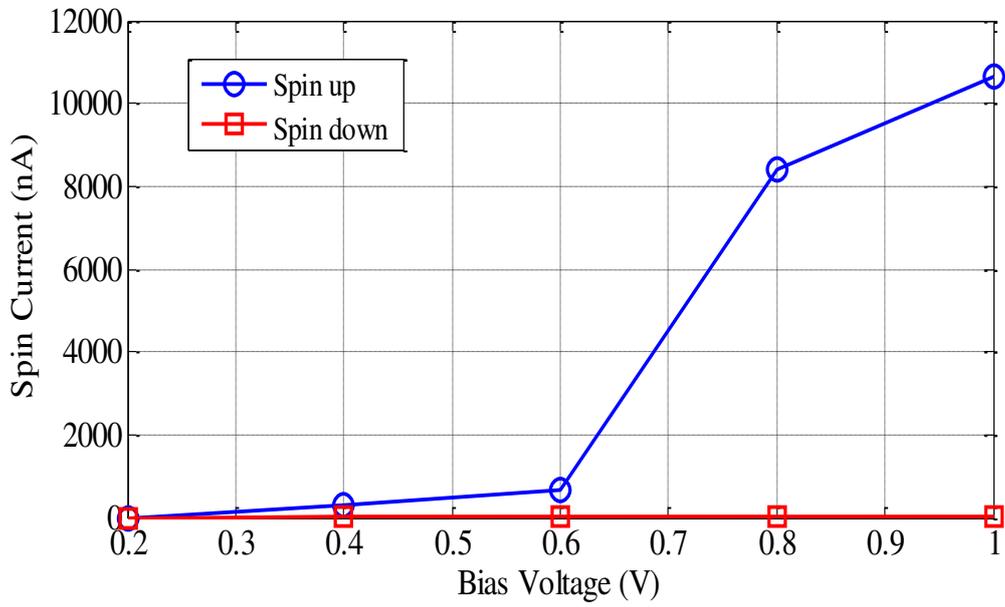


Fig 4: V-I characteristics curve for PC demonstrates total spin current (spin up+ spin down) is approximately equivalent to spin-up current. The spin-down current is roughly insignificant

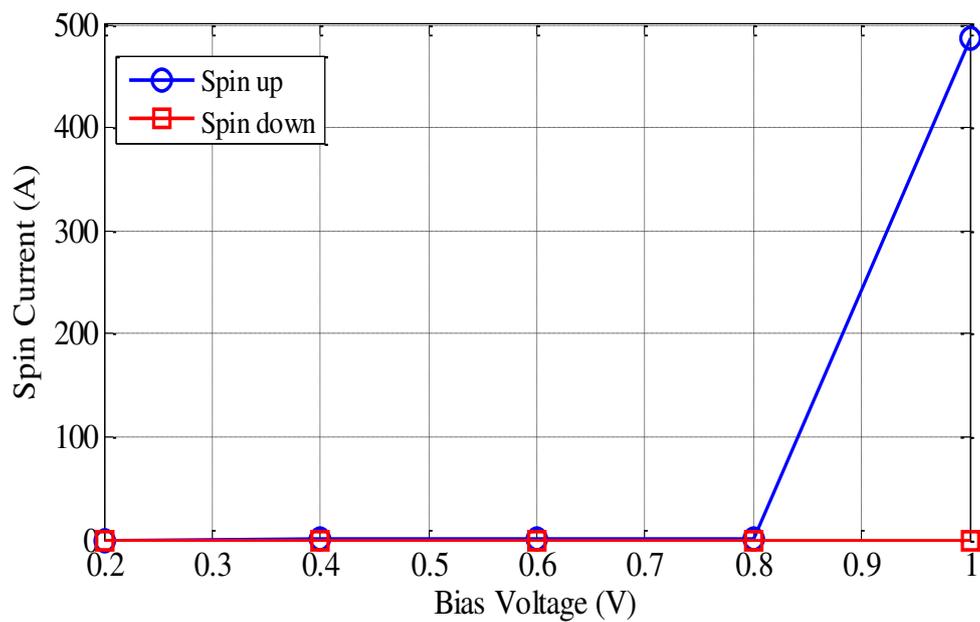


Fig .5. V-I characteristics curve for APC representing spin-up current which is larger than spin-down current when compared at higher bias voltages

Tunneling Organo Metallic Contact Resistance (TOMCR) can be calculated using the following formula which is shown in Eq. (4).

$$TOMCR = \frac{I_{PC} - I_{APC}}{I_{PC}} \dots \dots \dots (4)$$

In this Eq. (4),  $I_{PC}$  and  $I_{APC}$  are the sum of spin current (spin up and down) for PC and APC respectively for this bio-system. At 0V bias voltage, current is almost 0, therefore, TOMCR is calculated as 99.99% which is even increased to 99.9% and remains hold its constant value upto 0.4V bias voltage where  $I_{APC}$  is almost 0. TOMCR value is almost remains high upto 0.4V and then decreases due to the slight increased values in spin current for APC. TOMCR with respect to bias voltage is plotted in Fig. 6. This graph shows that almost constant line has been achieved due to the lower values of spin current of APC. Spin injection factor or spin current efficiency  $\eta$  is calculated using Eq. (5).

$$\eta = \frac{(\text{spin up current} - \text{spin down current})}{(\text{spin up current} + \text{spin down current})} \dots \dots \dots (5)$$

Spin current efficiency is plotted with respect to bias voltage and shown in Fig. 6. Spin current is almost negligible and considered as 0 at 0V bias voltage; therefore  $\eta$  has calculated using conductance at equilibrium. For PC  $\eta$  is obtained almost 100% at all bias voltage. Thus spin –filtration which is approximately 100% , has been obtained for this bio-molecular device for all bias voltage. It is observed from Fig. 7 that 100% spin filtration is also obtained for APC. This is due to the less difference between spin up and spin down current are obtained during APC. This leads to give almost 100% spin-filtering effect. The cross-tick table shows the novelty of this device when compared with existing spin dependent devices in Table 3.

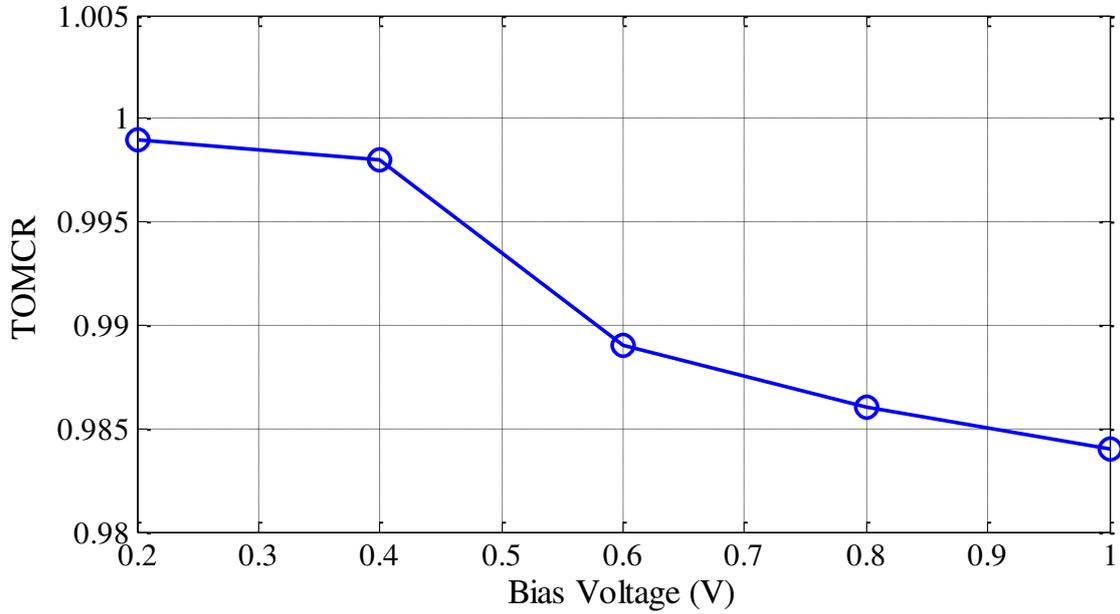


Fig 6: TOMCR vs. voltage. Extremely high values of TMR (~99.9 %) illustrates perfect organo-metallic contact resistance effect

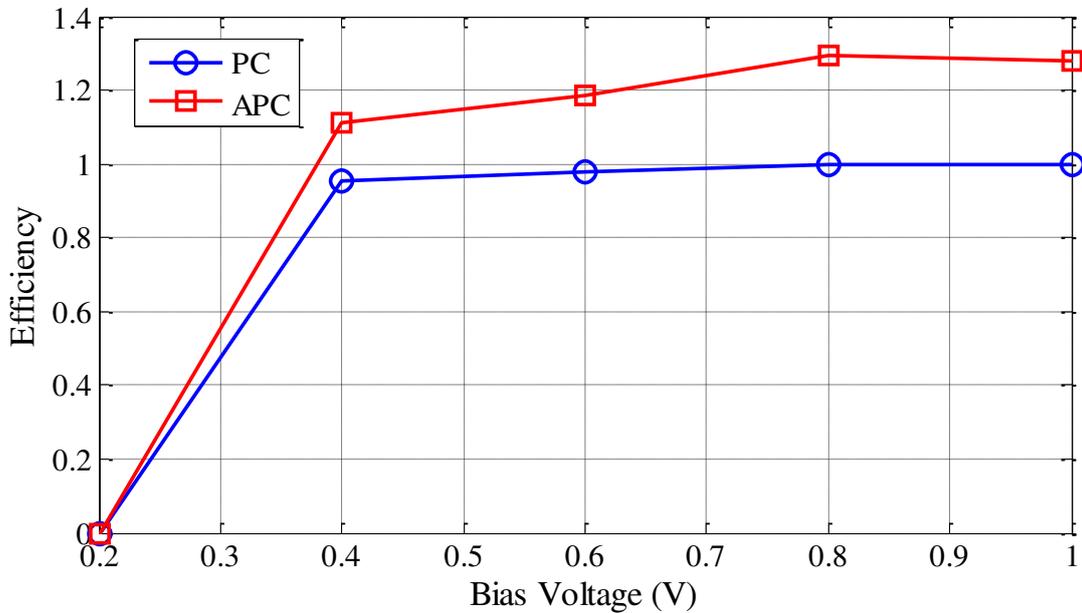


Fig 7: Spin injection factor ( $\eta$ ) or spin efficiency factor vs voltage. Incredibly large values of  $\eta$  shows ideal spin filtration at almost all bias voltages above 0.3V in PC and at larger voltages in APC

Table 3: Cross-tick table for the proposed spin dependent bio-molecular device with existing spin-dependent devices.

Table 3: Cross-tick table for the proposed spin dependent bio-molecular device with existing spin-dependent devices						
Features	[9]	[10]	[11]	[12]	[13]	This work
Bio-materials	√	×	√	×	√	√
High Resistance(TM R/TCR/TOMCR)	×	√	√	√	√	√
Large Current	×	×	×	×	√	√
Reduced Force	×	×	×	×	×	√

## Conclusion

The spin transport phenomenon is observed for this bio-molecular system both for PC and APC conditions. These results show that this device gives almost 100% spin filtration effect both for PC and APC at higher bias voltage. Spin transport current is high for spin up condition both for PC and APC. TOMCR is obtained approximately 99.9% for PC condition. This filtration effect is observed at room temperature operation. Comparative analysis of this device along with existing models proves novelty of this device. This device can be proved as a challenging candidate for future generation spin-dependent device.

## \*Declarations

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Conflicts of interest/Competing interests: *On behalf of all authors, the corresponding author states that there is no conflict of interest.*

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Code availability: *Not Applicable*

Authors' contributions: *All the authors have equally contribution to prepare the manuscript.*

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