Effect of Intra-Molecular Coupling Within Double Segmented Molecules on Equilibrium Magnetic Properties of Molecular Spintronics Devices

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Abstract

The intra-molecular coupling within multiple units of paramagnetic molecules can produce various effects on molecular spintronics devices (MSD). The effect of the nature of the strong magnetic coupling between a multi-segmented molecule with two ferromagnetic (FM) electrodes is unexplored. Such knowledge is of critical importance for magnetic tunnel junction-based molecular spintronics devices (MTJMSD). MTJMSD architecture experimentally allows very strong bonding between complex molecules and ferromagnetic electrodes. In our prior studies, we have extensively studied the atomic analog of the single molecular magnet. That means whole molecular geometry and internal features were approximated to appear as one atom representing that molecule. To advance the understanding of the impact of internal molecular structure on MTJMSD, we have focused on multi-segmented molecules. This research aims to fill the knowledge gap about the intramolecular coupling role in the magnetic properties of the MTJMSD. This study explored a double segmented molecule containing two atomic sections, each with a net spin state and interacting via Heisenberg exchange coupling within molecules and with ferromagnetic electrodes. The effect of thermal energy was explored on the impact of intra-molecular coupling on the MTJMSD Heisenberg model. We performed Monte Carlo simulations(MCS) to study various possibilities in the strong molecule-ferromagnet coupling regime. This resaerch provides insights into the influence of complex molecules on MSD that can be employed in futuristic computers and novel magnetic meta-materials.

I. Introduction

The manipulation of electron spin and its associated magnetic moment is now being applied with increasing pace in spin-based electronic devices; traditional electronics devices exploited just the electron charge. These spin-based electronics (or spintronics) came to light in the 1980s, offering major advantages in terms of speed, heat dissipation, and power consumption [1]. Molecular



Figure 1 3D illustrations of (a) Magnetic Tunnel Junction device (MTJ), (b)MTJ with molecular channels attached to the exposed edges (MTJMSD), (c) Ising model describing the intra-molecular Heisenberg exchange coupling (d) Ising model describing the positions of inter molecular Heisenberg exchange coupling between the molecule and the Ferromagnets (JmL and JmR) and the intra-molecular coupling (Jm).

spintronics devices(MSDs) present an interdisciplinary field at the junction between organic spintronics, molecular magnetism, molecular electronics, and quantum computing, which is advancing fast and promises enormous technological benefits[2, 3]. These devices operate by taking advantage of electrons' charge and spin properties within molecules and magnetic electrodes. Therefore, spin-based MSDs are promising to replace old technologies and produce novel forms of devices[4]. Molecules' small spin-orbit coupling and hyperfine splitting favor the application of molecules in spin devices. Molecules' internal structure can allow the spin to travel within with negligible spin scatterings that are almost impossible with many insulating spacers utilized in popular magnetic tunnel junctions (MTJs) employed in hard drives and heavily researched for the application in random access memory [5]. However, harnessing the molecule's internal quantum property in device forms depends on MSD fabrication. MSDs are produced by several methods (Fig.1a-d). Approaches where molecules are inserted between two magnetic electrodes are limited by vast randomness in producing a gap for molecule insertion between ferromagnetic electrodes. The chemical interaction of a molecule with the two ferromagnetic electrodes is probabilistic and may vary drastically over very weak to the strong range. Hence molecule-ferromagnetic electrode interfaces may create enormous Fermi-energy mismatch, and molecule spin and electrode spin interaction may become unfavorable to harness the true quantum properties of a magnificent molecule as an MSD element[6, 7]. Similarly, sandwiching molecules in multiple layers or monolayers creates difficulty because metal atoms from electrodes can diffuse via molecular layer to yield a system of molecules and atomic defects between two electrodes[8]. Molecule-metal interfaces and molecule-molecule interfaces can produce enormous hurdles in setting optimum spin pathways free from debilitating spin scaterings[9]. A promising MSD must allow an electronic spin state to travel without a change in spin direction for a longer time and distance in a molecule as compared to its inorganic counterparts[10]. We have demonstrated that a highly versatile mass-producible MSD can be realized by utilizing magnetic tunnel junctions (Fig.1c) as the testbed. Magnetic Tunnel Junction Molecular spintronic devices (MTJMSD) (Fig. 1d), are multilayer structures composed of two layers of ferromagnetic electrodes, separated by a ~2 nm insulator. The insulator is called a tunneling barrier that prevents the diffusion of electrode atoms toward the opposite electrode (Fig. 1e). If a voltage is applied, a small number of electrons can travel through the tunneling barrier from one electrode to the other in a wavelike form (Fig. 1e). Highly efficient spin channels, much more efficient than the tunneling barrier, are created by covalently connecting the two ferromagnets through molecular bridges (Fig.1e). Covalent bonds are the strongest form of interactions between two atoms and give MTJMSD an advantage in enabling the flow of spins between the two ferromagnets via the molecular tunnels with the least scattering at the interface and expected to create an ideal situation for Fermi energy matching (Fig.1e). In our previous study, we observed how unprecedented paramagnetic molecule-induced exchange coupling

impacted the microscopic ferromagnetic electrodes with the MTJMSD device approach[11]. One of the exemplary result is long range impact of paramagnetic molecules (Fig. 1f). Our experimental results suggested that molecules with multiple internal spin centers were strongly coupled with the ferromagnetic electrodes. Magnetic force microscopy(MFM) showed a two regular magnetic electrodes of a magnetic tunnel junction without any distinguishable difference in magnetic contrast (Fig.1g) started exhibiting large contrast and long range ordering due to molecular channels (Fig. 1f) [12]. We initially investigated the mechanism of molecule induced exchange coupling by considering octametallic paramagnetic molecule as a single atomic analog[13]. However, a octametallic molecular complex (OMC) used in our work [14, 15] is composed of multiple spin centers that are chemically conded to each other ferromagnetically or antiferromagnetically to manifest a net spin state. Understanding and addressing the challenges of the intra-molecular Heisenberg exchange couplings (J_m) within the magnetic core of the molecule is the knowledge gap that must be addressed for this MTJMSD technology to advance. However, simulating MTJMSD involving complex magnetic molecules, ferromagnetic electrodes, and thermal energy can be extremely challenging. In this paper, we have studied the effect of J_m on the complete cross junction-shaped MTJMSD by representing molecule with two spincenter entity (Fig.1i). This paper provides new understanding of J_m effect on the long-range properties of the ferromagnetic electrode of MTJMSD using Monte Carlo simulation.

Methodology

This paper investigates the effect of intra-molecular coupling (J_m) on the MTJMSD magnetic properties using Monte Carlo Simulation (MCS) (Fig. 1j). We varied J_m magnitude and sign and studied its impact on the MTJMSD magnetic properties at different thermal energies. This study uses the Monte Carlo Simulation (MCS) to investigate the interaction between the molecules and the ferromagnetic electrodes at the cross-junction of the MTJMSD and how the outcome affects the entire device functionality. Based on our studies, the MCS utilizes the Metropolis and iterate algorithm to generate random processes by means of a computer, arising naturally as part of the modeling of the real-life system. MTJMSD model (Fig. 1j) simulated in this study was inspired by our prior continuous spin MCS study explaining the experimental results on pillar-shaped MTJMSD, i.e., without any elongated FM electrodes [16]. In previous research, organometallic molecular clusters (OMC) were attached to two FM electrodes; these OMCs produced antiferromagnetic coupling with one FM electrode and ferromagnetic coupling with the other FM electrode. The magnitude of OMC induced coupling was ~0.5 the Hisenberg exchange coupling energy present between two nearest atoms of the FM electrodes. Hence, we surmise that OMC like paramagnetic molecules can yield very strong exchange coupling of the order of inter-atomic exchange coupling. Due to this reason in this paper we consider specifically molecule induced strong coupling. In this study, we are investigating, for the first time, the magnetic interaction between the molecular layers of the double molecules (intra-molecular coupling).

To avoid prohibitive computational complications associated with complex and transition metalbased molecules, we represented the molecule with a simple atomic-shaped analog involving two two atoms interacting via J_m [17](Fig.1i); hereafter referred to as a molecule or molecular analog in this manuscript. We represented molecule-FM electrode coupling as the Heisenberg exchange coupling and the Molecule-to-molecule couplings (Heisenberg exchange intra-molecular coupling). The size of the MTJMSD model in our MCS study is $H \times W \times L$ (=10×50×50), where Hrepresents the atomic height, W is the atomic width, and L is the atomic length. A molecular plane is a 4×5 atomic square with an empty interior inserted along the H dimension of the MTJ. For achieving the equilibrium state, the system's energy was minimized using the following equation:

$$E = -J_L\left(\sum_{i\in L}\vec{S}_i\vec{S}_{i+1}\right) - J_R\left(\sum_{i\in R}\vec{S}_i\vec{S}_{i+1}\right) - J_{mL}\left(\sum_{i\in L,i+1\in mol}\vec{S}_i\vec{S}_{i+1}\right) - J_{mR}\left(\sum_{i-1\in mol,i\in R}\vec{S}_{i-1}\vec{S}_i\right) - J_m\left(\sum_{i\in R}\vec{S}_i\vec{S}_{i+1}\right)$$

$$I1$$

Where *S* represents the spin of individual atoms of FM electrodes and molecule in the form of a unit magnitude 3D vectors, Figure1g represents the parameters associated with FM electrodes, FM-molecule, and molecule-molecule interactions. J_L , and J_R , are the Heisenberg exchange coupling strengths for the left and right FM electrodes, respectively, J_{mL} and J_{mR} are the Heisenberg exchange coupling strengths between the left FM electrode and molecules and right FM electrodes and molecules, respectively, and J_m , the Heisenberg exchange coupling strength of the molecule within the double molecular layers (Fig.1k). To simulate a wide range of weak to strong ferromagnetic and antiferromagnetic coupling possibilities between the molecular layers, we varied the nature and strengths of J_m , J_{mL} , and J_{mR} . Here, with three variables, J_m , J_{mL} , and J_{mR} , we supposed that inter-FM electrode exchange coupling is zero, and thus there is negligible or no leakage of current or conduction between ferromagnetic electrodes via the tunneling barrier. We

ensure that the intra-molecular coupling strength (J_m) was investigated at different molecular strength values of -1, 0, and 1 and focused on the strong coupling regime only. The equilibrium energy state is determined using the Metropolis algorithm and Markov process [17]. Each Monte Carlo simulation was run for 200 million iterations to achieve a stable low energy state. When the equilibrium state is attained, the spin vectors settle in any direction due to a continuous model used in our MCS study. The sum of the magnetic moment of the left and right FM electrodes and molecules gives the total device magnetic moment[18]. We also investigated the correlation between molecular spins in relation to the FM electrodes. Furthermore, we measured the molecular coupling impact on spatial magnetic susceptibility.

II. Results and Discussion

We conducted 200 M iterations to allow MTJMSD model reach equilibrium state aunder different combinations of intramolecular coupling and overall molecule coupling with the FM electrodes. After MCS simulations for 200M iterations MTJMSD was found to settle in different magnetic states with time as shown in Figure 2 and discussed elsewhere [11, 12]. Temporal evolution of MTJMSD's magnetic properties was studied for variety of couplings strengths and

nature between molecules and FM electrodes. We represented time in MCS as the simulation count. MTJMSD and FM electrodes' magnetic moment were recorded during the MCS period, typically 200 million counts. Based on the Ising Model utilized in this study, left-FM and right-FM electrodes can attain the maximum magnetization of 1200



Figure 2 Variation of total device magnetization with time at Thermal energy (Kt) = 0.1 for;(a) Jm =1, JmL = 1, JmR = 1, (b) Jm = 1, JmL = -1, JmR = 1, (c) Jm = -1, JmL = 1, JmL = 1, JmR = 1, (d) Jm = -1, JmL = -1, JmR = 1.

magnitude. The overall MTJMSD magnetic moment can be nearly 2432(Sum of magnetic moment of two ferromagnetic electrodes and molecules). Figure 2 represents time dependent evolution of magnetization of the overall MTJMSD, left FM, and right FM electrodes at different molecular strength. For the case of Jm = 1, JmL = 1, JmR = 1, MTJMSD's magnetization settled at approximately around 2000 approaching the maximum possible magnetic moment(Fig. 2a). It is noteworthy that thermal energy kT was set to 0.1 for this study to keep simulation relevant to experimental observation made near room temperature (Fig.1g-h)[12]. In this case, the molecules and the FM electrodes are aligned parallel to each other. This behavior indicates a strong intramolecular ferromagnetic magnetic coupling and ferromagnetic coupling between FM electrodes and molecules resulting a gradual attainment of high magnetization state (Fig. 2a). For the case of ferromagnetic intramolecular coupling and molecule ends making opposite strong antiferromagnetic coupling with two FM electrodes (Jm = 1, JmL = -1 and JmR = 1) two FM electrodes evolved to be antiparallel to each other (Fig. 2b). The MTJMSD magnetization evolution occurs gradually. Also, the trend observed in Fig. 2b is consistent with the timedependent experimental observation of various magnetic and transport characteristics during the initial stage of MTJMSD formation [11, 12]. In the case of Jm = 1 JmL = -1 and JmR = 1, the orientation of the molecular spin forces two large FM electrodes to align in an antiparallel state in which left-FM and right-FM electrode cancels each other magnetic moment and produce low magnetic. In this state MTJMSD's magnetization settled to close to ~400.

We realized that based on the molecule and FM electrode types there is a possibility where molecule's end points can form either antiferromagnetic (JmL=-1 and JmR=1) or ferromagnetic coupling (JmL=1 and JmR=1) with the two FM electrodes. We investigated the role of Jm when molecule made different complings with FM electrode. We simulated time evolution of MTJMSD for other possible scenarios. In this case we shifted the intra-molecular exchange strength from 1 to -1 as shown in Fig. 2c (Jm=-1 JmL=1 and JmR=1). Molecules' two segments aligned antiparallel to each other. Also, two FM electrodes stabilized in antiprallel direction to stabilized a low magnetic moment state (Fig. 2c). We observed that the magnetic moment of both right and left FM electrodes cancels out since they are aligned in an antiparallel fashion (Fig. 2c). In both cases (Fig.2b and 2c) two FM electrodes were forced to align in a antiparallel positions. This result suggests that the experimental observations where two FM electrodes assumed opposite magnetic orientations can also be due to the case when molecule made ferromagnetic coupling with two electrode by internally had a net antiferromagnetic coupling (Fig. 2b-c). We also investigated other possibility when molecule made net antiferromagnetic coupling with the two electrodes and possessed antiferromagnetic intramolecular coupling. For Jm = -1, JmL = -1 and JmR = 1 (*Fig. 2d*), the molecule layer aligned antiparallel with respect to right FM electrode and parallel to the left FM electrode. However, right segment of the molecule aligned antiprallel to the left segment. Hence, right segment of the molecule aligned as well as right FM electrode (Fig. 2d). Interestingly, for the last case (Fig. 2d) the rate of MTJMSD stabilization was significantly more than that observed in other cases Fig 2a-c.

For complex molecues, change in intramolecular coupling can produce long range effect on MTJMSD. We investigated the spatial range and variation of intramolecular coupling impact on by studying the stabilized 3D atomic spins obtained after the stabilization process discussed in figure 2. We used the lattice plots to show spatial distribution of atoms' spins orientation for the entire MTJMSD (Fig. 3).



Figure 3 3D simulated lattice plots, for (a.) Jm = 1, JmL = 1, JmR = 1, (b.) Jm =1, JmL = -1, JmR = 1, (c.) Jm = -1, JmL = 1, JmR = 1, (d.) Jm= -1, JmL = -1, JmR = 1

For Jm = 1, JmL = 1, JmR = 1

case, (Fig. 3a) the molecule and the FM electrode all aligned parallel to each other and resulted in uniform color in both the molecules and the FM electrodes. Changing magnetic exchange coupling between the FM electrodes and the molecule resulted in changing correlated states and coherent molecular spins direction. Keeping Jm = 1 we simulated the the case of JmL = -1, and JmR = 1

(Fig. 3b). In this case that the magnetic molecules made antiferromagnetic coupling with left FM electrode (JmL=-1) and ferromagnetic coupling with the right FM electrode (JmR=1). In this case two magnetic electrode aligned opposite to each other (Fig. 3b). As seen in figure 3(b), the FM electrodes' spin alignment strongly depends on the exchange couplings with magnetic molecules. This means that, molecules can force the FM electrodes' spins to take a different spin orientation with respect to each other. This behavior leads to magnetic moments cancellation and takes the overall device magnetization close to zero (Fig. 3c). In strong coupling regime, paramagnetic molecules can become highly coherent with respect to each other and the FM electrodes (Fig. 3c, 3d). We also learned that the molecules could influence MTJMSD magnetic properties dramatically. Conforming with MCS result in Fig. 3b, MFM study showed that thousands of molecules (Fig. 1g-h). This result suggests that the MTJMSD can be a platform to create highly correlated systems by combining molecular magnetism with the ferromagnets.

The simulated 3D lattice plots shown in figure 3 does not reflect the numerical value of correlation between molecules and the different regions of FM-electrodes. However computing dot product between molecular spin and the average of atomic spins in each row for each FM layer will represent the numerical value of correlation between molecules and the FM electrodes. The compution scheme for calculating the correlation is shown below in equation 2.

 $C = (S_m \vec{x} + S_m \vec{y} + S_m \vec{z}). (S_{FM} \vec{x} + S_{FM} \vec{y} + S_{FM} \vec{z})$ [2]



Figure 4 Correlation function for (a) Jm = 1, JmL = -1, JmR = 1, (b) Jm = 1, JmL = 0, JmR = 0, (c) Jm = 1, JmL = 1, JmR = 1

Figure 4 Illustrates the correlation between the molecules and the left and right FM electrodes with the Heisenberg couplings. In this case of Jm = 1, JmL = -1, JmR = 1, (Fig 4a), the molecular spin was positively correlated with the right FM electrode and negatively correlated with the left electrode. For the case of Jm = 1 JmL = 0, JmR = 0, we noticed that there is no correlation exists between FM atomic spin and molecular spin when there is no molecular connection (Fig. 4b). The correlation factor is about zero throughout each layer of the two FM electrodes (Fig. 4b). However, for Jm = 1, JmL = 1, JmR = 1, we noticed that the molecule induced strong correlation between itself and the FM electrodes. It is worth noting that the nature of molecular coupling with FM electrodes defines the spatial correlation state on each FM electrodes. The correlation factor (c) however, was seen to be relatively high within the FM electrodes and around the junction between the molecules and the FM electrode (Fig. 4c). Near FM-molecule junction there were several regions where c was ~0.9. Away from the junction, that is, within the FM electrodes, the correlation c was in the range of 0.75 to 0.8 (Fig. 4c).

We also calculated the spatial magnetic susceptibility, the measure of how much a material will become magnetized in an applied magnetic field. It is the ratio of magnetization (magnetic moment per unit volume) to the applied magnetizing field of intensity. This was calculated in different sections of MTJMSD (Fig. 5). The magnetic susceptibility calculation was carried out, taking in consideration the atoms present along the width of FM electrodes. In the event when Jm = 1, JmL = -1, JmR = 1, the molecular region for on the magnetic susceptibility plot was akin to right FM electrode. However, the left electrode exhibited that of FM electrodes. The molecule to FM bonding in this case is very significant.

Here switching of magnetic moment of molecule and FM electrodes can be extremely challenging (Fig. 5a). In Figure 5b where Jm = 1, JmL = 0, JmR = 0, molecules exhibited higher magnetic susceptibility as compared to the two electrodes (Fig. 5b). Molecules was about eight times more susceptible. Molecules in this situation can selectively respond to magnetic field and provide selective switching

In a similar manner, when Jm = 1, JmL=1, JmR=1 the magnetic susceptibility of the molecular region was in the range of (0.7-0.9) and comparable to that of the FM electrodes in the range of 0.4. Also, FM electrodes possessed non-uniform magnetic susceptibility distribution (Fig. 5c). It is clear that for Jm = 1, JmL=1, JmR=1 case molecule magnetic moment can not be made independently. In other words MTJMSD is completely inter-locked and no switching of magnetic molecule is possible.



Figure 5 Magnetic susceptibility between the double molecule layer and the FM electrodes for Jm = 1, at (a) JmL = -1, JmR = 1, (b) JmL = 0, JmR = 0, JmL = 1, JmR

In our MCS of the MTJMSD, we observed that at Jm = -1 produced strong antiferromagnetic coupling and at Jm = 1 favored strong ferromagnetic coupling between two segments of a molecule (Fig.1i). We investigated the effect of variations in intra molecular coupling for the two cases when molecule made strong ferromagnetic and antiferromagnetic with the two electrodes. It is apparent that major



Figure 6 Variation of device magnetization with respect to molecular coupling strength (Jm)

change in Jm effect start appearing when its magnitude fall below ~0.5. Other striking feature is that as soon as Jm change sign magnetization of MTJMSD also switch. It means an effective mean of controlling the intra-molecular couling may produce switchability. In our previous study we observed that such possibility was not there when molecule coupling strength with two FM electrode was varied. Molecule-FM electrode coupling has to pass a non-zero threshold to allow switching possibility.

Figure 7 shows the effect of Jm on the MTJMSD evolution under varying molecular coupling strengths that is at Jm = -1, Jm = 0, and Jm = 1, at three distinct conditions of increasing thermal energies(kT = 0.01, kT = 0.1, kT = 0.5 respectively) Our MCS results showed that Jm catalyzed a long-range impact on ferromagnetic (Jm = 1), antiferromagnetic (Jm = -1) and paramagnetic (Jm = 0) electrodes at low thermal energy. At higher thermal energy Jm was unable to sustain long range ordering and chaotic state appeared.



Figure 7 (a – c) Shows how increase in thermal energy for Antiferromagnetic coupling (Jm = -1) affects the total device magnetization. (d - f) shows the effect of increased thermal energy when there is no coupling (paramagnetic in the case Jm = 0) and (g – i) for ferromagnetic coupling (Jm = 1) increasing thermal energies, that is kt = 0.01, 0.1, 0.5.

III. Conclusion

In these studies, we used the Monte Carlo simulation to investigate the effect of intramolecular coupling strengths within a double segmented molecules on the magnetic property of the magnetic tunnel junction molecular spintronic device (MTJMSD). We noticed that when the molecules are ferromagnetically coupled (Jm = I), the total device magnetization is maximum within the range of 1800 - 1900. The same behavior was observed within the same range, when the two molecular layers are antiferromagnetically coupled (Jm = -1). By changing the molecular coupling strength position between the range of -1 to +1 in step size of 0.1, we observed that antiferromagnetic coupling was favored at low values of Jm (-1 to -0.1) showing high device magnetization which transitions around Jm = 0 to low. The same effect was observed, as the device showed a strong ferromagnetic coupling at high values of Jm (1 to 0.1) showing high device magnetization. It is interesting to note at this point that at Jm = 0, total device magnetization was about 1200, confirming that our molecule is magnetic in nature. Under the above-mentioned circumstances, it is fair to say that the total device magnetization was greatly influenced by the molecule. The result of our studies also showed that increase in thermal energy has an adverse effect on the magnetic properties of the device, irrespective of the molecular coupling strength. This paper also showed that molecule induced a coupling effect into the entire device this effect was strongest at Jm = -1, and Jm = 1. For our future studies, we aim at investigating the behavior of the same device, using the same parameter at extremely low temperatures using liquid nitrogen, as well as testing magnetic tunnel junction-based sensors.

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