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Non-Metallic Substitutes for New QTC

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***Abstract*: The purpose of this study is to investigate the usage of nonmetal materials to substitute metals currently used in quantum tunneling composites (QTCs). The molecule in focus in this study was C2H4Li2. All testing was done using computational chemistry programs such as Transiesta and Gabedit. The C2H4Li2 molecule was inserted in a lithium wire 11 atoms in length. A voltage was run across the wire while the molecule was inserted in between the wire and the current across the system was measured. The current was measured from voltages 0.00 to 2 eV. The same procedure was followed for a lithium wire 11 atoms in length with no atom inserted, which also served as control.**

***Keywords*: Voltage vs. current, non-conducting and QTC**

1. Introduction

The purpose of this study is to investigate if nonmetallic materials can be used in Quantum Tunneling Composites (QTCs) as a replacement of or supplement to metals. The basis of such a device is, of course, quantum tunneling. Tunneling is an effect observed in which a particle is able to "tunnel" or pass through a barrier which it classically would not be able to. The explanation of this phenomenon depends on the knowledge that particles lack an actual "position" until they are observed. Rather, they are described through the use of wave functions which give the probability of a particle being at a particular location (Kothoryansky, 2016). The integral from negative to positive infinity of the absolute value of the square of the wave function, if the function is normalized, should be equal to one (Washington, 2018). When a particle wave function encounters a barrier, the wave bounces off of the barrier, and is exponentially diminished in amplitude as it goes deeper into the barrier. However, its amplitude, and therefore the probability of the particle's position, never reaches zero. Thus, if an extremely thin barrier is considered, where the particle wave function is only somewhat diminished, the nonzero amplitude means that the wave may exit out the other side of the barrier. Therefore, when a particle hits a barrier, there is a certain probability that it will be reflected, and a certain probability that it will pass through, or tunnel. The shorter the barrier, the less diminished the amplitude of tunneling particles, and thus the greater the probability is of tunneling (Kothoryansky, 2016). Though tunneling can occur with any particle, its effects are most often observed with electrons. The tunneling of electrons leads to a tunneling current, which can be exploited for use in devices.

This study aims to investigate the possibility of a new type of nonmetallic material for use in Quantum Tunneling Composite materials. Such materials make use of quantum tunneling effects as a means of creating pressure sensitive, electrically conductive materials. In their present form, Quantum Tunneling Composites are systems which contain two electrodes, a non-conducting elastomeric matrix between them, and a conducting filler material in the matrix. The filler material consists of many spiked nanoparticles made of metal. The use of spikes increases the probability of tunneling at the tips. When the QTC has no pressure applied, the nanoparticles with their spikes are too far apart to conduct electricity (Washington, 2018). However, the application of external pressure on the QTC compresses the nanoparticles, bringing them closer together, and subsequently increasing the probability of tunneling. The more pressure that is applied, the closer the particles become, and the higher the tunneling current. Thus, QTCs have extensive application in devices which require extreme pressure sensitivity. Most notable at present is the development of robotics with a kind of sense of touch. The QTC (which is extremely flexible) can serve as a pressure sensitive skin, granting operators insight into the grip strength of the machines they are operating. The elastomeric nature of the QTC matrix is what grants the device its flexibility. As such, QTCs can be developed in thin sheets which can be folded, twisted, or compressed easily (Peratech, 2016). This was undertaken through the use of computer programs such as Transiesta and Gabedit which simulate molecules and the effect of applying voltages across them. The data collected determine the viability of a new type of QTC which makes use of nanowire-molecule systems rather than spiked particles. The use of such small, molecular scale systems means that they are inherently spiked.

2. Methods

Note- The data yielded from this study is entirely quantitative, since only computer simulations are being used. Additionally, a series of programs especially written for inserting molecules into the Lithium wire and running many voltages across it were used.

A. Methodology

The first step in the study was constructing the C2H4Li2 molecule that was to be used. Gabedit software was used to construct and obtain the optimum structure for the molecule and the Li chain. Using nwchem, an equilibrium structure search was conducted on each molecule using the hybrid functional option. The density functional used was B3LYP, with cc-pVDZ as the basis set. The study also made use of several programs

written in python just for this project. One of these programs was used to ensure the C2H4Li2 molecule fit into the Li chain. The Li chain with no molecules inserted has 11 Li atoms and is 27.1 angstroms long. The program requires that the molecule must have a Li atom on both ends so it can be integrated into the wire. The molecule C2H4Li2 fits this criterion. After the equilibrium structure search, the molecule coordinates were stored in a struct. fdf file. When transiesta is run using this file, it sends a set voltage across the system and records the current. In order to plot trends, large amounts of data are required so this file was run in transiesta repeatedly with varying voltages. Another program written in python was used to automate this process. The voltages varied from 0.00 to 2.00 eV with an increase of 0.1 eV each time. The same process was repeated for the Lithium wire with no insert. The aforementioned program was used to run transiesta 21 times on the Lithium wire. Thus, this data allows comparison between the conductivity of the two systems (with and without C2H4Li2) at the same voltages. Apart from this, it is also important to consider the conductivity of the wire with a gap. This gap was simulated by shifting every atom in the transiesta file by 0.1 lattice constants (2.4 angstroms). By doing so, it was possible to gauge the ideal size for each nanowire, in terms of maximizing conductivity. Gaps of 0.1 lattice constant were added in the center of each wire until the observed current became negligible, defined to be anything less than 1E-11 amps. Using the data gathered, it was necessary to determine how it would be applied in a QTC type device. The molecules would have to be at a minimum density, beyond which tunneling would occur. Essentially, it was necessary to determine the molecular concentration at which the molecules would be just touching, when any external pressure would cause tunneling to begin. The molecules, in this case, would be the nanowire-insert systems created earlier. An approximation of the volume of each nanowire-insert system, using the longest dimension therein, would be

$$Vo=(1/6)\pi d^3$$

The number of molecules of the nanowire-insert system when they are each just touching one anothe

$$Nmolecule= 1\ litre/Vmolecule$$

For the purposes of the calculation, a container volume of 1 liter is assumed. The number of moles of the molecule at overlap is

$$n\ overlap=Noverlap/\ N\ avagadro$$

Thus the concentration is

$$C= n\ overlap/1\ Litre$$

The fact that the concentration is given in molarity means that it holds true for any container volume.

3. Results

Table 1
Applied voltage and resulting current for Li nanowire with no insert

Table 1: Applied Voltage and Resulting Current for Li Nanowire with no insert

Applied Voltage (eV)	Current (amps): No Gap	Current (amps): 1 Gap	Current (amps): 2 Gaps
0	0	0	0
0.1	1.05E-12	2.35E-11	0
0.2	1.16E-12	3.12E-11	0
0.3	6.93E-12	1.78E-10	0
0.4	8.97E-12	1.3E-10	0
0.5	6.32E-11	3.67E-11	0
0.6	3.21E-10	6.89E-11	0
0.7	1.71E-10	8.78E-11	0
0.8	1.32E-10	2.94E-10	0
0.9	2.98E-10	2.58E-10	0
1.0	4.1E-10	3.67E-11	0
1.1	1.89E-10	6.10E-09	0
1.2	2.55E-10	3.98E-11	0
1.3	2.78E-10	8.86E-12	0
1.4	3.21E-10	6.69E-09	0
1.5	1.57E-10	1.59E-11	0
1.6	3.34E-10	5.58E-11	0
1.7	1.44E-10	1.46E-08	0
1.8	2.45E-10	7.10E-12	0
1.9	6.57E-10	1.62E-10	0
2.0	5.67E-12	1.86E-10	0

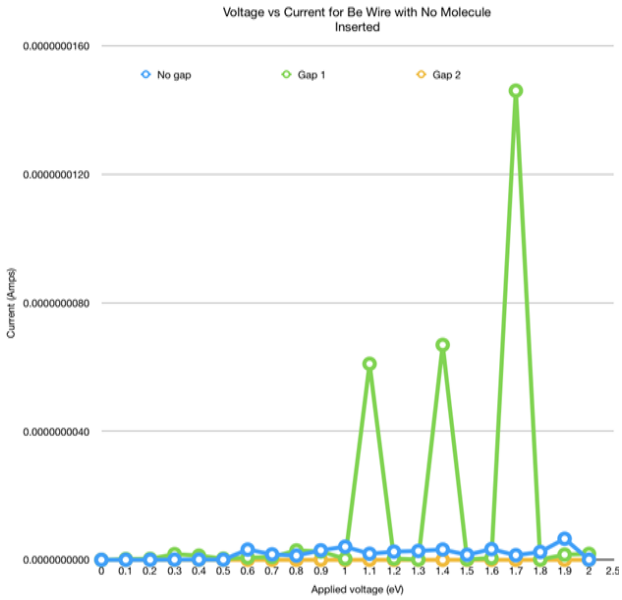


Fig. 1. Voltage vs. current for be wire with no molecule inserted

Table 2
Applied voltage and resulting current for Li nanowire with C2H4Li2 insert
Table2: Applied Voltage and Resulting Current for Li Nanowire with C2H4Li2 insert

Applied Voltage (eV)	Current (amps): No Gap	Current (amps): 1 Gap	Current (amps): 2 Gaps
0	0	0	0
0.1	2.35E-06	5.21E-06	5.89E-11
0.2	3.86E-06	8.02E-06	1.75E-10
0.3	7.86E-06	8.93E-06	9.92E-11
0.4	7.43E-06	9.76E-06	1.94E-10
0.5	8.26E-06	1.67E-05	1.68E-10
0.6	9.49E-06	1.89E-05	1.79E-10
0.7	1.02E-05	1.86E-05	2.59E-10
0.8	1.48E-05	2.02E-05	2.02E-10
0.9	1.32E-05	2.14E-05	1.96E-10
1.0	1.34E-05	1.94E-05	2.34E-10
1.1	1.63E-05	2.25E-05	1.97E-10
1.2	1.25E-05	2.37E-05	2.56E-10
1.3	9.85E-06	2.64E-05	2.78E-10
1.4	9.63E-06	2.58E-05	2.36E-10
1.5	9.01E-06	2.69E-05	2.79E-10
1.6	8.81E-06	2.87E-05	2.85E-10
1.7	8.17E-06	2.78E-05	2.67E-10
1.8	7.64E-06	2.86E-05	2.97E-10
1.9	7.78E-06	3.02E-05	2.82E-10
2.0	7.12E-06	3.16E-05	2.89E-10

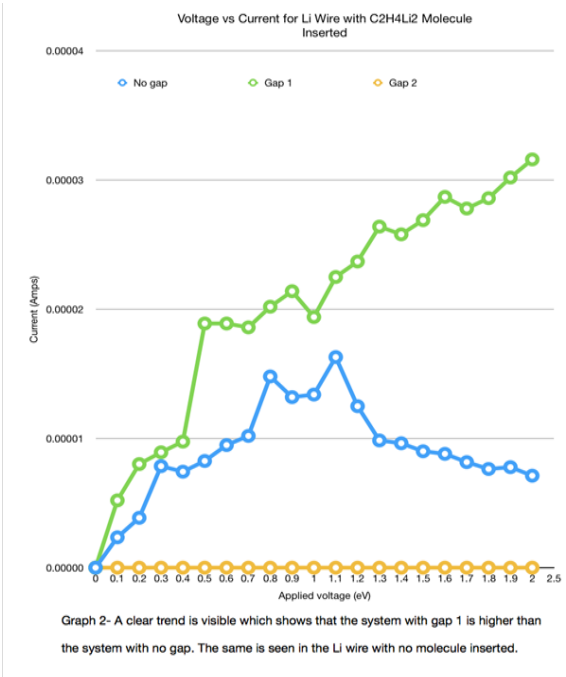


Fig. 2. Voltage vs. current for Li wire with C2H4LI2 molecule inserted

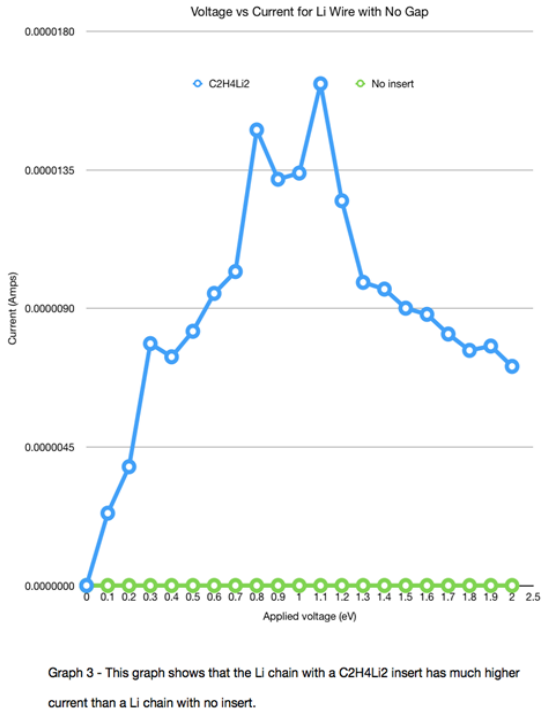


Fig. 3. Voltage vs. current for Li wire with no gap

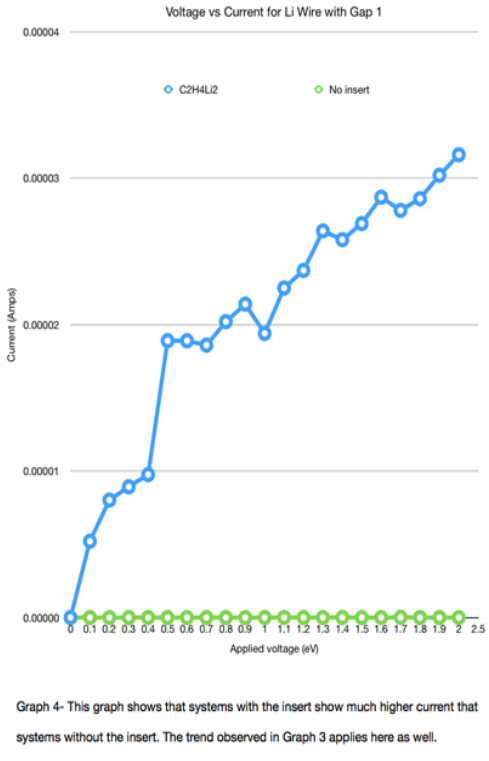
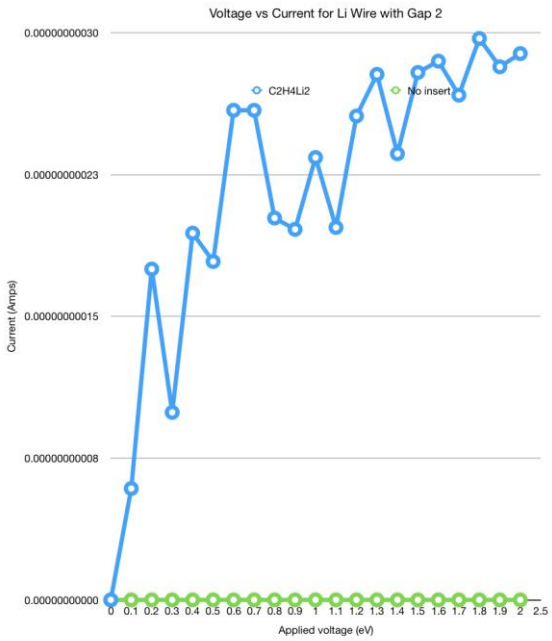


Fig. 4. Voltage vs. current for Li wire with gap 1



Graph 5- This graph shows that systems with the insert show much higher current that systems without the insert. The trend observed in Graph 3 applies here as well.

Fig. 5. Voltage vs. current for Li wire with gap 2

4. Discussion

The purpose of this study was to determine whether or not C2H4Li2 is a viable nonmetallic insert in a Lithium wire to create a QTC. It was originally hypothesized that C2H4Li2 would not be viable and would rather decrease conductivity, due to the usually superior conductivity of metals. The results of the experimentation, however, indicate that this hypothesis was incorrect. C2H4Li2 proved a strong conductive insert, raising conductivity by over a million times, compared to the Li wire. Rather than a flaw in experimental design, this points to misconceptions about how electrons were tunneling through the wire. It was thought previously that the reason that metals were so effective in QTCs was their loosely bound valence electrons, which would facilitate easy electron flow. This property of metals is only partially responsible for their usage in QTCs. It appears electron density plays a more important role in quantum tunneling than conductivity. The Carbon atoms in the C2H4Li2 molecule create a high electron density area due to its difference in electronegativity when compared to Hydrogen and especially Lithium. This region of high electron density facilitates quantum tunneling of electrons and thus increases current. In the Lithium wire without the insert, there would be a constant but low electron density since Lithium has only one valence electron. With the C2H4Li2 insert, due to the higher abundance and concentration of electrons, quantum tunneling is enhanced. The reason that the wires with a gap of 0.1 lattice constant in the center have a higher tunneling is less clear. The gap likely lowers the magnitude of electrostatic potential in the area around it. This could lower some of the obstacles to tunneling, essentially creating a smaller barrier for the electrons to tunnel through. Especially in the case of the Insert wire, the gap probably reduces negative electrostatic potential around Carbon, allowing electrons to become more attracted to the atoms, and thus more likely to flow in that direction.

5. Conclusion

The objective of the study was to determine whether or not nonmetal inserts like C2H4Li2 could increase tunneling through a Li nanowire. C2H4Li2 is an effective insert and accomplishes its target of increasing tunneling. It is likely that a new QTC can be developed which uses Li nanowire with nonmetallic inserts that act as pikes instead of spiked particles. The experiment, though useful in determining whether or not C2H4Li2 can be used as an insert in a QTC is limited by a computer simulation. The feasibility of actually creating particles described in the study is unknown. However, this is a basis towards another step in QTC technology.

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