

Hybrid Molecular-Junction Technique for Enhancement of Electrical Conductance and Non-exponential Conductance-Length Dependence

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Abstract

In an attempt to enhance electrical conductance and improve the formation probability of a molecular junction, a hybrid method was established. Charge transport and conductance-length dependence (exponential decay) in hybrid acene-based molecular junctions was investigated using Density Functional Theorem (DFT) in combination with Non-equilibrium Green's Function (NEGF) formalism. Lower acenes was employed to explore desired electronic functions in order to diversity the electrical properties and designs of molecular junctions by employing heterogeneous structures. The transmission coefficients $T(E)$, the Frontier Molecular Orbitals (FMO) in consideration of their gap (HOMO-LUMO gap) and the electrical conductance-length dependency were investigated. The results showed that hybrid molecular junctions enhanced electrical conductance and is recommended for anthracene and pentacene molecules. It also showed that the anchoring materials have a significant effect on the HOMO-LUMO gap of the junction. It is also observed that the hybrid molecular junctions showed a non-exponential conductance decay. Lastly, we recommend that the practical implementation of these hybrid molecular junction will bring about a lot discoveries of functionalities and applications in nano electrical circuits.

Keywords: Anthracene; conductance; DFT; HOMO; LUMO; NEGF; tetracene; transmission

1. Introduction

In recent years, there has been significant interest in the study of charge transport in Molecular Junctions (MJs). These systems consist of a molecule sandwiched between two metal electrodes. Understanding the nature of charge transport across these interfaces is of crucial importance for the improvement in molecular electronics. One class of molecules that has been studied as potential candidates for MJs is the acene family (Gozalvez *et al.*, 2019) which includes molecules such as anthracene, tetracene and pentacene. Acenes belong to the family of aromatic compounds that have received significant consideration for invention of electronic devices (Anthony, 2006; Thorley and Anthony, 2014; Yuan, *et al.*, 2021). These molecules have extended π -conjugation, which allows for efficient charge delocalization and transport. Acenes and polyacenes are capable for charge transport due to the strong conjugation between the benzene rings (Yang, *et al.*, 2016; He, *et al.*, 2020). Moreover, they represent good model structures for understanding the properties of more complex configurations (Shen, *et al.*, 2018; Zade and Bendikov, 2010; Ibrahim, *et al.*, 2022).

Some studies have shown that transport properties like conductance (G) depend on the system length (Bendikov, *et al.*, 2004; Lucas, *et al.*, 2021). At long-range, the molecular conductance generally indicates a linear length dependence linked with thermal activation and described by an illogical mechanism (Nichols, *et al.*, 2010). At short-range, the transport does not depend on the temperature (Yannick, 2020). At this range, the conductance exhibits an exponential decay with length of molecule and it is represented by equation (1) as given below (Valdiviezo, *et al.*, 2021);

$$G(L) = A \exp(\beta L) \quad (1)$$

where L is the molecular length, A is a prefactor that depends on the molecule-electrode contact, and β is the decay (attenuation) factor related to the tunneling barrier of the molecular region. The fast degeneration of the conductance with molecular length (Equation 1) restricts the formation of molecular-based electronic components. Some previous studies (Yannick, 2020; Fujii, *et al.*, 2020; Yelin, *et al.*, 2016), show the conductance of a chains of carbon-based compounds without anchoring groups. In these studies, the electrodes are joined directly to the π -orbital organic molecules and revealed a conductance to be high and independent of molecular length with a very low formation probability. Another study analyzed the conductance of a molecules connected to electrodes via anchoring groups predicted a near length-independent conductance (Gryn'ova, and Corminboeuf, 2019; Noori, *et al.*, 2021). Other studies have compared the conductance of MJs with anchoring groups showing that the anchoring design governs the electron transport path. These MJs has a high formation probability but low conductance value (Vincent, *et al.*, 2020; Yoo and Kim, 2015).

In an attempt to enhance electrical conductance of a MJs, and improve its formation probability at the same time, a hybrid method was established. Charge transport in hybrid molecular junctions has been a topic of recent research interest (Chen, *et al.*, 2020; Hu, *et al.*, 2022; Pinheiro, *et al.*, 2020). Hybrid molecular inorganic junctions have been investigated, showing a transition in the charge transport mechanism associated with the spin state conversion of the embedded spin crossover complex (Valdiviezo, *et al.*, 2021);

In this study, a combination of density functional theory (DFT) calculations and the non-equilibrium Green's function (NEGF) formalism were employed to investigate the charge transport properties of a hybrid acene-based MJs. DFT calculations are used to determine the electronic structure of the molecules and its interaction with the electrodes. This involves solving the Kohn-Sham equations to obtain the energy levels and wavefunctions of the system. The HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) energy levels of the acene molecules are crucial in understanding the charge transport behavior. The energy alignment of these levels with respect to the Fermi levels of the electrodes determines the charge injection and extraction process at the electrode-molecule interfaces. NEGF calculations are then performed to obtain the transmission spectrum. These theoretical investigations compliment experimental efforts and facilitate the design and optimization of molecular devices for various electronic applications.

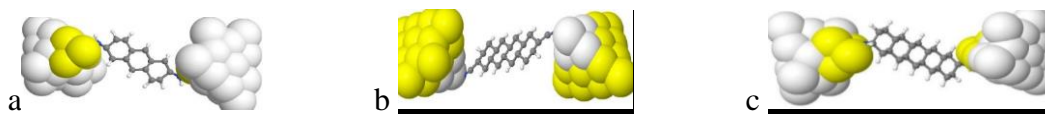


Figure 1: Acene-based MJs with Single Contact to Electrodes via Amines Anchor Group

2. Materials and Methods

This work involves a modelling of the extended structure, energy band calculations as well as charge transport simulations. Modellings of the structures was done using modelling and visualization software called Jmol. **Jmol.14.6.4 version** is an open-source viewer for three-dimensional chemical structures, with features for chemicals, crystals, materials and biomolecules. Figure 1, illustrates some of the MJs formed using some members of an acene group. Throughout this work, gold (Au) was maintained as an electrode (leads/reservoirs) and they are connected in *para*-positions (Pinheiro, *et al.*, 2020). The structure optimization and energy band calculations were performed using DFT technique as implemented in FHI-aims computer code (Blum, *et al.*, 2009), with the Perdew-Burke-Ernzerhof (PBE) exchange correlation. Transport properties of the system were investigated using Non-equilibrium Green's Function (NEGF) formalism approach as implemented in the Aitranss computer code (Arnold, *et al.*, 2007; Wilhelm, *et al.*, 2013; Bagrets, 2013).

In the first phase, hybrid MJs was investigated by comparing its properties to those that are made up using direct π -electrode contacts and π -anchor-electrode bindings. The first three acene member (i.e., anthracene, tetracene and pentacene) molecules connected to Au electrode via different anchoring groups (Reddy, *et al.*, 2007)

were considered. The anchoring materials used are amine (NH₂), cyanide (CN), sulphur (S) and thiol (SH). Figure 1 and 2 illustrate how an anchoring group are connected to a) anthracene b) tetracene and c) pentacene molecules in a single and hybrid modes respectively. In the second phase, exponential decay and length dependence of the electrical conductance of the hybrid MJs was investigated (Akbarabadi, *et al.*, 2020; Chen, *et al.*, 2020).

DFT is based on quite a rigid conceptual frame work. For many-body problem, the Schrodinger equation becomes

$$\left[\sum_i^N \left(\frac{-\hbar^2 \nabla_i^2}{2m} + V(r_i) \right) + \sum_{i<j} U(r_i, r_j) \right] \Psi(r_1, r_2, \dots, r_N) = E \Psi(r_1, r_2, \dots, r_N) \quad (2)$$

It is assumed that the full Hamiltonian of the extended molecule (Figure 2) has been a subject to partitioning into a sub-system M (molecule), a reservoir, R , and a mutual coupling.

$$H = H_M + H_R + V \quad (3)$$

The coupling V is of the form $V = \sum_{m,k} v_{mk} d_m^\dagger c_k + H.c.$ while d_m^\dagger , denote the creation/annihilation operators in M Hilbert space and, c_k the counterparts in R space. For a small voltage and low temperature limit, the electrical conductance G_e of the molecular junction can be express as

$$G_e = \frac{I}{V} = G_o \tau_e(E_F) \quad (4)$$

Where G_o is the quantum of electrical conductance and has a value of $\frac{2e^2}{h} \approx 77.48 \mu S$, E is energy $\tau_e(E)$ is the transmission function for electrons passing from one electrode to the other electrode via the molecule (which can also be written as T) and E_F is the Fermi energy (chemical potential) of the electrode material. Therefore, from equation (4), we have (Valdiviezo, *et al.*, 2021);

$$G/G_o = T(E_F) \quad (5)$$

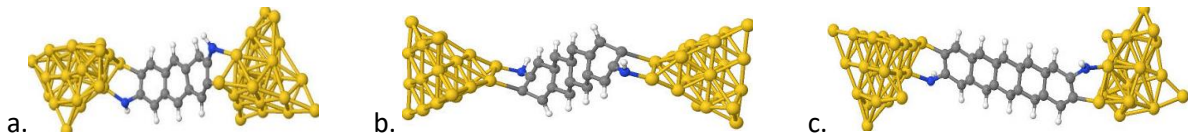


Figure 2: Double contact (Hybrid) acene-based MJs with amines as anchor groups (a. anthracene MJ, b. tetracene MJ and c. Pentacene MJ).

3. Results

The results are presented in two different segments. In the first segment, a comparative study between MJs formed without anchoring materials, the others that the anchoring materials were used as well as the double-contact version (hybrid). In the second segment, conductance-length dependence as stated above by equation 1 was scrutinized.

3.1 Double Contact MJs (Hybrid)

To improve the conductance as well as the formation probability of MJs, the hybrid (double-contact) MJs are formed. This is designed as a combination of direct-contact model and that of using anchor group simultaneously. In this mode, the charge transport path is assigned via direct π -electrode binding whereas anchoring of the molecule with the metal electrode is assign via molecule-anchor-electrode path. Here, the design, synthesis and structural characterization of hybrid MJs were performed. Four different anchoring materials (i.e., amines, cyanides, sulphides and thiols) were used to couple the molecules with electrodes.

3.1.1 Anthracene

At Fermi (E_F) level, the transmission coefficient $T(E_F)$ stands for the conductance of MJs as stated in equation 5. Figure 3 represents transmission coefficients for the MJs formed by three different techniques, which are the direct π -electrode binding, the direct π -anchor-electrode binding and the hybrid technique. Figure 5 represent the $T(E)$ of MJs made up using amines, cyanides, sulphides and thiols anchoring materials respectively.

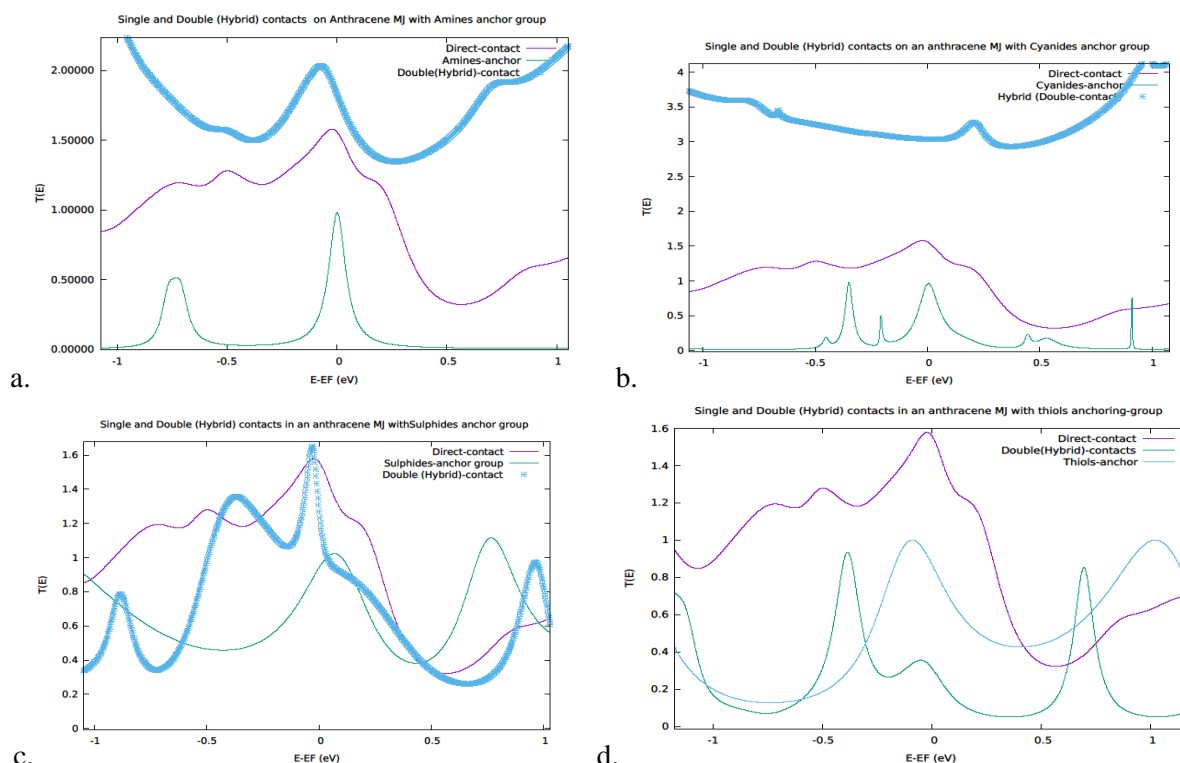


Figure 3: Variation of a transmission of an anthracene MJs with direct, anchor and double-contact (hybrid) molecule-electrodes intercept, for (a) amines, (b) cyanides, (c) sulphides, and (d) thiols anchoring groups.

As it can be noticed in Figure 3a, the hybrid MJ has the highest value of $T(E_F)$ which is around 1.83, thus it has a higher conductance. The direct contact had $T(E_F)$ value of 1.56, and then that with anchor material with $T(E_F)$ value of 0.98. When a cyanides anchor is used (Figure 3b), the similar results was obtained. The hybrid MJ has $T(E_F)$ value of 3.04 followed by the direct contact and then with anchor material whose $T(E_F)$ value is 0.95. For sulphides anchor material (Figure 3c), the $T(E_F)$ value of hybrid MJ is 1.61 and that of the anchor binding is 0.94. Lastly, for the thiol anchoring, hybrid MJ has $T(E_F)$ value of 0.31 while the anchoring binding has 0.88.

Table 1, is the frontier orbitals energies for the hybrid anthracene MJs formed using four different anchor materials. The HOMO-LUMO gap of these MJs ranges from 0.049 to 0.008 eV. It can be seen that, the sulphides anchor MJ, the gap is wider followed by cyanides and thiols with gap of 0.018 and 0.012 respectively. MJ made up with amines as anchor group has a least HOMO-LUMO gap of 0.008.

Anchor material	HOMO	LUMO	HOMO-LUMO gap
Amines	-4.4171	-4.4091	0.008
Cyanides	-4.5523	-4.5340	0.0183
Sulphides	-4.5321	-4.4835	0.0486
Thiols	-4.5674	-4.5549	0.0125

3.1.2 Tetracene

For the tetracene MJs, the transmission coefficients $T(E)$ for a MJs formed using direct-contact, π -anchor and hybrid methods against energy (E) are displayed in Figure 5 (a-d). In these figures, the MJs are designed using amines, cyanides, sulphides and thiols as anchor groups, respectively.

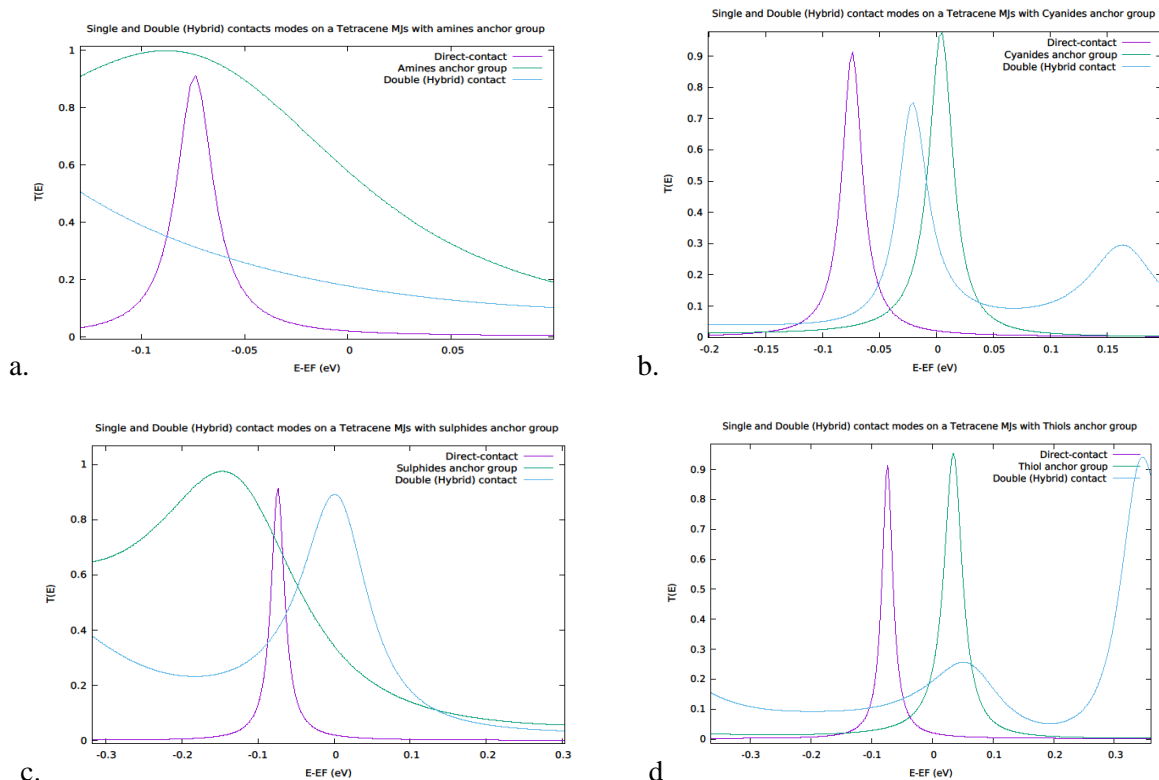


Figure 4: Variation of a transmission of tetracene MJs with direct, anchor and double-contact (hybrid) molecule-electrodes intercept, for (a) amines, (b) cyanides, (c) sulphides, and (d) thiols anchoring groups.

As it can be observed, the transmission of a tetracene MJ using direct method is 0.021. When amines were used as molecule-electrode anchor (Figure 4a), the $T(E_F)$ value rises to 0.59 and for a hybrid MJ, the $T(E_F)$ falls to 0.18. For the cyanides anchor tetracene MJs (Figure 4b), the $T(E_F)$ value is 0.91, while it is 0.32 for its hybrid. When the sulphides anchor groups are applied, the $T(E_F)$ value is 0.35, while it is 0.89 for its hybrid form. Lastly, the $T(E_F)$ value for tetracene MJ with thiols anchor group is 0.23 and it is 0.19 for the hybrid.

Table 2: HOMO, LUMO and gap of tetracene MJs with different anchor group

Anchor material	HOMO	LUMO	HOMO-LUMO gap
Amines	-4.7217	-4.7197	0.002
Cyanides	-4.7213	-4.7079	0.0134
Sulphides	-4.5648	-4.5117	0.0531
Thiols	-4.4761	-4.3986	0.0775

Table 2, shows the variation of HOMO and LUMO and their relative gap (HOMO-LUMO gap) with respect to the type of an anchoring material used. The maximum gap here is 0.078 eV for the thiols anchor group. Here also, the amines anchor hybrid MJ had the minimum HOMO-LUMO gap of 0.002 eV. Sulphides and cyanides anchored hybrid MJs has 0.053 and 0.013 eV, respectively.

3.1.3 Pentacene

Pentacene is the next member of acene after tetracene. Here also, the MJJs are made up of a pentacene. The transmission coefficients at Fermi energy level $T(E_F)$ are presented in Figure 5 below. The direct π -electrode, π -anchor-electrode and the hybrid modes of MJJs are investigated here.

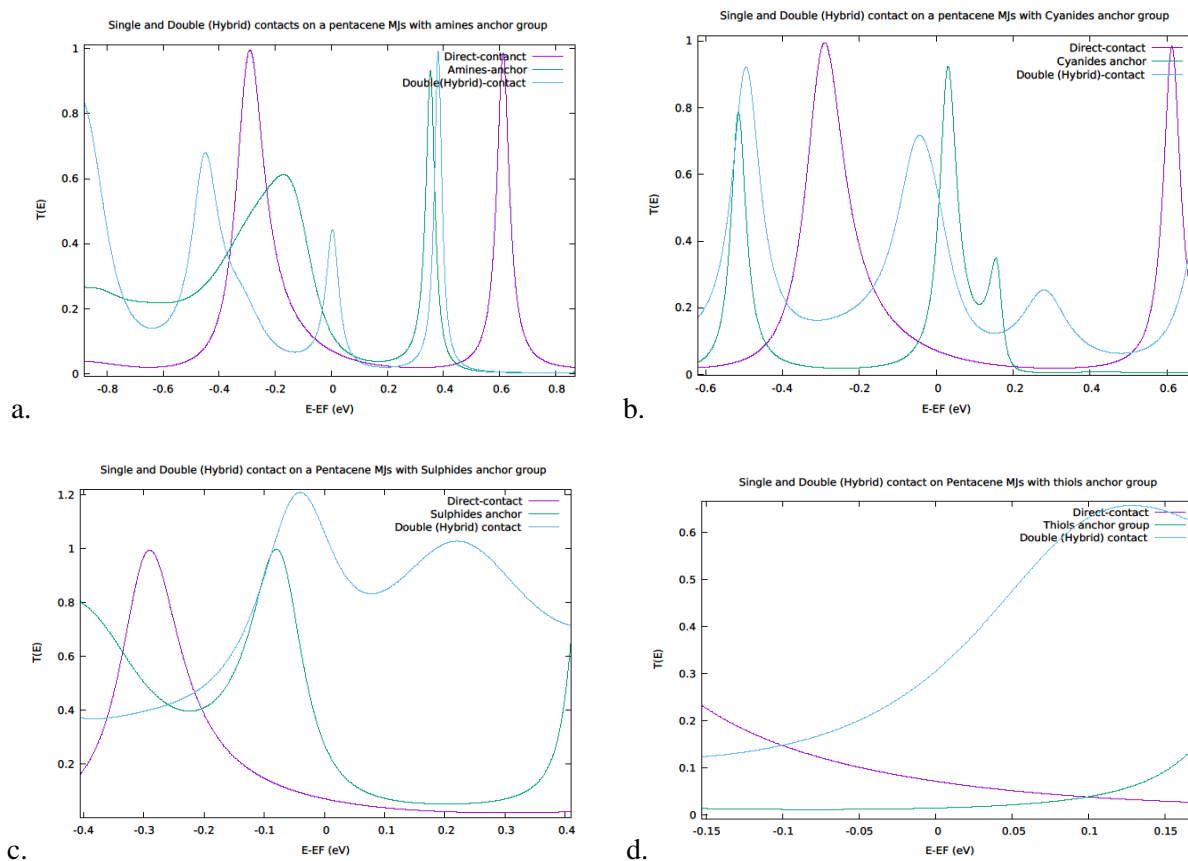


Figure 5: Transmission coefficient versus energy of pentacene MJJs with direct, anchor and double-contact (hybrid) molecule-electrodes binding using a) amines anchor group b) cyanides anchor group c) sulphides anchor group d) thiols anchor group.

For direct contact mode, the transmission coefficient at Fermi energy of an electrode $T(E_F)$ is 0.071. When amines anchor groups are used, the $T(E_F)$ is 0.12 and it is 0.42 for the hybrid MJ. The $T(E_F)$ of cyanides anchored MJ is 0.38, while it is 0.56 for the hybrid. For the sulphides and thiol anchored MJJs, the $T(E_F)$ values are 0.27 and 0.015 while for their corresponding hybrid MJJs, it is 1.07 and 0.30 respectively.

Table 3: HOMO, LUMO and gap of pentacene MJJs with different anchor group

Anchor material	HOMO	LUMO	HOMO-LUMO gap
Amines	-4.5641	-4.5458	0.0183
Cyanides	-4.7376	-4.7211	0.0165
Sulphides	-4.6591	-4.6364	0.0227
Thiols	-4.3696	-4.2144	0.1552

The frontier molecular orbitals of a hybrid pentacene MJJs varies according to the anchor group used in forming it. Thiols anchor group has the widest HOMO-LUMO gap of 0.16 eV. Next to this amount is sulphides

anchor group with gap of 0.023 eV. Amines and cyanides anchor groups are having the least gap with 0.018 and 0.017 respectively.

3.2 Length Dependence in Acene-based MJs

Here, the length dependency and exponential decay (equation 1) was investigated. The conductance at zero bias of the compounds anchored in different configurations (i.e., direct, anchored, and hybrid) was presented. Figure 6 (a-d) shows the conductance of these MJs within the exponential decay region (i.e., $N \leq 5$) (Valdiviezo, *et al.*, 2021).

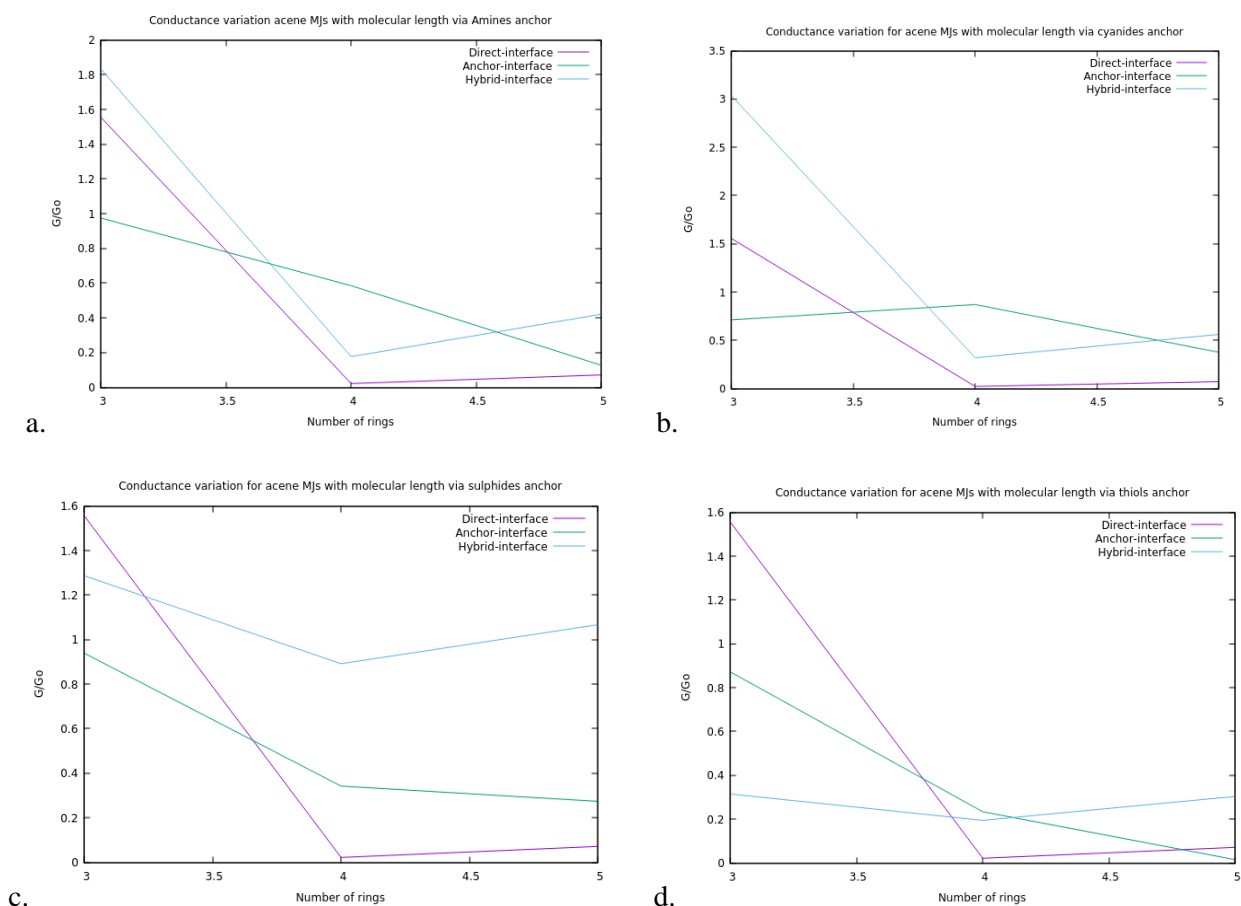


Figure 6: Zero bias conductance of acene-based MJs for different interfaces using (a) amines, (b) cyanides, (c) sulphides, and (d) thiols anchor groups.

For both anchoring groups (amines, cyanides, sulphides and thiols) in Figure 6 (a to d), the hybrid and direct π -electrode didn't show any definite conductance decay. The results shows that the conductance does not depends on the molecular length. For the case of π -anchor-electrodes formation, the conductance decays with molecular length except for the case of cyanides anchoring group (Figure 6b). The above results showed that, the anchoring materials plays a significant role in the nature of conductance behavior of MJ. It also shows that the hybrid MJ does not obey the exponential decay rule in equation 1.

4. Discussion

The findings show that, apart from improving the formation probability, the hybrid method increases the conductance of an anthracene MJ for all the anchor groups used. This may be attributed to the fact that the charge

transport path was enhanced. This is in line with the suggestions by Chen, *et al.*, (2020) and his co-workers. Also, the HOMO-LUMO gap varies with the type of anchoring material. The results showed that the amines anchor material increases the level of the FMOs and has a minimum HOMO-LUMO gap. It easily excites the molecules; thus, it is recommended as the better option for anchoring material. This claim is supported by Yuan, *et al.*, (2021).

Lastly, the results also demonstrate that, the lower acene derivatives have a non-exponential length dependence of the conductance when a hybrid-interface was used. The molecule-electrodes interface dictates the conductance behavior: molecules anchored through anchoring materials have a conductance decay with molecular length, whereas molecules anchored via hybrid method and those with direct π -metal contact exhibit conductance fluctuations with molecular length.

5. Conclusion

In conclusion, by using the DFT in combination with NEGF calculations, we have demonstrated that the hybrid method can improve the conductance and formation probability of an anthracene and pentacene MJs. The conductance of tetracene MJ can only be improve when sulphides are used as an anchoring group. Energy band calculations suggested that the anchoring groups influenced the variation of HOMO, LUMO and the gap between them. It shows that for anthracene and pentacene MJs, the amines anchor materials produced a minimum HOMO-LUMO gap.

Acknowledgments

We want to acknowledge the effort of Professor A. S. Gidado for the helpful discussions and professional advice. We also show our appreciation to Professor M. A. Hajara for the spot light in the field of Electronics.

References

- Akbarabadi, S.R., Soleimani, H. R., Golsanamlou, Z., Tagani, M. B. (2020). Enhanced thermoelectric properties in anthracene molecular device with graphene electrodes: the role of phononic thermal conductance. *Scientific Reports*, 10, 10922. DOI: <https://doi.org/10.1038/s41598-020-67964-w>.
- Anthony, J. E. (2006). Functionalized acenes and heteroacenes for organic electronics. *J. Chem. Rev.*, 106: 5028-5048. <https://doi.org/10.1021/cr050966z>.
- Arnold, A., Weigend, F., Evers, F. (2007). Quantum chemistry calculations for molecules coupled to reservoirs: Formalism, implementation, and application to benzenedithiol. *The Journal of Chemical Physics.*, 126(17): 174101. doi: 10.1063/1.2716664.
- Bagrets, A. (2013). Spin-polarized electron transport across metal-organic molecules: a density functional theory approach. *Journal of Chemical Theory and Computation*, 9(6): 2801-45. <https://doi.org/10.1021/ct4000263>.
- Bendikov, M., Wudl, F., Perepichka, D. F. (2004). Tetrathiafulvalenes, oligoacenes, and their buckminsterfullerene derivatives: the brick and mortar of organic electronics. *J. Chem. Rev.*, 104(11): 4891-4946. <https://doi.org/10.1021/cr030666m>.
- Blum, V., Gehrke, R., Hanke, F., Havu, P., Havu, V., Ren, X., Reuter, M. S. (2009). Ab initio molecular simulations with numeric atom-centered orbitals. *Computer Physics Communications*, 180(11): 2175-2196. DOI:10.1016/j.cpc.2009.06.022.
- Chen, H., Li, Y., Chang, S. (2020). Hybrid Molecular-Junction Mapping Technique for Simultaneous Measurements of Single-Molecule Electronic Conductance and Its Corresponding Binding Geometry in a Tunneling Junction *Anal. Chem.*, 92(9): 6423-6429. doi: 10.1021/acs.analchem.9b05549.
- Fujii, S., Madoka, I., Shunsuke, F., Tomofumi, T., Tomoaki, N., Masaichi, S., Manabu, K. (2020). Hybrid Molecular Junctions Using Au-S and Au- π Bindings. *The Journal of Physical Chemistry C*, 124(17): 9261-9268. <https://doi.org/10.1021/acs.jpcc.9b11725>.
- Gozalvez, C., Zafra, J. L., Saeki, A., Manuel, M., Casado, J., Mateo-Alonso, A. (2019). Charge Transport Modulation in Pseudorotaxane 1D Stacks of Acene and Azaacene Derivatives. *Chem. Sci.*, 10: 2743-2749. <https://doi.org/10.1039/C8SC04845B>.

- Gryn'ova, G., and Corminboeuf, C. (2019). Topology-Driven SingleMolecule Conductance of Carbon Nanothreads. *J. Phys. Chem. Lett.*, 10(4): 825-830. <https://doi.org/10.1021/acs.jpcclett.8b03556>.
- He, C., Zhang, Q., Gao, T., Liu, C., Chen, Z., Zhao, C., Nichols, R. J., Dappe, Y. and Yang, L. (2020). Charge Transport in Hybrid Platinum/Molecule/Graphene Single Molecule Junctions. *Phys. Chem. Chem. Phys.*, DOI: 10.1039/D0CP01774D.
- Hu, Y., Zhou, Y., Ye, J., Yuan, S., Xiao, Z., Shi, J., Yang, Y., Gemma, C. S., Hong, W. (2022). Σ -dominated charge transport in sub-nanometer molecular junction. *J. Fundamental Research*, 2667-3258. <https://doi.org/10.1016/j.fmre.2022.06.021>.
- Ibrahim, K. L., Babaji G. and Nura A. M. (2022). Charge Transport Enhancement in Anthracene Molecular Junction: Density Functional Theory Studies. *J. Mater. Sci. Res. Rev.*, 2022; vol. 10, no. 4, pp. 32-41, Article no.JMSRR.95693.
- Lucas, D., Hyunhak, J., Nayan, K. P., Juan, S. G. and Joshua, H. (2021). Multidimensional Characterization of Single-Molecule Dynamics in a Plasmonic Nanocavity. *Angew. Chem. Int.* <https://doi.org/10.1002/anie.202100886>.
- Nichols, R. J., Haiss, W., Higgins, S. J., Leary, E., Martin, S., Bethell, D. (2010). The experimental determination of the conductance of single molecules. *Phys. Chem. Chem. Phys.*, 12 (12): 2801-2815. <https://doi.org/10.1039/B922000c>.
- Noori, M. D., Sangtarash, S. and Sadeghi, H. (2021). The effect of anchor group on the phonon thermal conductance of single molecule junctions. *Appl. Sci.*, 11, 1066.
- Pinheiro, M., Machada, F.B.C., Plasser, F., Aquino, J.A., and Lischka, H. (2020). A system analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. *Material Chemistry C*. (DOI: 10.1039/C9TC06581D).
- Reddy, P., Jang, S. -Y., Segalman, R. A., Majumdar, A. (2007). Thermoelectricity in molecular junctions. *Science*, 315(5818), 1568-1571. doi: 10.1126/science.1137149.
- Shen, B., Tatchen, J., Sanchez-Garcia, E., Bettinger, H. F. (2018). Evolution of the optical gap in the acene series: undecacene. *Angew. Chem.*, 13; 57(33): 10506-10509. doi: 10.1002/anie.201802197.
- Stegmann, T., Franco-Villafane, J. A., Ortiz, Y. P., Deffner, M., Herrman, C., Kuhl, U., . . . Seligman, T. H. (2020). Current vortices in aromatic carbon molecules. *Physical Review B*, 102(7): 075405. DOI: <https://doi.org/10.1103/PhysRevB.102.075405>.
- Thorley, K. J. and Anthony, J. E. (2014). The electronic nature and reactivity of the larger acenes. *Isr. J. Chem.*, 54: 642-649. DOI: 10.1002/ijch.201400060.
- Valdiviezo, J., Rocha, P., Polakovsky, A., Palma, J. L. (2021). Nonexponential Length Dependence of Molecular Conductance in Acene-Based Molecular Wires *ACS Sens.*, 26; 6(2): 477-484. doi: 10.1021/acssensors.0c02049.
- Vincent, D., Valentin, D. C., Colin, V. D., ELke, S., Karine, C., Jerome, C. (2020). On the reliability of acquiring molecular junction parameters by Lorentzian fitting I/V curved. *Phys. Chem. Chem. Phys.*, 22: 26702-26706. <https://doi.org/10.1039/D0CP05372D>.
- Wilhelm, J., Walz, M., Stendel, M., Bagrets, A., Evers, F. (2013). Ab initio simulations of scanning-tunneling-microscope images with embedding techniques and application to C58-dimers on Au(111). *Phys. Chem. Chem. Phys.*, 15: 6684-6690. <https://doi.org/10.1039/C3CP44286A>.
- Yang, Y., Davidson, E. R. and Yang, W. (2016). Nature of ground and electronic excited states of higher acenes. *Proc. Natl. Acad. Sci. U. S. A.*, 113(35): E5098-E5107.
- Yannick, D. J. (2020). Attenuation Factors in Molecular Electronics: Some Theoretical Concepts. *Journal of Applied Sciences*, 10(18): 6162. <https://doi.org/10.3390/app10186162>.
- Yelin, T., Korytar, R., Sukenik, N., Vardimon, R., Kumar, B., Nuckolls, C., Evers, F., Tal, O. (2016). Conductance saturation in a series of highly transmitting molecular junctions. *Nat. Mater.*, 15(4): 444-9. doi: 10.1038/nmat4552.
- Yoo, P. S. and Kim, T. (2015). Linker-dependent Junction Formation Probability in Single-Molecule Junctions. *Bull. Korean Chem. Soc.*, 36(1): 265-268. DOI:10.1002/bkcs.10061.

- Yuan, S., Gao, T., Cao, W., Pan, Z., Liu, J., Shi, J., Hong, W. (2021). The characterization of electronic noise in the charge transport through single-molecule junctions. *Small Methods*, 5, 2001064. DOI: 10.1002/smt.202001064.
- Zade, S. S., Bendikov, M. (2010). Heptacene and beyond: the longest characterized acenes. *Angew. Chem., Int. Ed.*, 49: 4012-4015. <https://doi.org/10.1002/anie.200906002>.