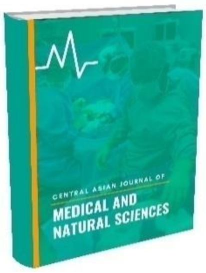
CENTRAL ASIAN JOURNAL OF MEDICAL AND NATURAL SCIENCES



Volume: 04 Issue: 02 | Mar-Apr 2023 ISSN: 2660-4159

http://cajmns. centralasianstudies. org

Promising Single Molecules for Laser Active Medium

1. **Safa Saleem Hussein**
2. **Shaymaa Sami Khleef**

Received 2nd Jan 2023,
Accepted 3rd Feb 2023,
Online 25th Mar 2023

[1,2] Department of Laser Physics, College of Science for Women, University of Babylon

Abstract: We provide a brief overview of recent calculations and predictions of electronic properties for single-molecules and discuss some principles underpinning strategies for enhancing their electronic performance. Quantum interference effects in the electronic properties of (Pyridine-2Cyclopentene Metallic) organometallic-type molecules possessing six aromatic rings were investigate theoretically. In this paper, electronic transmission properties were study for different types of organometallic molecules. A calculation also provides a powerful tool to estimate the electrical and electronic properties. Furthermore, to probe the electronic structure of all compounds in this study we compute the UV-visible, isosurface and energies calculations. It is finding that the (HOMO and LUMO) energy changing with replace metallic atoms as well as the energy gap changes as the metal different. Therefore, this indicates the energies depend on the type of the metallic atoms in the studied molecules. All calculations were performed using density functional theory at three parameters with the Lee-Yang-Parr functional (B3 LYP) levels with SDD basis sets.

Keywords: DFT, Organometallic molecules, UV-visible calculations.

1. Introduction

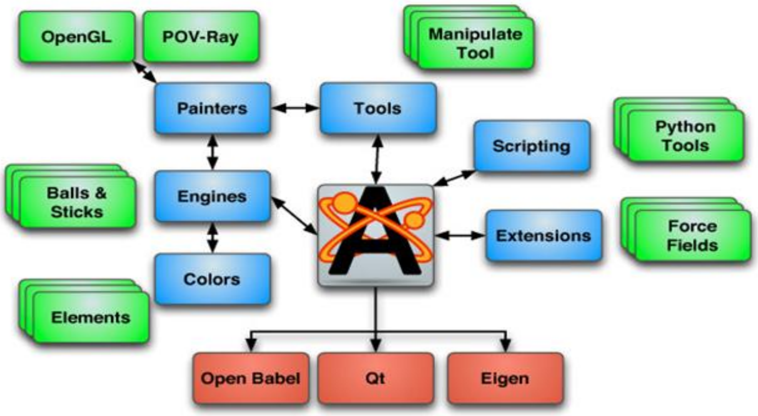
Nowadays, single molecules as electronic devices become one of the most useful routes to develop the computational architectures of sub-10nm [Paul F. B. et al., 1996]. The conductance of metal|molecule|metal junctions has been measured using different methods [Reed, et al., 1997; Di Ventra et al., 2000; Smit et al., 2002]. These techniques have attracted many investigations into molecular structure-property relationship [Ismael, D., et al., 2011; Thomas, H., et al., 2010; Venkataraman L., et al., 2006].Wide interesting has been focused on the molecular length of pi-conjugated oligomers, because the electrical conductance G of molecular wires decays gradually with the molecular length [Yamada, R., et al., 2008; Changsheng, W. et al., 2009]. In almost all molecular junctions measured to date, the Fermi energy of the metallic electrodes lies in the HOMO-LUMO gap of the molecule and therefore electron transport occurs via tunnelling. Consequently for large enough L, the electrical conductance varies as $G = A\exp-(E_F)L$, where the pre-factor A depends on details of the electrode-molecule interface, whereas for large L, the attenuation coefficient $\beta(E_F)$ is a property of the molecular wire and the Fermi energy E_F of the electrodes. Since (E_F) is minimised by reducing the offset between E_F and either the HOMO or LUMO levels, it is desirable to minimise the HOMO-LUMO gap and maximise the electronic coupling between adjacent monomer segments of long wires. Since the rotation of such segments can break conjugation and reduce the pi coupling between segments [Artem, M., et al., 2010; Artem M., et al., 2010;], it is advantageous to introduce constraints, which prevent rotation or alternatively to use wires made from segments which have no rotational degrees of freedom [Christopher, M., et al., 2008].

In this study we have investigated the geometrical properties such as molecular length of the structures, carbon-carbon double and single bonds in a gas phase and in a junction form. The electronic properties such as molecular orbitals distribution, charge transport mechanisms, binding energy, electrical conductance, decay constant and current-voltage characteristics of single molecular wires have been studied in this work using density functional theory (DFT) with using of SIESTA and GOLLUM codes and also Gaussian09 software package. The impact of molecular length on electronic properties of this kind of molecules has been explored and the results shown that the highest and lowest electrical conductance values are 0.4 and 0.3 μS respectively. In addition, the computations demonstrate that the high value of decay constant yields a low value of electrical conductance. Furthermore, the transport mechanisms through metal|molecule|metal junctions are studied and the results shown the mechanism is LUMO-based conduction mechanism.

2. Computational details

2. 1 Theoretical Building and Configuration

To get the structure of all systems in theory, I have been utilized Avogadro programming. Avogadro is a propelled particle manager and visualizer intended for cross-stage use in computational science, molecular modeling, bioinformatics, materials science, and related areas (see Figure 3.1). It offers flexible high quality rendering and a powerful plugin architecture [13].Avogadro offers a semantic compound developer and stage for perception and investigation. For clients, it offers a simple to-utilize manufacturer, incorporated help for downloading from basic databases, for example, PubChem and the Protein Data Bank, separating synthetic information from a wide assortment of arrangements, including computational science yield, and local, semantic help for the CML record position [14]. For progressively hypothetical insights regarding Avogadro and what it gives in, see [13,14]. All molecules under investigation in this thesis are shown in Figure X.



2.2 Iso-Surfaces Calculations.

In the quest to better understand the trends in conductance behavior, the electronic properties of the molecules and the electrical behavior of the junctions have been investigated by using DFT-based methods. Initial studies of the electronic structures of all molecules were carried out at the B3LYP level of theory [15] with 6-311G basis set [16-17]. Plots of the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO, respectively) are given in Figure XXX, and an analysis of the energy and distribution of the frontier molecular orbitals is summarized in Tables 1.

2.3 Density Functional Theory [DFT].

The explanation and understanding of the electronic properties of molecular wires can be understood by investigating the behaviour of electrons in the wires. This means finding a tool for solving the interacting electron problem. In order to solve this complex problem there are various theoretical and semi empirical techniques which are based on an ‘ab-initio’ method using fitted parameters with experimental data [17-18]. Density Functional theory (DFT) is one of these techniques and is based on two key theorems: the Hohenberg-Kohn Theorem (1964) and the Kohn-Sham Formulation[13,14]. This chapter will contain a brief outline of DFT and the computational code SIESTA) Spanish Initiative for Electronic Simulations with Thousands of Atoms) [8], which is used to carry out the later studies. The DFT code SIESTA is a software package to achieve DFT calculations for thousands of atoms and can be used to calculate properties such as band structures, bond lengths binding energies etc. Also, in this chapter, I have described how the underlying mean field Hamiltonian from SIESTA can be used as an input with a Green’s function scattering formalism which can be used to predict transport properties.

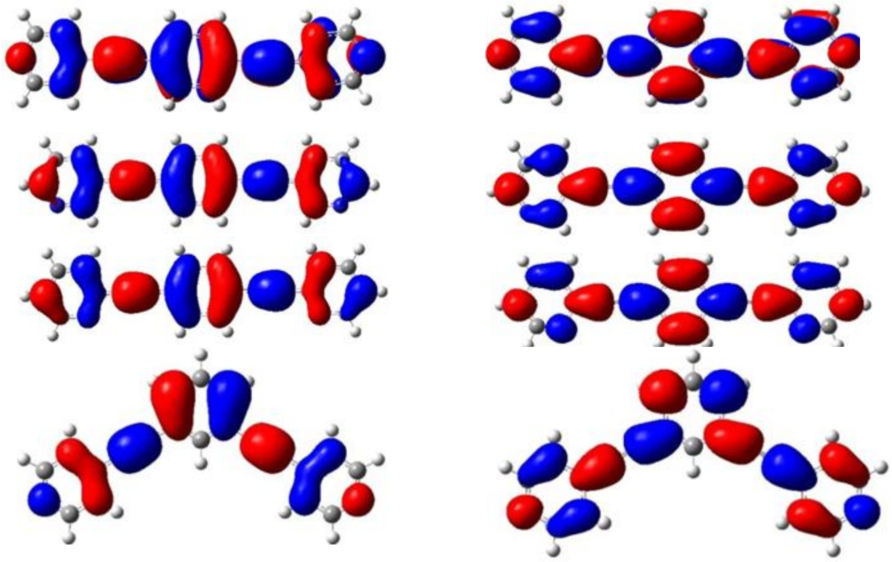
Undamental concept of DFT, Theoretical Methods for computing the ground state properties of metal, insulators and semiconductors [10], is dependent on the ground state energy; all electronic features of other ground state are note that decided by the electron density. Today, DFT it is one of the most used methods in this area. Time-dependent density functional theory (TD-DFT) spreads the important idea of the ground-state DFT which can be used to examine the excited state properties of” a system in the presence of timedependent potentials, such as electric or magnetic fields. The influence of fields on molecules could be studied with TD-DFT as an application for representative excitation energies, oscillator strength, wavelength, molecular orbital character and electronic transitions of the molecules [19-20].

3. Results and Discussion

1. Molecular Orbitals Distribution

The molecules have been optimized using the standard Gaussian09 software package. The B3LYP level of theory with basis set 6-311G, are used to computing the orbital energy levels.

HOMO LUMO



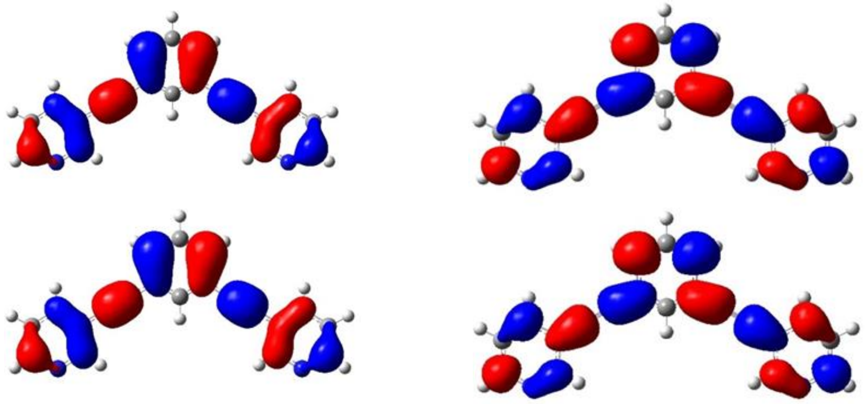


Figure 2. The iso-surfaces of the HOMOs and LUMOs for all molecules.

Molecular electronics is the next important step in the development of nanoscale electronic devices. However, the current challenge is the ability to wire electronic devices and exploit the properties of molecular wires to enhance the efficiency and carry current over long distances. Current research has studied a range of molecular wires and has demonstrated that molecules do show charge transport across rather large wires [37-40]. Monatomic linear carbon chains with alternating single, or polyynes which are carbon chains with large numbers of triple bonds are some of the most widely studied of molecules [41-49].

Theoretical and experimental studies demonstrate that the conductance of monatomic linear chains depends on the number of atoms and that conductance of odd –numbered chains is higher than that of even –numbered chains. This is called the odd-even effect [31, 32, 33-34]. In the literature there are experimental and theoretical studies of carbon chains with different end-groups to understand carbon chain properties as the value of the energy gap (Eg) and bond length alteration (BLA) which is the difference in the bond length between the central single and triple bonds. There is agreement that Eg and BLA decrease with the lengthening of the molecule [35-36].

These results provide a convenient point to commence discussion and a basis for comparison between the highest occupied and lowest unoccupied molecular orbitals HOMO and LUMO, respectively.

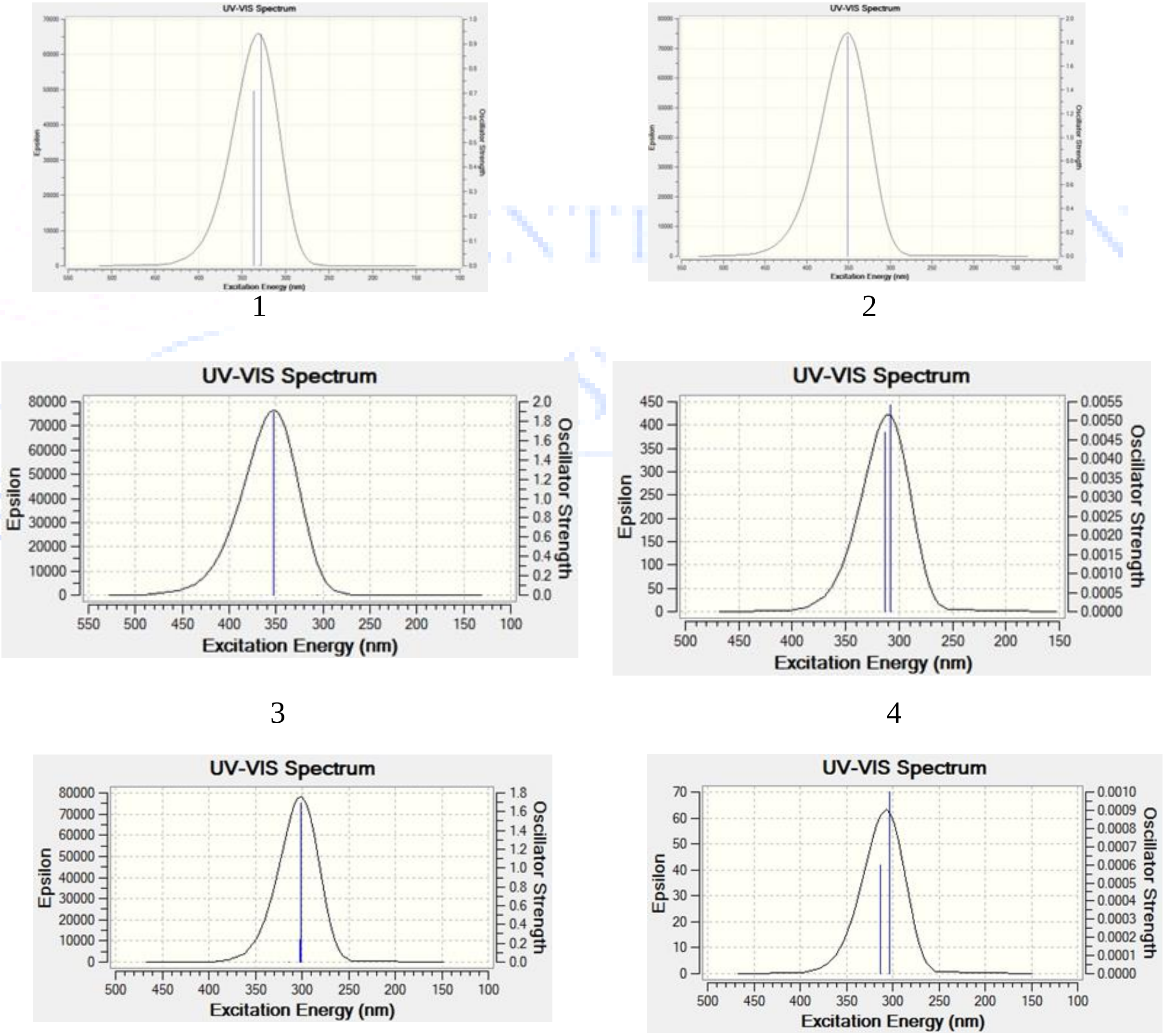
Unsurprisingly, the lowest and highest energy structures features arrangement the electronic structure with the frontier orbitals distributed almost evenly across the molecular backbone, making a linear, p-type conjugated pathway between the two nitrogen atoms. On the other hand, the lowest unoccupied molecular orbitals are localized on the (o-m-o) bonds and shown more contribution than that of the highest occupied molecular orbitals, which are concentrated on the (p-p-p) bonds. It is worth to mention that the weight of the LUMO on the pyridine anchor groups is noticeable, and higher than that of the HOMO. This result reflects two points. The first one is the transport mechanism of the charge carriers could be the LUMO-dominate transport mechanism. On the other hand, it is obvious that there is an important effect of the molecular length on the frontier molecular orbitals distribution, since the weight of HOMOs and LUMOs gradually decreases with increasing of the molecular length. In this kind of systems, it is known that the transport mechanism is the tunneling mechanism, so the increasing of molecular length leads to increasing the tunneling distance and that leads to decrease the concentration of molecular orbitals across the backbone. Finally, this kind of calculations could be a hint factor to explore the charge transport mechanism, which is a LUMO-dominate transport.

Table 1 | Most-probable experimental conductance, electrode separation zH * at the end of the high-conductance plateaus and JFP of pyridyl-terminated OPE derivatives from MCBJ and STM-BJ**.**

Moleculer	HOMO	LUMO	HOMO- LUMO
P-P-P	**6.16301939**	**2.122458**	**4.04056139**
m-p-m	**5.85907252**	**2.09034902**	**3.7687235**

o-p-p	**5.75022852**	**1.98857988**	**3.76164864**
p-m-p	**6.31921053**	**2.02232152**	**4.29688901**
m-m-m	**6.08111428**	**1.80191242**	**4.27920186**
o-m-o	**6.36329235**	**1.52626499**	**4.83702736**

“In terms of low electrical conductance offset by large thermal energy, our results presented in Table show that the lowest conductivity is obtained by BCP-Pt, which leads to a significant increase in the value figure of merit, and a high value of the Seebeckcoefficient”.“On the other side, there is clearly a strong link between the HOMOLUMO gap and the electronic and thermoelectric properties of these compounds, which definitely needs further investigation”.“Fig. 3 illustrate promising strategy to influence and control the thermoelectric properties of single-molecule junctions”. With obtained results, the emergence of destructive quantum interference this aplanning usedfor reduce conduction and escalate thermal energy. Obviously,“We can get from this phenomenon a lower transmission coefficient over a wide range of electron energy (-3 - 3eV) as illustrate in Fig. 3a,b.”



1 2

3 4

5 6

Figure 3

The conductances for p-p-p and m-m-m molecules is equal to the product of conductances for p-m-p and m-p-m molecules, and the qu antum circuit rule Gppp/Gpmp ¼ Gmpm/Gmmm is satisfied.

Further statistical analysis of conductance versus Dz curves provides information about the junction formation probability (JFP) and allows us to determine the most-probable relative electrode displacement (DzH*) at the end of the high-conductance plateaus. For every log(G/G0) versus Dz stretching trace, we determine the relative electrode displacement at the end of the high-conductance plateau, DzH, which is the largest Dz value within the range 0.34log(G/G0)4log(GH end/G0), where GH end is the end of high-conductance feature. The most-probable values of DzH (denoted DzH*) are obtained by constructing a histogram and fitting a Gaussian function to the largest maxima. Taking into account the snap-back length, the most-probable electrode separations at the end of the high-conductance plateau are zH* ¼ DzH* þ Dzcorr. The representative DzH histograms with Gaussian fitting functions are shown in Supplementary. The JFP is calculated as the ratio of the area under the fitted Gaussian function and the total area of the DzH histogram. If no distinct peak is observed in the DzH histogram, then the JFP is considered to be zero.

tical and experimental conductances.) Figure 4 demonstrates that for a wide range of Fermi energy choice, the theoretical and experimental conductances of the X-p-X molecules of group 1 are distinctly higher than those of the molecules in group 2, as expected from previous studies[21,22,23,24]. also shows that for wide range of energies in the gap between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), the ordering of the transmission coefficients follows the experimental conductance ordering. To demonstrate the resilience of the circuit rule, dotted lines are plots of (log Tmmm þ log Tppp)/2 and (log Tmpm þ log Tpmp)/2. The similarity of these two curves shows that the product rule is satisfied over a wide range of energies within the HOMO-LUMO gap. To demonstrate that QI effects associated with variations in the positions of the N atoms are suppressed owing to the presence of a parallel conductance path associated with the electrode-ring overlap, we performed transport calculations in which we artificially set to zero every .Hamiltonian and overlap matrix element that couples carbon and hydrogen atoms to gold atoms, leaving couplings between the nitrogen atoms and gold as the only possible transport path. The resulting transmission coefficients are shown as dashed lines in and demonstrate that without metal-ring interactions the meta link in the terminal ring of the m-p-m molecule reduces the conductance by orders of magnitude, which is comparable with the effect of a meta link in the central ring, whereas in the presence of metal-ring interactions meta coupling in the terminal rings has a much smaller effect(25).

4. Conclusions

We have presented charge transport studies of pyridyl terminated OPE derivatives, using the MCBJ and STM-BJ techniques, DFT-based theory and analytic Green's functions, and have investigated the interplay between QI effects associated with central and terminal rings in molecules of the type X-Y-X. Our results demonstrated that the contribution to the conductance from the central ring is independent of the para or meta nature of the anchor groups and the combined conductances satisfy the quantum circuit rule Gppp/Gpmp ¼ Gmpm/Gmmm. For the simpler case of a two-ring molecule, the circuit rule GppGmm ¼ G2 pm is satisfied (Supplementary Note 8). It should be noted that the circuit rule does not imply that the conductance GXYX is a product of three measureable conductances associated with rings X, Y and X. Indeed the latter property does not hold for a single molecule. On the other hand, provided sample to sample fluctuations lead to a broad distribution of phases within an ensemble of measurements, a product rule for ensemble averages of conductances can arise. This possibility is discussed in detail in Supplementary Notes 7 and 9. The qualitative relationship between the conductances agrees well with the simple QI picture of molecular conduction. It has been reported that destructive QI exists in benzene with the meta connectivity and is responsible for the observed reduction of conductance[26,27,28] whereas for para and ortho connectivities, constructive QI should be observed[29,30]. The transmission coefficient calculations through junctions where the metal-ring connection is artificially blocked (Fig. 5) show that the artificially coupled pyridyl ring exhibits similar behaviour to the benzene ring, with destructive QI in the case of the meta coupling significantly reducing the conductance compared with para and ortho connectivities. The dashed curves in the bottom panel in Fig. 5clearly demonstrate that when the conduction is through only the nitrogen atoms, the conductance of the meta isomer is much lower than in the para and ortho isomers. More realistically, however, in the presence of metal-ring overlap, the effect of varying the positions of the nitrogens in the anchors becomes much weaker, and as demonstrated by Fig. 4 the major changes in the molecular conductance are caused by the variations in the connectivity of the central ring. The dominant influence of the central ring is accounted for by the fact that the central ring is not in direct contact with electrodes and therefore no parallel conductance paths are present, which could bypass the ethynylene connections to the anchors. In a subnanometre scale molecular circuit, as in standard complementary metal-oxide-semiconductor (CMOS) circuitry, electrical insulation is of crucial importance. Destructive interference in a two-terminal device may not be desirable, because ofthe lower conductance. However, for a three-terminal device minimizing the conductance of the third terminal is highly desirable, because the third (gate) electrode should be placed as close to the molecule as possible, but at the same time, there should be no leakage current between the molecule and gate. One way of achieving this may be to use an anchor group with built-in destructive interference. Therefore, destructive QI may be a vital ingredient in the design of future three-terminal molecular devices and more complicated networks of interference-controlled molecular units.

References

1. **Paul F. B. *et al.,*** 1996, “Contemporary Issues in Electron Transfer Research”, J. Phys., 100, 13148-13168.
2. **Reed, M. A., Zhou, C., Muller, C. J., Burgin, T. P. & Tour, J. M.**, 1997, “Conductance of a molecular junction” Science 278, 252–254.
3. **Di Ventra, M., Pantelides, S. T. & Lang, N. D.**, 2000, “First-principles calculation of transport properties of a molecular device”, Phys. Rev. Lett. 84, 979–982.
4. **Smit, R. H. M. *et al.***, 2000, “Measurement of the conductance of a hydrogen molecule”, Nature 419, 906–909.
5. **Ismael, D., *et al.,*** 2011, “Controlling single-molecule conductance through lateral coupling of p orbitals”, Nat. Nanotech. 6, 226-231.
6. **Thomas, H., *et al.***, 2010; “Transition from Tunnelling to Hopping in Single Molecular Junctions by Measuring Length and Temperature Dependence”, J. AM. Chem. Soc. 132, 11658-11664.
7. **Venkataraman L., *et al.***, 2006, “Dependence of single-molecule junction conductance on molecular conformation”, Nature, 442, 904-907.
8. **Yamada, R., *et al***., 2008, “Electrical Conductance of Oligothiophene Molecular Wires”, Nano Lett. 8, 1237-1240.
9. **Changsheng, W. et al.**, 2009, “Oligoyne Single Molecule Wires”, J. AM. Chem. Soc. 131, 15647–15654.
10. **Artem, M., *et al.***, 2010, “Influence of Conformation on Conductance of Biphenyl-Dithiol Single-Molecule Contacts”, Nano Lett. 10, 156-163.
11. **Artem M., *et al.***, 2010; “Single-Molecule Junctions Based on Nitrile-Terminated Biphenyls: A Promising New Anchoring Group”, J. AM. Chem. Soc. 133, 184-187.
12. **Christopher, M., *et al.***, 2008, “Conformation dependence of molecular conductance: chemistry versus geometry”, J. Phys.: Condens. Matter, 20, 1-5.

13. **D.R. Kauffman,** D.C. Sorescu, D.P. Schofield, B.L. Allen, K.D. Jordan, A. Star Understanding the Sensor Response of Metal-Decorated Carbon Nanotubes ,Nano Lett. 2010, 10, 958.
14. **J.C. Ellenbogen,** J.C. Love Architectures for molecular electronic computers. I. Logic structures and an adder designed from molecular electronic diodes,Proc. IEEE 2000, 88, 386.
15. W. A. Chalifoux, R. R. Tykwinski, C. R. Chim. Synthesis of extended polyynes: Toward carbyne,2009, 12, 341– 358.5.
16. **P. Moreno-Garcia, M. Gulcur,** D. Z. Manrique, T. Pope, W. Hong, V. Kaliginedi, C. Huang, A. S. Batsanov, M. R. Bryce, C. Lambert and T. Wandlowski Single-molecule conductance of functionalized oligoynes: length dependence and junction evolution , J. Am. Chem. Soc., 2013, 135, 12228-12240.
17. **Moore, G.E.,** Cramming more components onto integrated circuits.1965,McGraw-Hill.
18. **Geim, A., Novoselov,** K. The rise of graphene. Nature Mater. 2007, 6(3), 183–191.
19. A. D. Slepkov, F. A. Hegmann, S. Eisler, E. Elliott, R. R Tykwinski .The surprising nonlinear optical properties of conjugated polyyne oligomers, J. Chem.Phys. 2004, 120, 6807 – 6810.
20. C. Wang, A. S. Batsanov, M. R. Bryce, S. Martin, R. J. Nichols, S. J. Higgins, V. M. Garcia-Suarez and C. J. Lambert Oligoyne single molecule wires, J. Am. Chem. Soc., 2009, 131, 15647-15654.
21. Aradhya, S. V. et al. Dissecting contact mechanics from quantum interference in single-molecule junctions of stilbene derivatives. Nano Lett. 12, 1643–1647(2012).
22. Arroyo, C. R. et al. Signatures of quantum interference effects on charge transport through a single benzene ring. Angew. Chem. Int. Ed. 52, 3152–3155 (2013).
23. Meisner, J. S. et al. Importance of direct metal p coupling in electronic transport through conjugated single-molecule junctions. J. Am. Chem. Soc. 134, 20440–20445 (2012).
24. Arroyo, C. R. et al. Quantum interference effects at room temperature in OPV-based single-molecule junctions. Nanoscale Res. Lett. 8, 1–6 (2013).
25. Chen, J., Reed, M. A., Rawlett, A. M. & Tour, J. M. Large on-off ratios and negative differential resistance in a molecular electronic device. Science 286, 1550–1552 (1999).
26. Ke, S.-H., Yang, W. & Baranger, H. U. Quantum-interference-controlled molecular electronics. Nano Lett. 8, 3257–3261 (2008).
27. 0. Markussen, T., Stadler, R. & Thygesen, K. S. The relation between structure and quantum interference in single molecule junctions. Nano Lett. 10, 4260–4265(2010).
28. Arroyo, C. R. et al. Signatures of quantum interference effects on charge transport through a single benzene ring. Angew. Chem. Int. Ed. 52, 3152–3155 (2013).
29. Hansen, T., Solomon, G. C., Andrews, D. Q. & Ratner, M. A. Interfering pathways in benzene: an analytical treatment. J. Chem. Phys. 131, 194704 (2009).
30. Solomon, G. C. et al. Understanding quantum interference in coherent molecular conduction. J. Chem. Phys. 129, 054701 (2008).
31. F. Diederich Carbon scaffolding: building acetylenic all-carbon and carbon-rich compounds ,Nature 1994, 369, 199 –207.
32. W. A. Chalifoux, R. R. Tykwinski, C. R. Chim. Synthesis of extended polyynes: Toward carbyne,2009, 12, 341– 358.5.

33. P. Moreno-Garcia, M. Gulcur, D. Z. Manrique, T. Pope, W. Hong, V. Kaliginedi, C. Huang, A. S. Batsanov, M. R. Bryce, C. Lambert and T. Wandlowski Single-molecule conductance of functionalized oligoynes: length dependence and junction evolution , J. Am. Chem. Soc., 2013, 135, 12228-12240.
34. Huber, R.; Gonza´lez, M. T.; Wu, S.; Langer, M.; Grunder, S.; Horhoiu, V.; Mayor, M.; Bryce, M. R.; Wang, C.; Jitchati, R.; Scho¨nenberger, C.; Calame, MElectronic properties of linear carbon chains: Resolving the controversy. J. Am. Chem. Soc. 2008, 130, 1080–1084.
35. Salomon, A.; Cahen, D.; Lindsay, S.; TomfohEnhanced Conduction through Isocyanide Terminal Groups in Alkane and Biphenylene Molecules Measured in Molecule/Nanoparticle/Molecule Junctionsr, J.; Engelkes, V. B.; Frisbie, C. D. AdV. Mater. 2003, 15, 1881–1890.
36. Pauly, F.; Viljas, J. K.; Cuevas, J. C.; Scho¨n, G. Density-functional study of tilt-angle and temperature-dependent conductance in biphenyl dithiol single-molecule junctions Phys. ReV. B 2008, 77, 155312.
37. Moore, G.E., Cramming more components onto integrated circuits. 1965,McGraw-Hill.
38. Tour, J.M., Molecular electronics. Synthesis and testing of components. Accounts of Chemical Research, 2000. 33(11): p.791-804.
39. Aviram, A. and M.A. Ratner, Molecular rectifiers. Chemical Physics Letters, 1974. 29(2): p. 277-283.
40. Xu, B. and N.J. Tao, Measurement of single-molecule resistance by repeated formation of molecular junctions. Science, 2003. 301(5637): p. 1221-1223.
41. Geim, A., Novoselov, K. The rise of graphene. Nature Mater. 2007, 6(3), 183–191.
42. D.R. Kauffman, D.C. Sorescu, D.P. Schofield, B.L. Allen, K.D. Jordan, A. Star Understanding the Sensor Response of Metal-Decorated Carbon Nanotubes ,Nano Lett. 2010, 10, 958.
43. J.C. Ellenbogen, J.C. Love Architectures for molecular electronic computers. I. Logic structures and an adder designed from molecular electronic diodes,Proc. IEEE 2000, 88, 386.
44. F. Diederich Carbon scaffolding: building acetylenic all-carbon and carbon-rich compounds ,Nature 1994, 369, 199 –207.
45. W. A. Chalifoux, R. R. Tykwinski, C. R. Chim. Synthesis of extended polyynes: Toward carbyne,2009, 12, 341– 358.5.
46. J. Cornil, D. Beljonne, J. P. Calbert, J. L. Bredas Interchain Interactions in Organic π-Conjugated Materials: Impact on Electronic Structure, Optical Response, and Charge Transport, Adv. Mater. 2001,13, 1053 –1067.
47. A. D. Slepkov, F. A. Hegmann, S. Eisler, E. Elliott, R. R Tykwinski .The surprising nonlinear optical properties of conjugated polyyne oligomers, J. Chem.Phys. 2004, 120, 6807 – 6810.
48. Z. Crljen and G. Baranovic Unusual Conductance of Polyyne- zBased Molecular Wires, Phys. Rev. Lett., 2007, 98, 116801.
49. C. Wang, A. S. Batsanov, M. R. Bryce, S. Martin, R. J. Nichols, S. J. Higgins, V. M. Garcia-Suarez and C. J. Lambert Oligoyne single molecule wires, J. Am. Chem. Soc., 2009, 131, 15647-15654.