Advances in Energy and Materials Research
https://jaem.qom.ac.ir/

Fluorenone as a Promising Candidate for Nanoelectronics: Electric Field Effects Explored: computational approach

Reza Safari [1] and Hamid Hadi ✉[2]

1. *Department of Chemistry, Faculty of Sciences, University of Qom, Qom, Islamic Republic of Iran*
2. *Department of Chemistry, Physical Chemistry group, Lorestan University, Khorramabad, Islamic Republic of Iran*
Corresponding author. hadi.ha@fs.lu.ac.ir

Article Info

Article type:
Research Article

Article history:
Received 4 Jan 2025
Received in revised form 15 Mar 2025
Accepted 5 May 2025
Published online 25 Jun 2025

Keywords:
Fluorenone, Field effect, Nano wire, Landauer theory, I-V curve.

ABSTRACT

Fluorenone has attracted considerable interest in nanoelectronics owing to its favorable electronic properties. In this work, the influence of an external electric field on fluorenone is investigated to evaluate its potential for nanoelectronic applications using density functional theory (DFT) and Landauer theory (LT). The electronic response of fluorenone is analyzed systematically as a function of electric-field strength, with particular attention to the energy gap, dipole moment, electron spatial extent (ESE), cohesive energy, and current–voltage (I–V) characteristics. The results show that cohesive energy and bond lengths are largely insensitive to the applied field, whereas the energy gap decreases significantly under increasing field strength. Moreover, both the dipole moment and the ESE distribution increase markedly, indicating enhanced field-induced polarization and electron delocalization. The I–V characteristics exhibit a pronounced rise in current with increasing electric-field intensity, suggesting that fluorenone is a promising candidate for field-effect molecular devices, such as molecular wires. Overall, the present study demonstrates the strong sensitivity of fluorenone to external electric fields and provides quantitative insights into the tunability of its electronic properties, thereby supporting its potential implementation in next-generation nanoscale electronic systems.

Cite this article: Safari, R., & hadi, H. (2025). Fluorenone as a Promising Candidate for Nanoelectronics: Electric Field Effects Explored: computational approach. Advances in Energy and Materials Research, 2(6), 19-27.
https://doi.org/10.22091/jaem.2025.14884.1035

DOI: 10.22091/jaem.2025.14884.1035
Publisher: University of Qom.

1. Introduction

In the realm of electronics, the quest for miniaturization and enhanced functionality has led to the exploration of single molecule electronics, a frontier where nanowires stand as indispensable components [1-3]. At the nanoscale, where individual molecules become building blocks of electronic devices, nanowires serve as crucial conduits, enabling precise manipulation and control over molecular-scale interactions and functionalities [4, 5]. This burgeoning field holds promise for revolutionizing electronics by leveraging the unique properties of molecules to achieve unprecedented levels of device integration, sensitivity, and efficiency. Among nanoelectronic devices, the design of nanowires in single molecule electronics is critical for several reasons [6-8]. Nanowires not only facilitate the electrical interfacing with individual molecules but also provide a versatile platform for integrating diverse molecular species into functional circuits. Their nanoscale dimensions and tunable properties enable tuning of electrical, optical, and mechanical properties [9-12]. So far, several compounds have been proposed and studied for their potential as nanowires, each offering distinct advantages and applications. From traditional semiconductors such as silicon and germanium to new materials such as carbon nanotubes and metal oxides [13-17]. The diversity in the design of nanowires reflects the pursuit of superior conductivity, mechanical flexibility, chemical stability, and other properties suitable for advanced electronic circuits and devices [18, 19]. In this study, fluorenone was proposed as a new candidate for use as a nanowire in quantum nanoelectronic systems. Fluorenone, a versatile compound known for its unique properties, can be used as a compelling candidate for nanowire applications in electronic circuits [20-22]. The utilization of fluorenone nanowires promises significant advancements in electronic device design and performance due to its superior characteristics compared to other designed nanowires. These attributes include exceptional electrical conductivity, robust chemical stability, precise dimensional control, and compatibility with diverse materials [23-26]. Such qualities not only enhance the efficiency and reliability of electronic circuits but also pave the way for innovative applications in miniaturization, optical functionalities, and beyond. In this research, computational chemistry knowledge was used to predict the performance of fluorenone in the presence and absence of an electric field. The structural and electronic properties of the proposed structure for use in nanoelectronic systems have been optimized under the influence of an external electric field using DFT density theory and the CAM-B3LYP/6-311G* level of theory. Then the effect of the external electric field with different intensities on the structural and electronic properties was investigated, Figure 1.

2. Computational method

Based on the density function theory (DFT), geometry optimization and calculation of the structural and electronic properties (such as ESE, DOS, and energy gap HLG=$|E_{LUMO}-E_{HOMO}|$) and vibrational characterizations of the Fluorenone field-effect molecular wire have been carried out at CAM-B3LYP/6-311G* level of theory, under different EF intensities applied along the x-axis (Figure 1), using G09 program [27-29]. Also, for the gold atoms of the end electrodes, LANL2DZ pseudopotential is used.

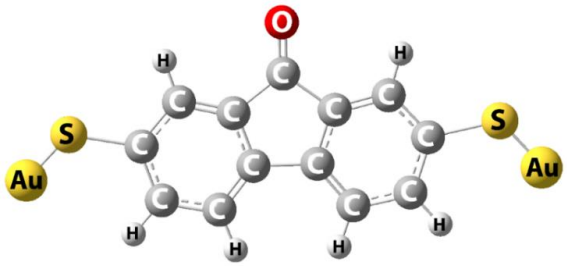

Figure 1. The structure of the studied molecule (fluorenone) in this work after binding to the gold electrode.

Landauer's formula/theory (LT, Eq. 1-3) was used to predict the current-voltage diagram (I-V curve) of this field-effect molecular wire [30]. In this regard, the temperature-independent direct-tunneling electric conduction (G) of a single-molecule nanoelectronics system can be evaluated using the Landauer formula as follows:

$$\mathbf{G} = \frac{\mathbf{1}}{\mathbf{R}} = \frac{\mathbf{2e^2\tau_e}}{\hbar} \quad (1)$$

$$\tau = \exp(-\beta L) \quad (2)$$

$$\beta = \left(\frac{2m^*\alpha\varphi}{\hbar^2}\right)^{\frac{1}{2}} \quad (3)$$

where $\hbar$ is $\frac{h}{2\pi}$, φ is the potential barrier height for tunneling through the HOMO or the LUMO level, which is equivalent to the energy difference between the Fermi energy and the molecular HOMO or LUMO level, m* is the effective mass of the electron (m*=0.16m0, m0 is the free electron mass), and α is the symmetry parameter in the potential profile, in this symmetric case, α= 1 [31, 32].

3. RESULTAS AND DISCUSSION

3.1. Structural properties

3.1.1 Bond Length

The performance of nanoelectronic devices often relies on precise control over nanoscale material properties. Changes in molecular length under an electric field can affect the overall behavior of these materials. By studying this effect, the performance and efficiency of the device can be optimized [33, 34]. For this purpose, the effect of electric field in different intensities on the studied molecule was investigated (Figure 2). Changes in the length of the molecule at the intensity of electric fields 0, 20×10^{-4} (au), 40×10^{-4} (au), 60×10^{-4} (au), 80×10^{-4} (au) and 100×10^{-4} (au) were obtained as 10.52 (A), 10.51 (A), 10.50 (A), 10.49 (A), 10.48 (A) and 10.47 (A) respectively. The obtained results show that the applied electric fields do not have a significant effect on the length of the molecule. The results indicate a relatively favorable stability along the length of the molecule.

For many applications, especially in electronics and nanotechnology, it is important to maintain a stable molecular length under the application of an electric field. Unwanted changes in length can lead to instability in device performance and have a detrimental effect on device performance, whereas a fixed molecular length ensures predictable and stable performance [35, 36].

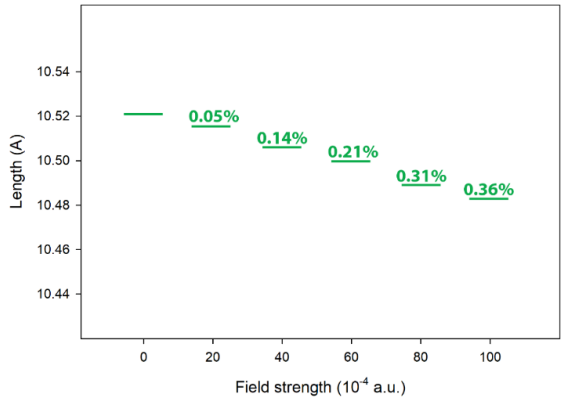

Figure 2. Changes in the length of the molecule in the intensity of different electric fields (zero electric field was used as a reference).

3.1.2 Cohesive energy

Cohesive energy is a measure of the energy required to break a substance into its constituent atoms [37]. Cohesive energy analysis provides valuable information to predict the stability of studied compounds [38, 39].

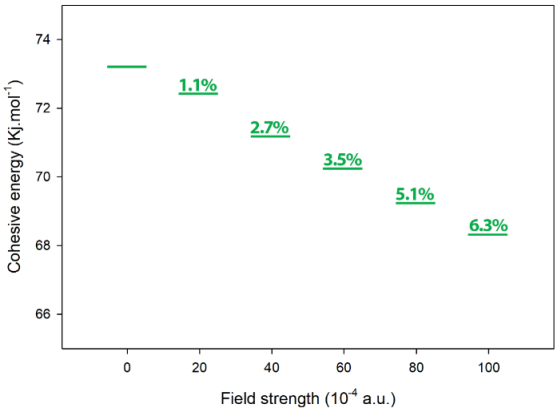

Figure 3. Cohesive energy values at different electric field intensities.

The cohesive energy values for the studied structure due to the application of the electric field with different intensities are shown in Figure 3. The cohesive energy changes in the intensity of electric fields 20×10^{-4} (au), 40×10^{-4} (au), 60×10^{-4} (au), 80×10^{-4} (au) and 100×10^{-4} (au) compared to zero field were obtained by 1.1%, 2.7%, 3.5%, 5.1% and 6.3%, respectively. According to the obtained results, after applying the electric field, there was no significant change in the coherent energy values, which indicates the acceptable stability of the system in the presence of the electric field. Cohesive energy stability ensures that the studied structure can maintain its structural integrity over a long period of time [40, 41]. This property is very important for applications that require long-term stability, such as nanoelectronic devices (such as wires, switches or molecular transistors).

3.2 Electronic properties

3.2.1 Energy of HOMO/LUMO frontier orbitals and energy gap

Investigating the energy of HOMO/LUMO boundary orbitals and the energy gap between them in nanoelectronic devices (such as wires, switches, and molecular transistors) after applying an electric field is crucial for optimizing device performance, understanding the fundamental properties of materials, and searching for new capabilities. Examining these properties enables researchers to use quantum effects to create new properties in molecules [42-46]. Table 1 shows the obtained values for the energy of HOMO/LUMO orbitals and the energy gap between them.

Table 1. The obtained values of the energy of HOMO/LUMO boundary orbitals and the energy gap in the intensity of different electric fields (All values are in eV).

Field Strength (10-4 a.u.)	LUMO	HOMO	HLG
0	-3.88	-6.45	2.57
20	-3.93	-6.39	2.46
40	-4.0	-6.18	2.18
60	-3.88	-5.78	1.90
80	-3.83	-5.5	1.67
100	-3.81	-5.08	1.27

The value of the energy gap in the absence of an electric field was calculated to be 2.57 eV. In the presence of electric fields 20×10^{-4} (au), 40×10^{-4} (au), 60×10^{-4} (au), 80×10^{-4} (au), and 100×10^{-4} (au), the energy gap value was 2.46 eV, 2.18 eV, 1.90 eV, 1.67 eV and 1.27 eV, respectively. The obtained values show that the energy gap decreases as the intensity of the electric field increases, and there is a non-linear relationship between the energy gap and the intensity of the applied electric field. According to the values obtained in Table 1, Applying an electric field has caused a disturbance in the distribution of electrons and energy levels and has a significant impact on the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), which is often called the energy gap. A smaller energy gap typically means that electrons can more easily move between different molecular orbitals. This enhances charge transport properties, allowing for better conductivity or mobility of charge carriers within the molecule. This is crucial for creating efficient electronic devices where rapid and efficient electron transfer is desired. Also, reducing the energy gap due to the application of an electric field facilitates the phenomenon of quantum tunneling between the electrode and the molecule and increases the conductivity of the molecule. This feature helps to design suitable materials (such as wire and molecular switches) for use in nanoelectronic circuits [47-51]. A DOS (Density of State) plot is a great way to show the energy gap in materials [52]. In order to more closely examine the energy gap in the studied structure, the DOS diagram was shown in Figure 4.

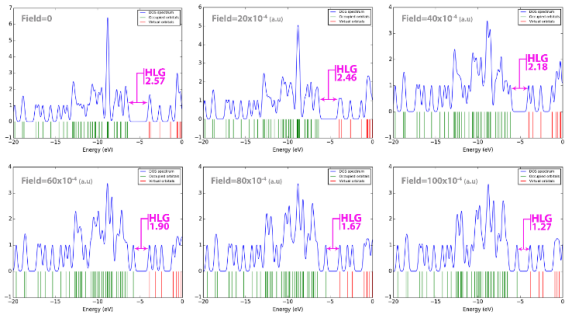

Figure 4. DOS plot of the studied structure in the intensity of different field effect.

3.2.2 Dipole moment

Dipole moment is a prominent feature in determining the electronic properties of components used in nanoelectronic systems. In the design of nanoelectronic materials and devices, understanding the effect of electric field on dipole moments helps to optimize material properties. Adjusting this feature through electric fields can lead to the design of high-performance electronic components [53-57].

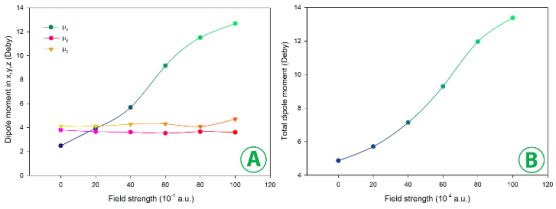

Figure 5. External field effect on electric dipole moment vectors (A) and total dipole moment (B) of the molecular system.

The values of total dipole moment in the absence of electric field were 4.86 Debye. After applying the electric field, the total dipole moment increased dramatically. The obtained values for the dipole moment in the intensity of applied electric fields, 20×10^{-4} (au), 40×10^{-4} (au), 60×10^{-4} (au), 80×10^{-4} (au) and 100×10^{-4} (au), were calculated as 5.70 Debye, 7.14 Debye, 9.29 Debye, 11.96 Debye, and 13.38 Debye respectively. According to the obtained results, the application of an external electric field caused the separation of positive and negative charge centers as well as a change in the dipole moment in the studied molecular system (Figure 5). The results showed that the dipole moment in the direction of the length of the molecule is more affected by the field, so that due to the application of the electric field, we see a symmetrical and linear pattern.

3.2.3 Electronic spatial extent (ESE) and Molecular electrostatic potential (MEP) analysis

Examining Electronic Spatial Extent (ESE) is essential in nanoelectronic device design to harness quantum effects, optimize performance, and ensure efficient operation at the nanoscale [58, 59].

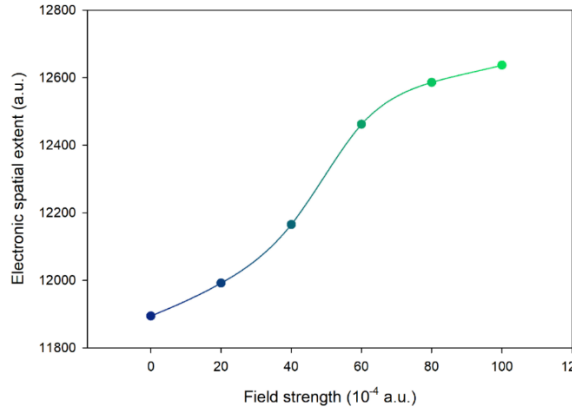

Figure 6. Changes in Electronic Spatial Extent (ESE) due to application of electric field with different intensities.

According to the results obtained in Figure 6, ESE increased due to the application of the electric field. Due to the increase of the electronic spatial extent under the influence of the electric field, the charge carriers (electrons) experience less dispersion and can move more freely. This leads to improved mobility of charge carriers, which is very important for the performance of electronic devices.

MEP analysis provides valuable insight into the three-dimensional distribution of molecular charges. Areas of high charge density are usually shown in yellow and red, while blue areas represent areas of relatively lower charge density. Neutral areas are also usually shown in green. The greater the width between the red and blue colors, the greater the dipole moment of the molecule and thus the charge distribution [60-62]. The MEP results for the studied structure in the presence of (2 and 3) and the absence of electric field are shown in Figure 7. These results show that the charge density along the length of the molecule increases with the increase in electric field intensity, which can be related to the extension of the π-conjugated bond along the length of the molecule (along the x-axis).

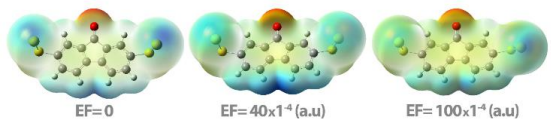

Figure 7. MEP maps for the studied molecule in EF= 0, 20×10^{-4} (au), 80×10^{-4} (au).

3.2.4 I-V Curve

Studying the Current-Voltage (I-V) characteristics of a molecule using Density Functional Theory (DFT) is crucial in understanding its electronic transport properties [63, 64]. DFT provides a theoretical framework to calculate the electronic structure and properties of molecules, and I-V curves offer insights into the conductance behavior [65, 66]. Analysis of the I-V curve reveals valuable information about the electronic/quantum properties of the molecular structure, such as electrical conductivity, energy levels, and potential applications of the molecule in electronic devices (such as molecular junctions or nanoscale electronics) [67, 68]. For this purpose, the I-V curve of the studied molecular system was studied computationally (Figure 8).

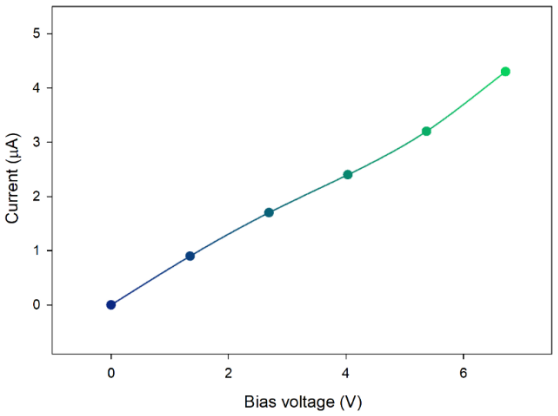

Figure 8. Current-voltage curve (I-V) of the studied structure in the intensity of applied currents.

According to the calculations, the current obtained in each of the applied electrical fields is 20×10-4 (au), 40×10-4 (au), 60×10-4 (au), 80×10-4 (au) and 100×10-4 (au) equal to 0.9 μA, 1.7 μA, 2.4 μA, 3.2 μA and 4.3 μA respectively. These results showed that there is a linear relationship between applied field intensity and current. Also, the obtained results show that the response of the studied structure to the applied electric field is significant. The reason for the increase in current can be related to the increase in electronic transitions in the molecule, which leads to higher populations in excited states and thus affects the intensity of the current.

Also, increasing the intensity of the electric field facilitates the movement of π-electrons along the length of the molecule and provides the possibility of charge transfer along the length of the molecule, thus affecting the increase in current. These features indicate the application of the case structure in molecular electronics as a molecular wire or sensor.

4. Consolation

In conclusion, this study employed density functional theory at the CAM-B3LYP/6-311G* level, combined with Landauer transport analysis, to evaluate the electronic response of fluorenone under external electric fields. Structural optimization and systematic field-dependent calculations provided detailed insights into its stability and transport characteristics.

The results indicate that cohesive energy and bond lengths remain essentially unchanged under varying electric-field intensities, confirming the structural stability of fluorenone and supporting its suitability for device integration. In contrast, the energy gap decreases significantly with increasing field strength, demonstrating strong electronic tunability—an essential feature for field-effect nanoelectronic applications.

Furthermore, the marked increase in dipole moment and electron spatial extent with applied field highlights enhanced polarization and charge redistribution within the molecule. This field-induced electronic modulation is reflected in the current–voltage characteristics, which exhibit a substantial increase in current as the electric field intensifies.

Collectively, these findings identify fluorenone as a promising candidate for molecular nanoelectronic devices, including molecular wires and potential switching elements. Its structural robustness combined with pronounced field-dependent electronic behavior underscores its potential role in the development of next-generation nanoscale electronic systems.

Conflicts of Interest

The authors declare no conflict of interest.

Acknowledgments

The authors wish to gratefully thank the Research Affairs Division at University of Qom and Lorestan University, for financial support.

Authors' Contributions

All aspects of this study were performed collaboratively by both authors. Both authors contributed equally and approved the final manuscript.

5. Reference

[1] Lu, W., & Lieber, C. M. (2007). Nanoelectronics from the bottom up. Nature materials, 6(11), 841-850. DOI: https://doi.org/10.1038/nmat2028

[2] Chau, R., Doyle, B., Datta, S., Kavalieros, J., & Zhang, K. (2007). Integrated nanoelectronics for the future. Nature materials, 6(11), 810-812. DOI: https://doi.org/10.1038/nmat2014

[3] Akinwande, D., Petrone, N. and Hone, J., 2014. Two-dimensional flexible nanoelectronics. Nature communications, 5(1), p.5678. DOI: https://doi.org/10.1038/ncomms6678

[4] Ferry, D. K. (2008). Nanowires in nanoelectronics. Science, 319(5863), 579-580. DOI: https://doi.org/10.1126/science.1154446

[5] Lin, Y. F., & Jian, W. B. (2008). The impact of nanocontact on nanowire based nanoelectronics. Nano letters, 8(10), DOI: 3146-3150. https://doi.org/10.1021/nl801347x

[6] Patolsky, F., Timko, B. P., Zheng, G., & Lieber, C. M. (2007). Nanowire-based nanoelectronic devices in the life sciences. MRS bulletin, 32(2), 142-149. DOI: https://doi.org/10.1557/mrs2007.47

[7] Lieber, C. M., & Wang, Z. L. (2007). Functional nanowires. MRS bulletin, 32(2), DOI: 99-108. https://doi.org/10.1557/mrs2007.41

[8] Ferry, D. K., Gilbert, M. J., & Akis, R. (2008). Some considerations on nanowires in nanoelectronics. IEEE Transactions on Electron Devices, 55(11), 2820-2826. DOI: https://doi.org/10.1109/TED.2008.2005171

[9] Lu, W., & Lieber, C. M. (2007). Nanoelectronics from the bottom up. Nature materials, 6(11), 841-850. DOI: https://doi.org/10.1038/nmat2028

[10] Khan, M.I., Wang, X., Bozhilov, K.N. and Ozkan, C.S., 2008. Templated fabrication of InSb nanowires for nanoelectronics. Journal of Nanomaterials, 2008(1), p.698759. DOI: https://doi.org/10.1155/2008/698759

[11] Zhou, W., Dai, X., Fu, T. M., Xie, C., Liu, J., & Lieber, C. M. (2014). Long term stability of nanowire nanoelectronics in physiological environments. Nano letters, 14(3), 1614-1619. DOI: https://doi.org/10.1021/nl500070h

[12] Kenry, Yong, K. T., & Yu, S. F. (2012). AlN nanowires: synthesis, physical properties, and nanoelectronics applications. Journal of Materials Science, 47, 5341-5360. DOI: https://doi.org/10.1007/s10853-012-6388-0

[13] Choi, W. B., Bae, E., Kang, D., Chae, S., Cheong, B. H., Ko, J. H., ... & Park, W. (2004). Aligned carbon nanotubes for nanoelectronics. Nanotechnology, 15(10), S512. DOI https://doi.org/10.1088/0957-4484/15/10/003

[14] Che, Y., Chen, H., Gui, H., Liu, J., Liu, B., & Zhou, C. (2014). Review of carbon nanotube nanoelectronics and macroelectronics. Semiconductor Science and Technology, 29(7), 073001. DOI https://doi.org/10.1088/0268-1242/29/7/073001

[15] Avouris, P. (2004). Carbon nanotube electronics and optoelectronics. Mrs Bulletin, 29(6), 403-410. DOI: https://doi.org/10.1557/mrs2004.123

[16] Mallakpour, S., & Khadem, E. (2016). Carbon nanotube–metal oxide nanocomposites: Fabrication, properties and applications. Chemical Engineering Journal, 302, 344-367. DOI: https://doi.org/10.1016/j.cej.2016.05.038

[17] Kumar, N., Navani, N. K., & Manhas, S. K. (2021). Effect of metal oxide nanoparticles on carbon nanotube device characteristics. Journal of Electronic Materials, 50(2), 528-536. DOI: https://doi.org/10.1007/s11664-020-08579-9
[18] Baraban, L., Ibarlucea, B., Baek, E., & Cuniberti, G. (2019). Hybrid silicon nanowire devices and their functional diversity. Advanced Science, 6(15), 1900522. DOI: https://doi.org/10.1002/advs.201900522
[19] Arjmand, T., Legallais, M., Nguyen, T. T. T., Serre, P., Vallejo-Perez, M., Morisot, F., ... & Ternon, C. (2022). Functional devices from bottom-up Silicon nanowires: A review. Nanomaterials, 12(7), 1043. DOI: https://doi.org/10.3390/nano12071043
[20] Andrews, L. J., Deroulede, A., & Linschitz, H. (1978). Photophysical processes in fluorenone. The Journal of Physical Chemistry, 82(21), 2304-2309. DOI: https://doi.org/10.1021/j100510a011
[21] Semin, S., Li, X., Duan, Y., & Rasing, T. (2021). Nonlinear optical properties and applications of fluorenone molecular materials. Advanced Optical Materials, 9(23), 2100327. DOI: https://doi.org/10.1002/adom.202100327
[22] Shi, Y., & Gao, S. (2016). Recent advances of synthesis of fluorenone and fluorene containing natural products. Tetrahedron, 72(14), 1717-1735. DOI: https://doi.org/10.1016/j.tet.2016.02.022
[23] Kuboyama, A. (1964). Electronic spectrum of fluorenone. Bulletin of the Chemical Society of Japan, 37(10), 1540-1544. DOI: https://doi.org/10.1246/bcsj.37.1540
[24] Yoshihara, K., & Kearns, D. R. (1966). Spectroscopic Properties of the Lower-Lying Excited States of Fluorenone. The Journal of Chemical Physics, 45(6), 1991-1999. DOI: https://doi.org/10.1063/1.1727883
[25] Becker, K., Lupton, J. M., Feldmann, J., Nehls, B. S., Galbrecht, F., Gao, D. Q., & Scherf, U. (2006). On-Chain Fluorenone Defect Emission from Single Polyfluorene Molecules in the Absence of Intermolecular Interactions. Advanced Functional Materials, 16(3), 364-370. DOI: https://doi.org/10.1002/adfm.200500550
[26] Murphy, R. S., Moorlag, C. P., Green, W. H., & Bohne, C. (1997). Photophysical characterization of fluorenone derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 110(2), 123-129. DOI: https://doi.org/10.1016/S1010-6030(97)00191-3
[27] Orio, M., Pantazis, D. A., & Neese, F. (2009). Density functional theory. Photosynthesis research, 102, 443-453. DOI: https://doi.org/10.1007/s11120-009-9404-8
[28] Boudjella, A., Gougam, A. B., & Alizadeh, H. (2008). Electron transport in molecular wires. Japanese journal of applied physics, 47(6S), 4969. DOI: https://doi.org/10.1143/JJAP.47.4969
[29] Yanai, T., Tew, D. P., & Handy, N. C. (2004). A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP). Chemical physics letters, 393(1-3), 51-57. DOI: https://doi.org/10.1016/j.cplett.2004.06.011
[30] Emberly, E. G., & Kirczenow, G. (2000). Landauer theory, inelastic scattering, and electron transport in molecular wires. Physical Review B, 61(8), 5740. DOI: https://doi.org/0.1103/PhysRevB.61.5740
[31] Hadi, H., & Safari, R. (2024). Computational evaluation of some optical and quantum electronics properties (performance) of an organic molecular switch. Optical and Quantum Electronics, 56(4), 575. DOI: https://doi.org/10.1007/s11082-023-06221-6
[32] Frank, M. P. (2018, August). Physical foundations of Landauer's principle. In International Conference on Reversible Computation (pp. 3-33). Cham: Springer International Publishing. DOI: https://doi.org/10.1007/978-3-319-99498-7_1
[33] Bhadra, P., & Siu, S. W. (2021). Effect of concentration, chain length, hydrophobicity, and an external electric field on the growth of mixed alkanethiol self-assembled monolayers: A molecular dynamics study. Langmuir, 37(5), 1913-1924. DOI: https://doi.org/10.1021/acs.langmuir.0c03414
[34] Sancho-Garcıa, J. C., Horowitz, G., Brédas, J. L., & Cornil, J. (2003). Effect of an external electric field on the charge transport parameters in organic molecular semiconductors. The Journal of chemical physics, 119(23), 12563-12568. https://doi.org/10.1063/1.1625918
[35] Pandey, P. (2022). Role of nanotechnology in electronics: A review of recent developments and patents. Recent patents on nanotechnology, 16(1), 45-66. DOI: https://doi.org/10.2174/1872210515666210120114504
[36] Yu, B., & Meyyappan, M. (2006). Nanotechnology: Role in emerging nanoelectronics. Solid-state electronics, 50(4), 536-544. DOI: https://doi.org/10.1016/j.sse.2006.03.028
[37] Farid, B., & Godby, R. W. (1991). Cohesive energies of crystals. Physical Review B, 43(17), 14248. DOI: https://doi.org/10.1103/PhysRevB.43.14248
[38] Srivastava, G. P., & Weaire, D. (1987). The theory of the cohesive energies of solids. Advances in Physics, 36(4), 463-517. DOI: https://doi.org/10.1080/00018738700101042
[39] Ye, Y., Ahn, C. C., Witham, C., Fultz, B., Liu, J., Rinzler, A. G., ... & Smalley, R. E. (1999). Hydrogen adsorption and cohesive energy of single-walled carbon nanotubes. Applied physics letters, 74(16), 2307-2309. DOI: https://doi.org/10.1063/1.123833
[40] Lazaridis, T. (2001). Solvent size vs cohesive energy as the origin of hydrophobicity. Accounts of Chemical Research, 34(12), 931-937. DOI: https://doi.org/10.1021/ar010058y
[41] Turchanin, M. A., & Agraval, P. G. (2008). Cohesive energy, properties, and formation energy of transition metal alloys. Powder Metallurgy and Metal Ceramics, 47, 26-39. DOI: https://doi.org/10.1007/s11106-008-0006-3
[42] Huang, Y., Rong, C., Zhang, R., & Liu, S. (2017). Evaluating frontier orbital energy and HOMO/LUMO gap with descriptors from density functional reactivity theory. Journal of molecular modeling, 23, 1-12. DOI: https://doi.org/10.1007/s00894-016-3175-x
[43] Minsky, A., Meyer, A. Y., & Rabinovitz, M. (1985). Paratropicity and antiaromaticity: role of the homo-lumo

energy gap. Tetrahedron, 41(4), 785-791. DOI: https://doi.org/10.1016/S0040-4020(01)96458-0

[44] Matamala, A. R., & Alarcón, A. A. (2012). A simple model for the calculation of HOMO and LUMO energy levels of benzocatafusenes. International Journal of Quantum Chemistry, 112(5), 1316-1322. DOI: https://doi.org/10.1002/qua.23135

[45] Kim, B. G., Ma, X., Chen, C., Ie, Y., Coir, E. W., Hashemi, H., & Kim, J. (2013). Energy level modulation of HOMO, LUMO, and band-gap in conjugated polymers for organic photovoltaic applications. Advanced Functional Materials, 23(4), 439-445. DOI: https://doi.org/10.1002/adfm.201201385

[46] Huang, Y., Rong, C., Zhang, R., & Liu, S. (2017). Evaluating frontier orbital energy and HOMO/LUMO gap with descriptors from density functional reactivity theory. Journal of molecular modeling, 23, 1-12. DOI: https://doi.org/10.1007/s00894-016-3175-x

[47] Lin, L. Y., Chen, Y. H., Huang, Z. Y., Lin, H. W., Chou, S. H., Lin, F., ... & Wong, K. T. (2011). A low-energy-gap organic dye for high-performance small-molecule organic solar cells. Journal of the American Chemical Society, 133(40), 15822-15825. DOI: https://doi.org/10.1021/ja205126t

[48] Doffek, C., Wahsner, J., Kreidt, E., & Seitz, M. (2014). Breakdown of the energy gap law in molecular lanthanoid luminescence: the smallest energy gap is not universally relevant for nonradiative deactivation. Inorganic chemistry, 53(7), 3263-3265. DOI: https://doi.org/10.1021/ic500017a

[49] Nolan, M., O'Callaghan, S., Fagas, G., Greer, J. C., & Frauenheim, T. (2007). Silicon nanowire band gap modification. Nano letters, 7(1), 34-38. DOI: https://doi.org/10.1021/nl061888d

[50] Arora, N., & Joshi, D. P. (2017). Band gap dependence of semiconducting nano-wires on cross-sectional shape and size. Indian Journal of Physics, 91(12), 1493-1501. DOI: https://doi.org/10.1007/s12648-017-1052-9

[51] Ganji, M. D., Aghaei, H., & Gholami, M. R. (2008). Design of nanoswitch based on C20-bowl molecules: A first principles study. Microelectronics journal, 39(12), 1499-1503. DOI: https://doi.org/10.1016/j.mejo.2008.04.017

[52] Hussain, A., Ullah, S., & Farhan, M. A. (2016). Fine tuning the band-gap of graphene by atomic and molecular doping: a density functional theory study. RSC advances, 6(61), 55990-56003. DOI: DOI: https://doi.org/10.1039/C6RA04782C

[53] Veit, M., Wilkins, D. M., Yang, Y., DiStasio, R. A., & Ceriotti, M. (2020). Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles. The Journal of chemical physics, 153(2). DOI: https://doi.org/10.1063/5.0009106

[54] Roussy, T. S., Caldwell, L., Wright, T., Cairncross, W. B., Shagam, Y., Ng, K. B., ... & Cornell, E. A. (2023). An improved bound on the electron's electric dipole moment. Science, 381(6653), 46-50. DOI: DOI: https://doi.org/10.1126/science.adg4084

[55] Xu, F., Su, H., van der Tol, J.J., Jansen, S.A., Fu, Y., Lavarda, G., Vantomme, G., Meskers, S. and Meijer, E.W., 2024. Supramolecular polymerization as a tool to reveal the magnetic transition dipole moment of heptazines. *Journal of the American Chemical Society*, *146*(23), pp.15843-15849. DOI: https://doi.org/10.1021/jacs.4c02174

[56] De Visser, S. P., Mukherjee, G., Ali, H. S., & Sastri, C. V. (2021). Local charge distributions, electric dipole moments, and local electric fields influence reactivity patterns and guide regioselectivities in α-ketoglutarate-dependent non-heme iron dioxygenases. Accounts of chemical research, 55(1), 65-74. DOI: https://doi.org/10.1021/acs.accounts.1c00538

[57] Stuyver, T., Danovich, D., Joy, J., & Shaik, S. (2020). External electric field effects on chemical structure and reactivity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 10(2), e1438. DOI: https://doi.org/10.1002/wcms.1438

[58] Ghiasi, R., & Rahimi, M. (2021). Complex formation of titanocene dichloride anticancer and Al 12N 12 nano-cluster: A quantum chemical investigation of solvent, temperature and pressure effects. Main Group Chemistry, 20(1), 19-32. DOI: https://doi.org/10.3233/MGC-210034

[59] Ghiasi, R., Sofiyani, M. V., & Emami, R. (2021). Computational investigation of interaction of titanocene dichloride anti-cancer drug with carbon nanotube in the presence of external electric field. Biointerface Res. Appl. Chem, 11, 12454-12461. DOI: https://doi.org/10.33263/BRIAC114.1245412461

[60] Saral, A., Sudha, P., Muthu, S., Sevvanthi, S., & Irfan, A. (2022). Molecular structure spectroscopic Elucidation, IEFPCM solvation (UV–Vis, MEP, FMO, NBO, NLO), molecular docking and biological assessment studies of lepidine (4-Methylquinoline). Journal of Molecular Liquids, 345, 118249. DOI: https://doi.org/10.1016/j.molliq.2021.118249

[61] Vennila, M., Rathikha, R., Muthu, S., Jeelani, A., & Irfan, A. (2022). Theoretical structural analysis (FT-IR, FT-R), solvent effect on electronic parameters NLO, FMO, NBO, MEP, UV (IEFPCM model), Fukui function evaluation with pharmacological analysis on methyl nicotinate. Computational and Theoretical Chemistry, 1217, 113890. DOI: https://doi.org/10.1016/j.comptc.2022.113890

[62] Mumit, M. A., Pal, T. K., Alam, M. A., Islam, M. A. A. A. A., Paul, S., & Sheikh, M. C. (2020). DFT studies on vibrational and electronic spectra, HOMO–LUMO, MEP, HOMA, NBO and molecular docking analysis of benzyl-3-N-(2, 4, 5-trimethoxyphenylmethylene) hydrazinecarbodithioate. Journal of molecular structure, 1220, 128715. DOI: https://doi.org/10.1016/j.molstruc.2020.128715

[63] Song, X., Han, B., Yu, X., & Hu, W. (2020). The analysis of charge transport mechanism in molecular junctions based on current-voltage characteristics. Chemical physics, 528, 110514. DOI: https://doi.org/10.1016/j.chemphys.2019.110514

[64] TURUT, A. (2020). On current-voltage and capacitance-voltage characteristics of metal-semiconductor contacts. Turkish Journal of Physics, 44(4), 302-347. DOI: https://doi.org/10.3906/fiz-2007-11

[65] Upendranath, K., Venkatesh, T., Nayaka, Y. A., Shashank, M., & Nagaraju, G. (2022). Optoelectronic, DFT and current-voltage performance of new Schiff base 6-nitro-benzimidazole derivatives. Inorganic Chemistry Communications, 139, 109354. DOI: https://doi.org/10.1016/j.inoche.2022.109354

[66] Hassanien, A. M., Altalhi, T. A., Refat, M. S., Shakya, S., Atta, A. A., Alsawat, M., & Asla, K. A. (2022). Exploring microstructural, optical, electrical, and DFT/TD-DFT studies of boron subphthalocyanine chloride for renewable energy applications. Optik, 263, 169367. DOI: https://doi.org/10.1016/j.ijleo.2022.169367

[67] Papadopoulou, P., Ovaliadis, K., Philippousi, E., Hanias, M. P., Magafas, L., & Stavrinides, S. G. (2024). The Effect of Temperature on a Single-Electron Transistor IV Curve. Symmetry, 16(3), 327. DOI: https://doi.org/10.3390/sym16030327

[68] Evers, F., Korytár, R., Tewari, S., & Van Ruitenbeek, J. M. (2020). Advances and challenges in single-molecule electron transport. Reviews of Modern Physics, 92(3), 035001. DOI: https://doi.org/10.1103/RevModPhys.92.035001