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Fluorenone as a Promising Material for Nanoelectronics: Electric Field Effects Investigated

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ABSTRACT

Fluorenone has attracted significant interest in nanoelectronics due to its promising electronic properties. This study investigates the effects of an electric field on fluorenone to evaluate its suitability for nanoelectronic applications using density functional theory (DFT) and Landauer theory. The electronic properties of fluorenone, including the energy gap, dipole moment, electron spatial extent (ESE), cohesive energy, and current-voltage characteristics, were systematically analyzed under varying electric field strengths. Results show that while cohesive energy and bond lengths remain largely unaffected, the energy gap decreases significantly with increasing electric field strength. Additionally, the dipole moment and ESE distribution increase substantially. The current-voltage profile exhibits a sharp rise in current with increasing field intensity, underscoring fluorenone's potential as a strong material for field-effect molecular devices, such as molecular wires. These findings highlight fluorenone's sensitivity to external electric fields, supporting its viability for advancing nanoelectronic technologies. This study provides critical insights into the tunability of fluorenone's electronic properties, paving the way for its integration into next-generation nanoscale electronic systems.

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1. Introduction

The pursuit of miniaturization and enhanced functionality in electronics has driven the exploration of single-molecule electronics, where nanowires are essential components [1-3]. At the nanoscale, individual molecules serve as building blocks for electronic devices, and nanowires act as critical conduits, enabling precise control over molecular-scale interactions and functionalities [4, 5]. This emerging field promises to revolutionize electronics by leveraging molecular properties to achieve unprecedented device integration, sensitivity, and efficiency. In single-molecule electronics, nanowires are vital for electrically interfacing with individual molecules and providing a versatile platform for integrating diverse molecular species into functional circuits [6-8]. Their nanoscale dimensions and tunable properties allow for customization of electrical, optical, and mechanical characteristics [9-12]. Various compounds, including traditional semiconductors (e.g., silicon, germanium), carbon nanotubes, and metal oxides, have been studied for their potential as nanowires, each offering unique advantages [13-17]. The diversity in nanowire design reflects the pursuit of superior conductivity, mechanical flexibility, chemical stability, and compatibility with advanced electronic circuits [18, 19].

This study proposes fluorenone as a novel material for nanowires in quantum nanoelectronic systems. Fluorenone, known for its unique properties, is a compelling material for nanowire applications in electronic circuits [20-22]. Fluorenone nanowires offer significant advantages over other nanowire materials, including exceptional electrical conductivity, robust chemical stability, precise dimensional control, and compatibility with diverse materials [23-26]. These attributes enhance the efficiency and reliability of electronic circuits and enable innovative applications in miniaturization and optical functionalities. In this research, computational chemistry was employed to predict fluorenone’s performance under varying electric field conditions. The structural and electronic properties of fluorenone, optimized for nanoelectronic applications, were analyzed under the influence of an external electric field using density functional theory (DFT) at the CAM-B3LYP/6-311G* level of theory. The effects of electric fields with different intensities on these properties were investigated, as shown in Figure 1.

2. Computational method

Using density functional theory (DFT), geometry optimization and calculations of structural and electronic properties, including electron spatial extent (ESE), density of states (DOS), energy gap (HLG = |ELUMO - EHOMO|), and vibrational characteristics, were performed for the fluorenone field-effect molecular wire at the CAM-B3LYP/6-311G* level of theory. These calculations were conducted under varying electric field intensities applied along the x-axis, as shown in Figure 1, using the Gaussian 09 program [27-29]. For the gold atoms in the end electrodes, the LANL2DZ pseudopotential was employed.

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

Landauer theory (Eqs. 1–3) was employed to predict the current-voltage (I-V) characteristics of the fluorenone field-effect molecular wire [30]. The temperature-independent direct-tunneling electrical conductance (G) of a single-molecule nanoelectronic system was evaluated using the Landauer formula, as described below:

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

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

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

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. Results and Discussion

3.1. Structural Properties

3.1.1 Molecular Length

The performance of nanoelectronic devices often depends on precise control of nanoscale material properties. Variations in molecular length under an electric field can influence device behavior, and understanding these effects is critical for optimizing performance and efficiency [33, 34]. The impact of electric fields of varying intensities on the molecular length of fluorenone was investigated, as shown in Figure 2. Molecular lengths were calculated at electric field intensities of 0, 20×10^{-4}, 40×10^{-4}, 60×10^{-4}, 80×10^{-4}, and 100×10^{-4} atomic units (au), yielding values of 10.52 Å, 10.51 Å, 10.50 Å, 10.49 Å, 10.48 Å, and 10.47 Å, respectively. These results indicate that the applied electric fields have a minimal effect on the molecular length, suggesting favorable structural stability.

For many applications in electronics and nanotechnology, maintaining a stable molecular length under electric fields is essential. Unwanted length variations can lead to performance instability, whereas consistent molecular dimensions ensure predictable and reliable device behavior [35, 36].

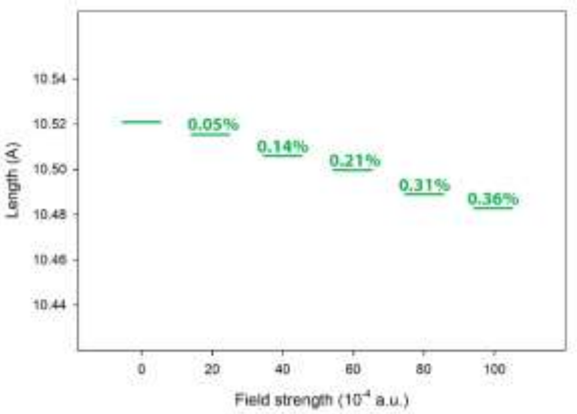

Figure 2. Changes in the length of the molecule in the intensity of different electric fields (zero electric field was used as a reference).

3.1.2 Cohesive Energy

Cohesive energy, defined as the energy required to dissociate a molecule into its constituent atoms, is a key indicator of structural stability [37]. Analysis of cohesive energy provides critical insights into the stability of fluorenone under varying electric field conditions [38, 39].

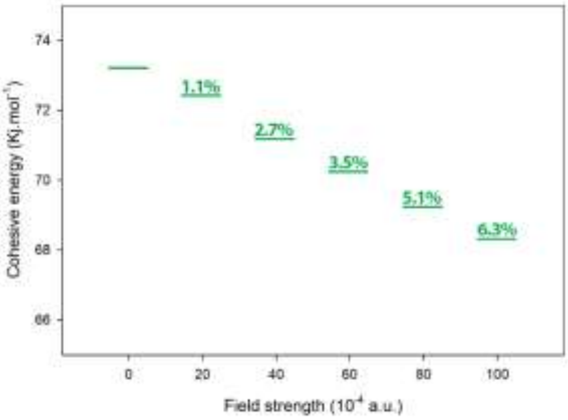

Figure 3. Cohesive energy values at different electric field intensities.

Cohesive energy values for fluorenone under varying electric field intensities are presented in Figure 3. Compared to the zero-field condition, cohesive energy changes at electric field intensities of 20×10^{-4}, 40×10^{-4}, 60×10^{-4}, 80×10^{-4}, and 100×10^{-4} atomic units (au) were 1.1%, 2.7%, 3.5%, 5.1%, and 6.3%, respectively. These results indicate minimal changes in cohesive energy upon application of electric fields, suggesting acceptable structural stability of the system. Stable cohesive energy ensures that fluorenone maintains its structural integrity over extended periods, a critical property for long-term reliability in nanoelectronic applications, such as molecular wires, switches, or transistors [40, 41].

3.2 Electronic Properties

3.2.1. HOMO/LUMO Frontier Orbitals and Energy Gap

The energies of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), along with the energy gap between them, are critical for optimizing the performance of nanoelectronic devices, such as molecular wires, switches, and transistors. Investigating these properties under electric fields provides insights into the fundamental characteristics of materials and enables the exploration of quantum effects to engineer novel molecular functionalities [42-46]. The calculated HOMO and LUMO energies and the corresponding energy gap for fluorenone under varying electric field intensities are presented in Table 1.

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 energy gap of fluorenone in the absence of an electric field was calculated to be 2.57 eV. Under electric field intensities of 20×10^{-4}, 40×10^{-4}, 60×10^{-4}, 80×10^{-4}, and 100×10^{-4} atomic units (au), the energy gap decreased to 2.46 eV, 2.18 eV, 1.90 eV, 1.67 eV, and 1.27 eV, respectively, as shown in Table 1. These results demonstrate a non-linear decrease in the energy gap with increasing electric field intensity. The application of an electric field perturbs the electron distribution and energy levels, significantly reducing the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). A smaller energy gap facilitates electron transitions between molecular orbitals, enhancing charge transport properties and improving conductivity or charge carrier mobility within the molecule. This is critical for designing efficient nanoelectronic devices, such as molecular wires and switches, where rapid electron transfer is essential. Additionally, the reduced energy gap promotes quantum tunneling between the molecule and electrodes, further increasing molecular conductivity. These characteristics make fluorenone a promising material for nanoelectronic circuits [47-51]. A density of states (DOS) plot effectively illustrates the energy gap in materials [52]. To further examine the energy gap of fluorenone, the DOS is presented in Figure 4.

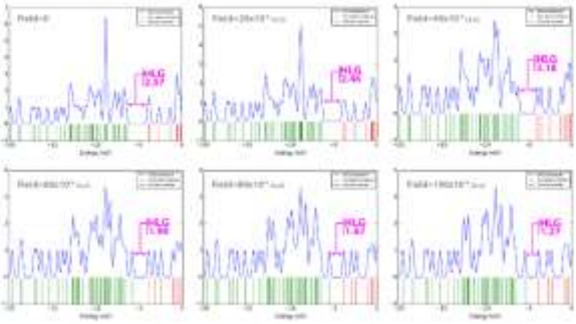

Figure 4. DOS plot of the studied structure in the intensity of different field effect.

3.2.2. Dipole Moment

The dipole moment is a critical property influencing the electronic behavior of materials in nanoelectronic systems. Understanding the effect of electric fields on the dipole moment of fluorenone is essential for optimizing material properties in the design of nanoelectronic devices. By tuning the dipole moment through applied electric fields, high-performance electronic components, such as molecular wires and switches, can be developed [53-57].

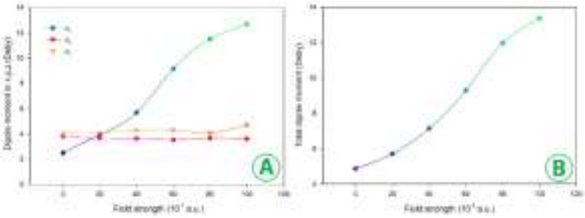

Figure 5. External field effect on electric dipole moment vectors (A) and total dipole moment (B) of the molecular system.

In the absence of an electric field, the total dipole moment of fluorenone was calculated to be 4.86 Debye. Under applied electric fields of 20×10^{-4}, 40×10^{-4}, 60×10^{-4}, 80×10^{-4}, and 100×10^{-4} atomic units (au), the dipole moment increased significantly to 5.70 Debye, 7.14 Debye, 9.29 Debye, 11.96 Debye, and 13.38 Debye, respectively, as shown in Figure 5. These results indicate that the external electric field induces a separation of positive and negative charge centers, leading to a substantial increase in the dipole moment of fluorenone. The dipole moment along the molecular axis is particularly sensitive to the electric field, exhibiting a linear and symmetric response to increasing field intensity.

3.2.3. Electronic Spatial Extent (ESE) and Molecular Electrostatic Potential (MEP) Analysis

The electronic spatial extent (ESE), which quantifies the spatial distribution of electrons, is crucial for designing nanoelectronic devices to leverage quantum effects, optimize performance, and ensure efficient operation at the nanoscale. Similarly, molecular electrostatic potential (MEP) analysis provides insights into charge distribution and intermolecular interactions, aiding in the development of high-performance materials [58, 59].

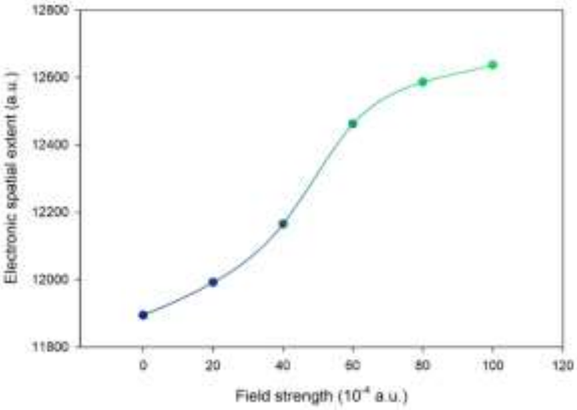

Figure 6. Changes in Electronic Spatial Extent (ESE) due to application of electric field with different intensities.

As shown in Figure 6, the electronic spatial extent (ESE) of fluorenone increases with the application of an electric field. This increase in ESE reduces electron dispersion, allowing charge carriers (electrons) to move more freely. Enhanced charge carrier mobility is critical for improving the performance of nanoelectronic devices, such as molecular wires and switches.

Molecular electrostatic potential (MEP) analysis provides insights into the three-dimensional charge distribution of fluorenone. In MEP maps, regions of high electron density are typically depicted in red and yellow, while regions of low electron density appear in blue, with neutral areas shown in green. A larger separation between red and blue regions indicates a greater dipole moment and more pronounced charge distribution [60-62]. The MEP results for fluorenone in the absence and presence of electric fields (2 and 3) are presented in Figure 7. These results reveal that charge density along the molecular axis (x-axis) increases with increasing electric field intensity, likely due to the extension of the π-conjugated system along the molecule's length.

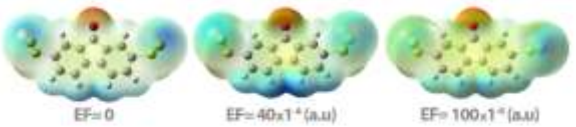

Figure 7. MEP maps for the studied molecule in EF= 0, 20×10^{-4} (au), 80×10^{-4} (au).

3.2.4 I-V Curve

The current-voltage (I-V) characteristics of fluorenone, calculated using density functional theory (DFT), are essential for understanding its electronic transport properties [63, 64]. DFT provides a robust framework for analyzing the electronic structure and transport behavior of molecules, with I-V curves revealing insights into conductance properties [65, 66]. Analysis of the I-V curve yields critical information about the quantum and electronic properties of fluorenone, including electrical conductivity, energy level alignment, and potential applications in nanoelectronic devices, such as molecular junctions and nanoscale circuits [67, 68]. The I-V curve of fluorenone under varying electric field conditions was computationally investigated, as presented in Figure 8.

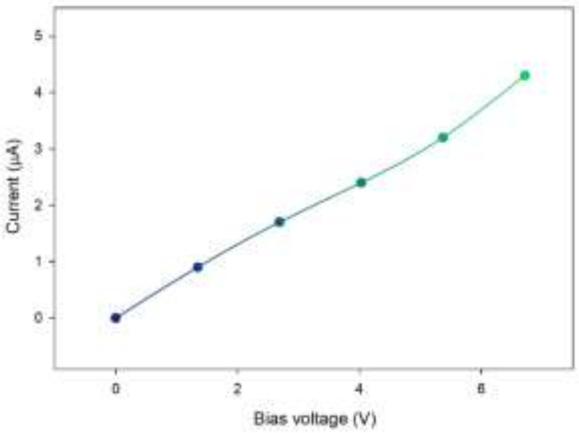

Figure 8. Current-voltage curve (I-V) of the studied structure in the intensity of applied currents.

The calculated currents for fluorenone under applied electric field intensities of 20×10^{-4}, 40×10^{-4}, 60×10^{-4}, 80×10^{-4}, and 100×10^{-4} atomic units (au) were 0.9 μA, 1.7 μA, 2.4 μA, 3.2 μA, and 4.3 μA, respectively, as shown in Figure 8. These results demonstrate a linear relationship between electric field intensity and current, indicating a significant response of fluorenone to the applied field. The increase in current is attributed to enhanced electronic transitions within the molecule, leading to higher populations in excited states and thus greater current intensity. Additionally, higher electric field intensities facilitate the movement of π-electrons along the molecular axis, enabling efficient charge transfer and further contributing to the current increase. These characteristics highlight fluorenone's potential as a molecular wire or sensor in nanoelectronic applications.

4. Consolation

This study employed density functional theory (DFT) at the CAM-B3LYP/6-311G* level to investigate fluorenone's potential in quantum nanoelectronic systems, revealing critical insights into its structural and electronic properties under varying electric field intensities. The key findings are summarized as follows:

First, fluorenone exhibits remarkable structural stability, with cohesive energy and molecular length remaining largely unaffected by electric fields, making it suitable for reliable device integration. In contrast, the energy gap, a critical parameter for electronic applications, decreases significantly with increasing electric field intensity, indicating fluorenone's responsiveness as a field-effect molecular component. Additionally, the dipole moment and electronic spatial extent (ESE) show substantial increases under stronger electric fields, highlighting fluorenone's ability to modulate its electronic properties dynamically. The current-voltage (I-V) characteristics further confirm this responsiveness, displaying a linear increase in current with escalating electric field intensity, consistent with enhanced charge transport.

These findings collectively position fluorenone as a promising material for quantum nanoelectronic applications, such as molecular wires or switches. Its pronounced response to electric fields underscores its potential to enhance the performance and efficiency of next-generation nanoscale electronic devices..

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