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IMPLEMENTATION OF A NANOSCALE OPTOELECTRONIC SWITCH FOR NANOROBOTS: A FIRST-PRINCIPLES APPROACH

IMPLEMENTACIJA NANOMETRSKEGA OPTOELEKTRONSKEGA STIKALA ZA NANOROBOTE: PRVI NAČELNI PRISTOP

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Nanotechnology is an emerging field that provides insights into multidisciplinary scientific research. Nanoscale optical switches are a key area for researchers. An optoelectronic molecular switch is also used in nanorobotics. In this study, a bio-inspired molecular optical switch is investigated and characterized for potential use in future nanorobotics systems. It is developed using an Adenine-Thymine-Guanine-Cytosine-based molecular chain, which is the basic building block of DNA. The self-assembly nature of DNA fragments helps the development of this opto-molecular switch. The article describesits characteristics and features. Its density of states, transmission spectra, and current-voltage characteristics are investigated and analyzed. Density Functional Theory (DFT) combined with the Non-Equilibrium Green's Function (NEGF) method, based on first-principlescalculations, is used to theoretically derive the electronic characteristics of the biomolecular switch. It operates with high efficiency, and its distinct 'ON' and 'OFF' states are clearly demonstrated. Hence,it will be applicable in future generations of nanorobotic systems. In summary, this opto-molecular switching device represents a significant advance toward the development of nanorobotic system modelling.

Keywords: DFT, NEGF, optical switch, nanorobot, DNA

Nanotehnologija je razvijajoča se nova tehnologija, ki zahteva multi-disciplinarno znanstveno-raziskovalno sodelovanje. Nanodimenzionalna optična stikala so danes eno od najbolj razvijajočih se področij delovanja raziskovalcev. Optomolekularna stikala se lahko uporabljajo v nanorobotskih sistemih. V tem članku avtorji opisujejo raziskavo in karakterizacijo novega biomolekularnega stikala in možnosti njegove prihodnje uporabe v nanorobotskih sistemih. V članku avtorja opisujeta razvoj biomolekularnega stikala z uporabo molekularne verige na osnovi adenin-timin-gvanin-citozina, ki je osnovni gradnik dezoksiribonukleinske kisline (DNK). Naravna sposobnost samo-sestavljanja posameznih delov (fragmentov) DNK jima je pomagala pri razvoju optomolekularnega stikala. V članku so predstavljene značilnosti in lastnosti tega optomolekularnega stikala. Avtorja sta raziskala in analizirala gostoto stanj naprave, transmisijske spektre in tokovno-napetostne značilnosti optomolekularne naprave. Za teoretično izpeljavo elektronskih značilnosti tega biomolekularnega stikala sta uporabila vzorec delovanja po *pristopu prvega načela* (angl.: first principle approach), ki temelji na teoriji funkcionalne gostote (DFT) in neravnovesni Greensovi funkciji (NEGF). Ta biološko navdihnjena molekularna naprava je zelo učinkovita in ključni stanji »VKLOP« in »IZKLOP« te stikalne naprave sta vizualizirani. Zato se bo ta biomolekularna naprava lahko učinkovito uporabljala v prihodnji generaciji nanorobotskih sistemov in kot takšna predstavlja korak naprej pri modeliranju novih nanorobotskih sistemov.

Ključne besede: teorija funkcionalne gostote, neravnovesna Greensova funkcija, optično stikalo, nanorobot, dezoksiribonukleinska kislina

1 INTRODUCTION

With advancementsin the nanoscale industry, researchers are highly motivated to design nanoscale robots. It is important to develop efficient and reliable nanoscale devices and assemble theminto a nanorobot. This nanorobotic era faces challenges in various fields, such as drugdelivery systemsused for human health in medical research.[1–10] However, a full control of these captivating molecular robots is the result of miniaturization and innovation approaches of artificial intelligence (AI).[11–16] In this framework, integrated opto-molecular switches along with other nanodevices provide the space for nanoscale robots. Opto-molecular switches influence the interaction between a material and light, manipulating the transmission of charge carriers and providing enormous speed and efficiency. Theseunparalleled devices provide unique and efficient features to nanorobots. Opto-molecular switches exhibit combined features of optics, electronics and quantum-ballistic mechanics used for faster and more efficient operations with high precision applicable in the nanorobot development. Nanoscale memories, ALU, transistors, logic gates, and diodes represent the future of the nanorobotics era.[17–25] In today's world, AI-based nanoscale-device designing isrequired and the demand is steadily increasing. These tiny devices play a crucial role in our lives. The involvement of AI is driving major breakthroughs in the quantum era. Their remarkable achievements establisheda revolutionary trademark in the field of nanotechnology. Nanorobots are composed of several key subsystems. The main ones are

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miniaturization and precision,enhanced functionality,efficiency and reliability, integration and assembly.Moreover, nanoscale electronic eyes and skin can be made possible with the help of AI. Many research areas are brought together to create a nanoscale robotic system, such as nanotechnology, robotics, materials science, biology, and computer science. These robots include nanoscale sensors, actuators, power sources, communication modules, and control systems,integrated into a unified nanorobotic platform. Each component must be carefully designed and optimized to ensure compatibility, functionality, and reliability within a nanorobotic system.[26–30] There are several reasonsfor implementing a nanoscale optoelectronic switch into nanorobots:

- Miniaturization: As technology advances, there is a growing demand for smaller and more efficient devices, especially in fields like robotics where size constraints are significant. Nanoscale optoelectronic switches offer the potential to create incredibly small components suitable for nanorobots, enabling them to perform tasks in confined spaces or at microscopic scales.
- Optoelectronics: The study and application of electronic devices that source, detect, and control light, is a rapidly evolving field with numerous potential applications. By leveraging optoelectronic principles at the nanoscale, researchers can develop devices with enhanced performance and functionality, such as faster operation and lower power consumption.
- Switching functionality: Switches play a crucial role in electronic circuits, allowing for the control over the flow of electricity. In the context of nanorobots, nanoscale switches can rapidly and precisely control various functions, enabling complex behaviors and interactions at the nanoscale.
- First-principles approach: This approach derives the behavior of a system from fundamental principles, such as the laws of physics or quantum mechanics, instead of relying solely on empirical data or pre-existing models.

This approach enables researchers to gain deeper insights into the underlying mechanisms governing the behavior of nanoscale optoelectronic switches, leading to more robust designs and potentially uncovering novel phenomena. Overall, the motivation behind this research is to advance the capabilities of nanorobots by developing nanoscale optoelectronic switches using a rigorous first-principles approach, with the goal of enabling more efficient, precise, and versatile functionality at the nanoscale.

Motivation and Background: The miniaturization of electronic components has been a cornerstone of modern technological advancements, propelling the development of nanoscale devices with unprecedented speed, efficiency, and integration capabilities. Among the most promising applications of this miniaturization trend is the field of nanorobotics, which aims to develop robotic systems on the nanometer scale for operations in confined or inaccessible environments – such as targeted drug delivery, cellular surgery, and in-situ sensing within biological or hazardous systems. For such nanorobots to function autonomously and respond to environmental stimuli, the integration of compact, energy-efficient, and high-speed switching devices is critical.

Traditional transistor-based switches face fundamental limitations when scaled down to the nanometer regime, including quantum tunneling effects, increased power dissipation, and fabrication challenges. These limitations necessitate the exploration of novel switching mechanisms that exploit quantum mechanical principles and can function reliably at such small scales.

In this context, nanoscale optoelectronic switches offer a compelling solution. These devices utilize light as a control signal, enabling ultrafast switching, low-power operation, and minimal heat dissipation – attributes essential for the constrained operational environment of nanorobots. Recent advances in two-dimensional (2D) materials, nanowires, and molecular electronics have demonstrated the feasibility of designing optoelectronic devices at the atomic and molecular scale. However, the design and optimization of such switches require a deep understanding of their electronic and optical behavior at the quantum level. First-principles methods based on DFT and NEGF formalism provide powerful tools for investigating the charge transport and optoelectronic properties of nanoscale systems with high accuracy and predictive power. Our work is motivated by the growing demand for intelligent, responsive nanoscale systems and the lack of compact, reliable switching elements that can operate under optical control. By leveraging a first-principles approach, this research aims to design and characterize a nanoscale optoelectronic switch suitable for integration into nanorobots. The study not only enhances the fundamental understanding of light-induced switching phenomena at the atomic scale but also provides a pathway for the practical implementation of optically controlled nanodevices in future nanorobotic systems.

2 MODEL AND METHODS

This paper presents a comprehensive study of the implementation of nanoscale robots using molecular parts of DNA. Adenine (A), Thymine (T), Cytosine (C) and Guanine (G) are used for molecular switches to build a nanorobot. The DFT- and NEGF-based first-principles approach formalism is used for the development of this robot. The current-voltage (IV) characteristics and quantum transmission spectra of the molecular switch show that this optical switch is almost similar to the conventional switches. The proposed opto-biomolecular switch is based on the fundamental building blocks of DNA. The quantum-ballistic transmission of this switch shows the efficiency required for a nanorobot. The self-assembly of the A, T, C, G molecules facilitates the dynamic configuration of the nanorobot. This phenomenon stimulates the nanorobot. This nanorobotlays the foundation for next-generation frameworks in the emerging era of drug delivery systems. The main objectives of this study are as follows:

- Investigation of the electronic structure of the opto-biomolecular switch.
- Design of the algorithm for the proposed nanoscale robot.

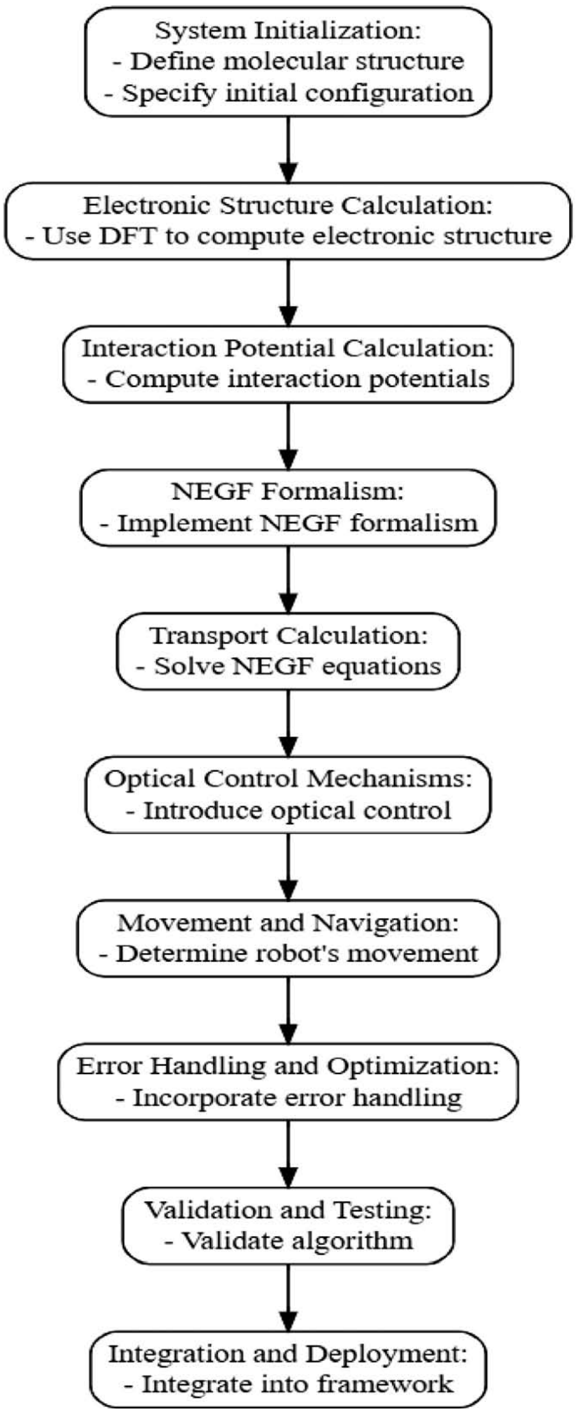

Figure 1: Detailed flowchart of the proposed nanorobot

- Assessment of the efficiency and implications of the nanorobotic system.As mentioned in the abstract, it will be quite easy to follow theset rules, as long as the user replaces the provided 'content' without modifying the 'form'.

This investigation satisfactorily demonstratesthe efficiency and future potentials of the strategic framework for the A-T-C-G based nanorobot. A detailed block diagram for the design of thenanorobot based on a biomolecular optical switch is shown in **Figure 1**. Detailed simulation parameters are listed in **Table 1**. The modeling and design of nanoscale optoelectronic switches for integration into nanorobotsrequire an accurate understanding of the material's behavior at the atomic scale. Density Functional Theory (DFT), a quantum mechanical modeling method, offers a robust first-principles framework for investigating fundamental properties of materials without relying on empirical parameters. For nanoscale systems, where classical models fail to capture quantum effects, DFT serves as an indispensable tool. In the context of this research, DFT plays a pivotal role in several key aspects:

1. Electronic Structure Analysis

DFT enables a precise calculation of the electronic structure of the active material used in the optoelectronic switch. By solving the Kohn-Sham equations for the interacting electron system, DFT provides:

- Band structure and density of states (DOS), revealing semiconducting, metallic, or insulating behavior.
- Identification of the bandgap nature (direct or indirect), which is crucial for the optoelectronic response.
- Charge distribution and localization, crucial for understanding switching mechanisms.
- The above information is vital in selecting or engineering materials with desirable optoelectronic properties such as high on/off ratio, low power consumption, and rapid response to optical stimuli.

2. Optical Properties Prediction

- Using time-dependent DFT (TDDFT) or perturbative methods within DFT, optical properties such as:
- Dielectric function,
- Absorption spectra,
- Exciton binding energies can be calculated. These properties determine a material's sensitivity to light, thus allowing the design of the photo-responsive element in the switch.

3. Charge Transport Characteristics

- By coupling DFT with Non-Equilibrium Green's Function (NEGF) formalism, it is possible to model:
- Current-voltage (I–V) characteristics under bias,
- Photon-assisted transport,
- Quantum tunneling effects at the nanoscale,
- Switching behavior under different illumination conditions.

- This combination of tools allows a simulation of real operational conditions for the switch, enabling predictive modeling of its performance within the nanorobot.

4. Material Stability and Structural Optimization

- DFT provides insights into:
- Structural relaxation to find the most stable configuration of atoms,
- Total energy minimization,
- Evaluation of binding energies, formation energies, and mechanical stability.
- These are crucial for ensuring that the material used in the nanorobot's switching element remains structurally and thermodynamically stable under operational stress.

5. Interface and Contact Modeling

- In nanoscale devices, the interface between the optoelectronic material and electrodes significantly influences the performance. DFT allows:
- Modeling of metal-semiconductor or heterojunction interfaces,
- Evaluation of Schottky barriers or tunneling contacts,
- Alignment of Fermi levels and potential drops at interfaces.
- These insights allow the design of efficient and low-resistance contacts in the nanoswitch.

6. Scalability and Miniaturization Insights

By evaluating how electronic and optical properties change with:

- Dimensional reduction (from bulk to 2D to molecule),
- Quantum confinement effects,
- Different geometries and chiralities (e.g., in nanotubes or nanowires),
- DFT helps identify scaling limits and optimal configurations for miniaturized robotic components.

Table 1: Simulation parameters

S. No.	Parameters	Details
1	System geometry	Inclusion of A-T-C-G
2	Computational software	DFT+ NEGF + Quantum-ATK
3	Exchange correlation function	Generalized Gradient Approximation (GGA), Perdew-Burke-Ernzerhof (PBE)
4	Basis set	Gaussian
5	K-point sampling	1×1×75
6	Electron temperature	300K
7	External perturbation	optical excitation and electrical biasing
8	Analytical tools	IV characteristics+ transmission spectra
9	Convergence criteria	Force and stress
10	Simulation steps	200

3 RESULTS AND ANALYSIS

Advanced quantum mechanical simulations and computations are required to design an algorithm for an optical molecular robot, built with A-T-C-G chains, employing NEGF- and DFT-based first-principles approach. The basic building block of this robot is an A-T-C-G based optical switch. The schematic diagram of this opto-biomolecular switch is shown in **Figure 2**. It shows that biomolecules are connected to each other by hydrogen bonds. However, the A-T-C-G bonding interactions are more complex than the example in the schematic. In it, only an A-T-C-G single chain is considered and no biomolecules are repeated. On the other hand, in complex designs, enormous numbers of repetitions are considered. In our schematic, it is clear that the two-way arrows carry the information to each node. Therefore, genetic information or data can flow in both directions. This is a simple schematic representation of DNA-based biomolecular switch, which is part of a nanorobot. The electronic structure calculation of this biomolecular switch is based on DFT calculations. It is associated with charge density, energy levels, and wave functions of the molecules. The calculation also determines the molecular orbitals and their energies. The I-V characteristics of the opto-molecular switch is shown in **Figure 3**. From this figure, it is evident that the switch is activated in both directions, but the maximum current is obtained in the forward-bias condition, thus considered as the 'ON' condition of the switch. Sufficient current is obtained for the switch, proving the efficiency of the proposed model compared to the conventional devices.

3.1 Computational Methods

The present study utilizes first-principles computational techniques based on Density Functional Theory (DFT) and the Non-Equilibrium Green's Function (NEGF) formalism to model and simulate the behavior of a nanoscale optoelectronic switch intended for integration into nanorobotic systems. These methods enable accurate predictions of electronic, optical, and transport properties of the proposed nanoscale device without relying on empirical data. The overall computational workflow can be summarized as follows:

1. Geometry Optimization

The atomic structure of the nanoscale optoelectronic switch, including active materials and electrodes, is first optimized using DFT. The total energy of the system is minimized until the forces on each atom are below a specified convergence threshold (typically <0.1 eV/nm), ensuring a stable equilibrium structure.

Exchange-Correlation Functional: Generalized Gradient Approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional is typically employed.

Pseudopotentials: Norm-conserving or projector augmented-wave (PAW) pseudopotentials are used to treat core electrons.

Basis Set: A double-zeta polarized (DZP) or plane-wave basis set is used depending on the software and system.

k-Point Sampling: Monkhorst-Pack scheme is applied for Brillouin zone sampling. Denser grids are used for periodic systems (e.g., nanoribbons or 2D materials).

2. Electronic Structure Calculations

Once optimized, the electronic properties are calculated to understand the material's semiconducting or metallic behavior and its suitability for switching applications.

Band Structure and Density of States (DOS): These are evaluated to determine the bandgap, electronic transitions, and energy level alignment.

Charge Density and Mulliken Population Analysis: Used to understand charge redistribution and interfacial interactions under external perturbations (e.g., light).

3. Optical Properties Evaluation

Evaluating the light-sensitivity and optoelectronic response of the material:

Dielectric Function (ε): Real and imaginary parts are computed to derive absorption spectra.

Optical Conductivity and Absorption Coefficient: These parameters help in assessing the suitability of the material for photon-induced switching.

Time-Dependent DFT (TDDFT): Used for precise optical transition analysis, particularly for molecular or low-dimensional systems.

4. Quantum Transport Simulations (DFT + NEGF)

The switching behavior of the device under external bias and optical excitation is studied using the DFT-NEGF formalism, which combines the quantum transport theory with first-principles calculations.

Device Configuration: A two-probe system is modeled, consisting of left and right electrodes connected through a central scattering region (the active switch).

Transmission Spectrum (T(E)): Calculated to evaluate electron transmission probability at different energy levels.

Current–Voltage (I–V) Characteristics: Computed using the Landauer-Büttiker formula.

Photonic Excitation: Simulated by modifying the Hamiltonian with light-matter interaction terms or by injecting photo-generated carriers.

5. Simulation Tools

The following software tools are used in the simulations:

QuantumATK or AtomistixToolKit (ATK): For DFT + NEGF-based transport simulationsneeds.

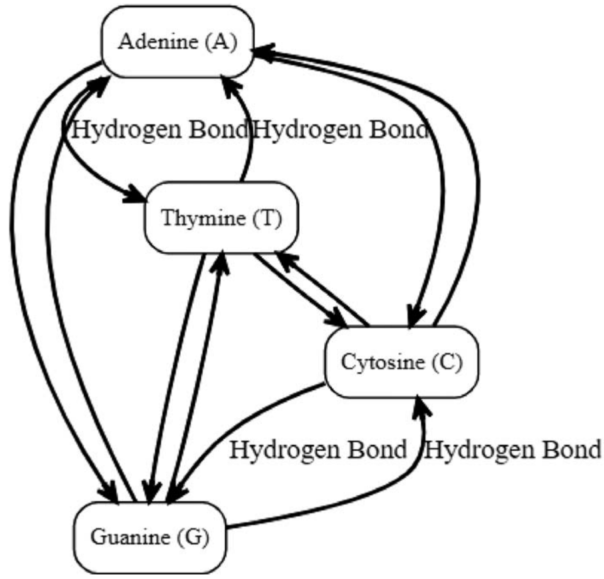

Figure 2: Schematic diagram of the A-T-C-G based opto-molecular switch

6. Convergence and Validation

All calculations are carefully converged with respect to: energy cutoff values (typically 300–500 eV for plane-wave basis), k-point density, supercell size to eliminate periodic image interactions, and vacuum padding (>1,5nm for non-periodic directions). Validation is performed by comparing calculated results with available experimental or high-level theoretical data, where applicable.

3.2 Effect of Transmission Spectra on the Nanorobot in the Context of a Nanoscale Optoelectronic Switch

1. Transmission Spectrum as an Indicator of Switching Capability

The transmission spectrum, T(E), describes the probability of electrons transmitting through the switch at dif-

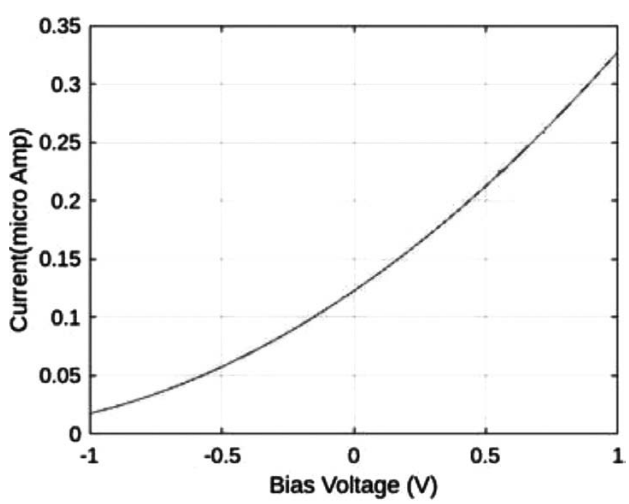

Figure 3: I–V characteristics of the A-T-C-G opto-switch

ferent energy levels, EEs. It is especially important in evaluating on-state and off-state conductance:

- High transmission peaks near the Fermi level (or under optical excitation) indicate low resistance and high current – the 'ON' state.
- Suppressed transmission (T(E) ≈ 0) implies poor carrier conduction – the 'OFF' state.
- Thus, the ability to modulate T(E) with external stimuli (e.g., light) defines the switch's responsiveness and determines its binary logic behavior inside the nanorobot.

2. Light-Induced Modulation of Transmission

In an optoelectronic switch, incident light alters the electronic structure or induces photo-generated carriers, which can open or close conductive channels in the transmission spectrum:

- When illuminated, if new transmission peaks emerge at or near the Fermi level, it indicates an enhanced carrier flow and a transition to the ON state.
- Without light, these pathways are suppressed or blocked, maintaining the system in the OFF state.
- This photonically controlled modulation is key to enabling logic and control operations in nanorobots, where mechanical switches are impractical.

3. Effect on Current–Voltage (I–V) Characteristics

The transmission spectrum is directly linked to the I–V response of the device through the Landauer-Büttiker formula.

Here, changes in T(E) under varying voltage or illumination conditions translate into a change in the current flow. This governs the switching speed, sensitivity, and power consumption of the nanorobot's logic or actuation module.

4. Selective Filtering and Signal Integrity

The shape and width of the transmission spectrum can also filter energy-specific carriers, allowing selective transport of electrons based on their energy. This is especially useful in:

- minimizing noise or thermal leakage currents
- maintaining signal integrity for communication between nanorobotic subsystems
- ensuring low-power operation, a critical constraint for autonomous nanoscale systems

5. Quantum Confinement and Size Effects

For devices operating in the nanometer regime, quantum confinement leads to discrete transmission states. This makes the transmission spectrum highly sensitive to:

- device dimensions
- electrode coupling
- interface quality

Fine-tuning these parameters enables precise control over switching thresholds and operating voltages, making it possible to design compact and energy-efficient switches suitable for nanorobots.

The detailed algorithm of this proposed nanorobot is given below.

DesignAlgorithm: Biomolecular robot design using DFT and NEGF

System Initialization:

Define Molecular Structure ():

- Define the molecular structure using adenine (A), guanine (G), thymine (T), and cytosine (C) molecules.
- Initialize the coordinates and orientations of the molecules.

Electronic Structure Calculation:

Perform DFT Calculation ():

- Use Density Functional Theory (DFT) to compute the electronic structure of the molecular system.
- Calculate the electronic density, energy levels, and wavefunctions of the molecules.
- Determine the molecular orbitals and their energies.
- Interaction Potential Calculation:
  Compute Interaction Potentials ():
- Compute the interaction potentials between adjacent molecules based on their electronic structures.
- Utilize DFT calculations to determine van der Waals interactions, hydrogen bonding, and other non-covalent interactions between nucleobases.

NEGF Formalism:

Implement NEGF Formalism ():

- Implement the Non-Equilibrium Green's Function (NEGF) formalism to describe the transport properties of the molecular system.
- Define the Hamiltonian matrix representing the electronic structure of the system.
- Incorporate self-energies to account for interactions with the electrodes or external environment.

Transport Calculation:

Solve NEGF Equations ():

- Solve the NEGF equations to calculate the electron density, current, and charge distribution within the molecular system.
- Simulate electron transport through the molecular junction formed by the robot.

Optical Control Mechanisms:

Introduce Optical Control ():

- Introduce optical control mechanisms to manipulate the electronic properties of the molecular system.
- Apply external optical fields or stimuli to modulate the energy levels, excitations, or electronic transitions within the molecules.
- Utilize DFT to simulate the response of the molecules to optical excitation and photon absorption.

Movement and Navigation:

Determine Robot Movement ():

- Utilize the calculated electronic properties and interaction potentials to determine the movement of the molecular robot.
- Design algorithms to control the motion of the robot based on changes in the electronic structure induced by optical stimuli or environmental factors.
- Implement feedback mechanisms to adjust the robot's trajectory in real-time.

Error Handling and Optimization:

Implement Error Handling ():

- Incorporate error handling mechanisms to correct deviations from the desired trajectory or functionality.
- Optimize the algorithm parameters, such as the molecular arrangement, optical control parameters, and NEGF simulation settings, to improve the efficiency and reliability of the robot.

Validation and Testing:

Validate Algorithm ():

- Validate the algorithm through a comparison of experimental data and benchmark calculations.
- Test the performance of the molecular robot in simulated environments and realistic scenarios.
- Iterate on the algorithm design based on feedback and validation results.

Integration and Deployment:

Integrate Algorithm ():

- Integrate the algorithm into a computational framework or platform suitable for practical applications.
- Deploy the molecular robot algorithm for specific tasks, such as molecular sensing, manipulation, or transport, in various investigations or industrial settings.

Based on the above algorithm, a schematic diagram of the A-T-C-G based nanorobotic system is shown in **Figure 4**. In this robotic system, we consider only the forward and backward movements of the line follower robot. This is the simplest form of the robot,based on A-T-C-G, which are the basic building blocks of DNA.

The transmission spectra of A-T-C-G based opto-molecular switch provides the information regarding the intensity of transmitted light as a function of wavelength of light. This function is capable to present the information on transmission spectrum of each molecule. A-T-C-G are the basic building blocks of DNA and RNA. Their distinct electronic structures, energy levels and light absorption capabilities make these molecules capable to interact with light. Optical switches show their optical properties in response to the external stimulants, for example light, bias voltage, electric field, etc. Our A-T-C-G opto-switch uses these stimulants for the transmission properties which are again influenced by optical excitation or environmental features. Transmission spectra measure the amount of transmitted light through a matter at different wavelength. This spectrum provides the information regarding the material's interaction with light along with its optical properties. **Figure 5** shows how A-T-C-G molecules absorb and transmit light at different wavelengths due theirdifferent structures. Each of them has the property of light absorption and transmission characteristics whose cumulative result is shown in **Figure 5**. Adenine typically absorbs light in the UV region and its transmission peaks at around 260–280 nm. Thymine's absorption peak is at around 260–270 nm, which is similar to Cytosine's peak. Guanine's peak is at around 250–270 nm. The changes in the transmission peaks are the indicators of the optical switching behavior of the molecular switch.

To develop a line follower A-T-C-G based nanorobot, we need to consider many features. The algorithm is shown below.

Algorithm for the line follower bionanorobot:
Initialization or Start:

- Define the initial configuration of the nanorobot, including the arrangement of Adenine, Thymine, Cytosine, and Guanine molecules.

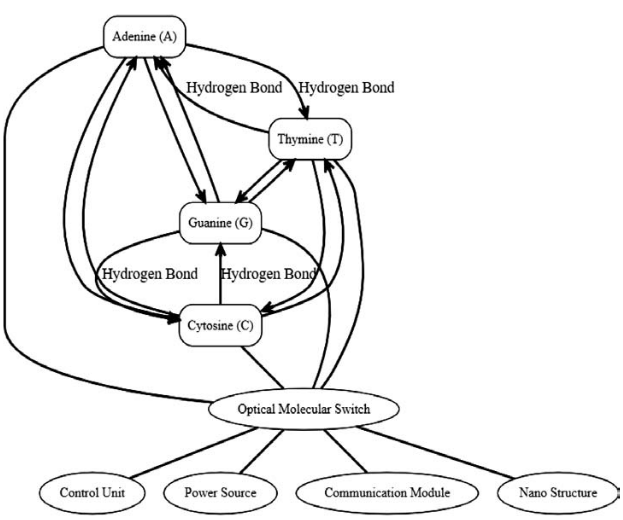

Figure 4: Schematic diagram of the bionanorobotic system

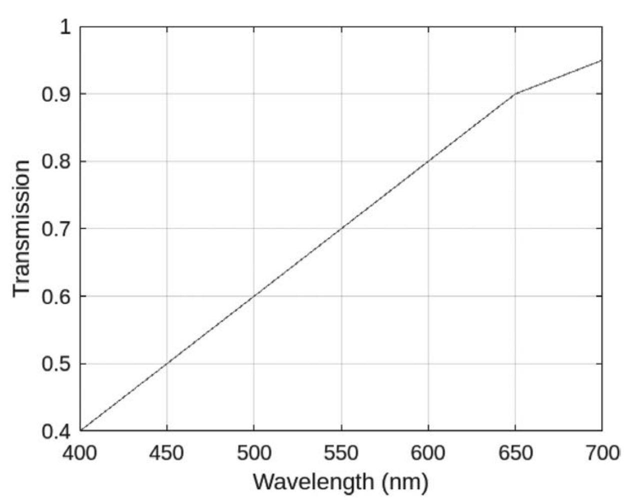

Figure 5: Transmission spectra of the biomolecular switch

- Specify the starting position and orientation of the nanorobot.

Sensing and Feedback

- Implement sensors to detect environmental cues or signals for navigation.
- Continuously monitor the nanorobot's surroundings for obstacles or target locations.
- Incorporate feedback mechanisms to adjust the robot's movement based on sensor inputs.

Control Mechanics:

- Utilize optical control mechanisms to manipulate the molecular structure and properties of the nanorobot.
- Apply external optical fields or stimuli to induce changes in the robot's configuration.
- Implement algorithms to translate optical signals into specific movements or actions.

Movement Algorithm:

- Design algorithms to control the movement of the nanorobot based on optical stimuli or environmental cues.
- Determine the desired trajectory or path for the robot to follow.
- Break down the movement into smaller steps or commands for precise control at the molecular level.

Motion Execution:

- Execute the movement commands to initiate the motion of the nanorobot.
- Implement algorithms for precise manipulation of Adenine, Thymine, Cytosine, and Guanine molecules to achieve the desired movement.
- Ensure that movements are performed within the constraints of the nanoscale environment to avoid unintended interactions or disruptions.

Feedback and Adjustment:

- Continuously monitor the progress of the nanorobot's movement.

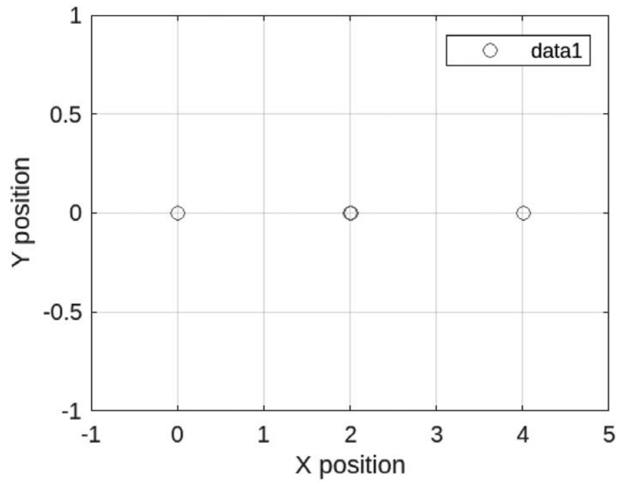

Figure 6: Movement of the optical biomolecular switch-based line follower nanorobot

- Incorporate feedback loops to make real-time adjustments to the robot's trajectory or behavior.
- Handle any unexpected obstacles or deviations from the planned path.

Termination:

- Define conditions for terminating the movement algorithm, such as reaching the target location or completing a specific task.
- Implement termination procedures to safely halt the robot's motion and deactivate any control mechanisms.

Error Handling:

- Include error-handling routines to address any failures or malfunctions during movement.
- Implement safety protocols to prevent unintended consequences of movement commands.

Optimization:

- Optimize the movement algorithm for efficiency and reliability.

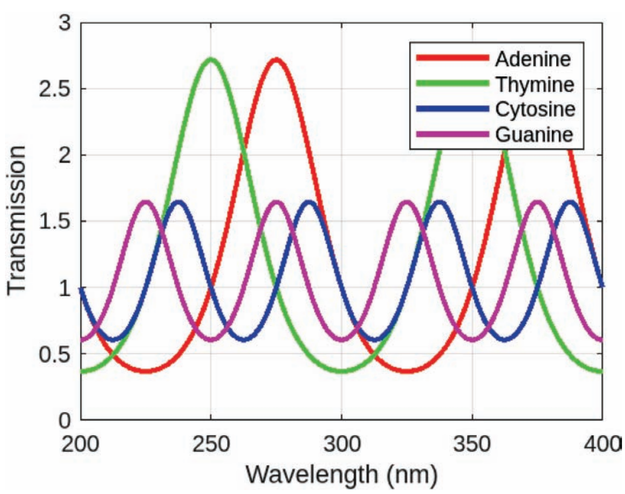

Figure 7: Transmission spectra of the optical biomolecular switch-based line follower nanorobot

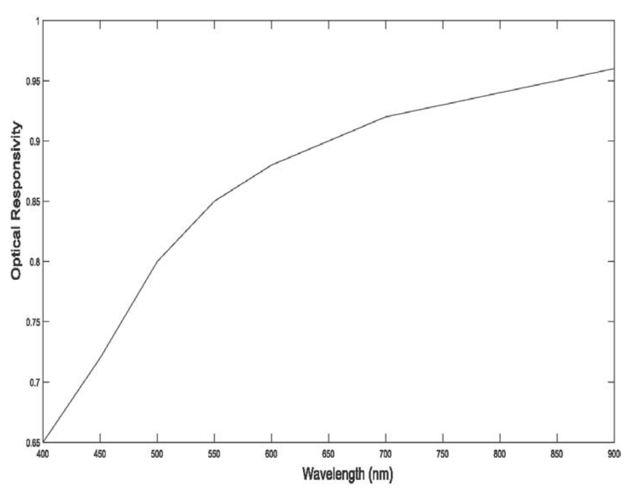

Figure 8: Wavelength vs optical responsivity for the nanorobot

Table 2: Comparative analysis

Feature	CMOS transistor (nanoscale)	Proposed optoelectronic switch (DFT-based)
Switching mechanism	Electric field-induced	Photon-induced electron excitation
Miniaturization limit	≈5–7 nm (quantum tunneling limits)	<5 nm feasible (atomic-scale modeling)
Energy consumption	High (leakage current at small scales)	Low (no standby current under light control)
Switching speed	Limited by gate capacitance	Ultrafast (ps–fs range, photon-limited)
Integration in nanorobots	Difficult (heat dissipation, bulkiness)	Excellent (minimal footprint, optical control)
Scalability	CMOS scaling is near its limit	Quantum-based design scalable with DFT

- Fine-tune parameters such as movement speed, responsiveness to stimuli, and energy consumption.

Validation and Testing:

- Validate the movement algorithm through simulation or experimental testing.
- Verify that the nanorobot can navigate its environment effectively and perform designated tasks.

The movement of the A-T-C-G based line follower nanoscale robot is shown in **Figure 6**. The middle red point shows the overlapping of the two points of the line follower robot when an optical stimulant has excited the molecular chain. This is the linear arrangement of the biomolecules. The stimuli are presented with red dots. The straight line in **Figure 6** shows the line path for the bionanorobot. The transmission spectra of this line follower bionanorobot are shown in **Figure 7**. It shows that due to the variation in the light absorption by the A-T-C-G, the transmission peaks of the line follower robot vary. These differences in light absorption act as the driving forces of the robot.

Figure 8 shows the optical response of the nanorobottodifferent wavelengths. This graph demonstrates that the response of the nanorobot increasesas the wavelength rises from 400 nm to 550 nm, after which the optical responsivity continues to increasemore gradually. A comparative analysis of a CIMOS transistor and our proposed switch is shown in **Table 2**.

4 CONCLUSION

In this work, we used a first-principles method to investigate the development of a nanoscale optoelectronic switch for nanorobots. Multidisciplinary research has provided several options thanks to the growth of nanotechnology, with optical nanoswitches emerging as a major area of study. These opto-molecular switches have enormous potential to advance nanorobotics systems, especially for drug delivery applications.

Using A-T-C-G based molecular chains, we developed a bio-inspired,optical molecular switch-based line follower nanorobot. We successfully built and analyzed this line-followingbionanorobottheoretically, considering its potential applications in next-generation nanorobotics systems, using the self-assembly nature of DNA fragments.

We carried outour work using first-principles paradigms based on NEGF and DFT. Transmission spectra, and current-voltage characteristics were examined as part of our investigation, and our findings shed light on the operation and functionality of the line follower bionanorobot. With distinct ON and OFF states visible during switching, the results showed great efficiency of the suggested molecular device. Additionally, the study laid foundation for upcoming developments in nanorobotics by presenting a thorough algorithm for the movement of optical molecular switch-based nanorobots using adenine, thymine, cytosine, and guanine. In summary, our work offers a bio-inspired solution with prospective applications in medicine and other sectors, marking a major advancement in the development of nanorobotics systems. As these molecular devices are further developed and optimized, we pave the way for the development of highly intelligent nanorobots that can carry out challenging tasks with hitherto unheard-of efficiency and precision.

Ethical Approval

Not Applicable.

Competing interests

The corresponding author states that there is no conflict of interest.

Authors' contributions

All the authors have equal contribution. XiaobaoXie planned the work and simulated the data. Yixiong He wrote the manuscript and all the authors finally checked the manuscript.

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All of the material is owned by the authors and/or no permissions are required.

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