

ISSN: 2582-7219



International Journal of Multidisciplinary Research in Science, Engineering and Technology

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)



Impact Factor: 8.206

Volume 8, Issue 6, June 2025



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET) (A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

NanoIntelligence: Designing Computation at the Molecular Scale using Interdisciplinary Science

Sharvil Ganesh Nikam¹, Rohit Ravindra Patil², Dr. Poonam Kaswan³

UG Student, Dept. of IT, AISSMS IOIT, Pune, Maharashtra, India¹

UG Student, Dept. of ENTC, AISSMS IOIT, Pune, Maharashtra, India²

Assistant professor, Dept. of Industrial Chemistry, AISSMS IOIT, Pune, Maharashtra, India³

ABSTRACT: By using molecular systems to process information beyond the capabilities of conventional silicon-based devices, nanocomputers represent a revolutionary change in computational design. The multidisciplinary integration of quantum physics, molecular biology, and synthetic chemistry in the creation of next-generation nanocomputing architectures is examined in this review. Scalable and reconfigurable molecular circuits are now possible in chemistry thanks to developments in dynamic reaction networks, luminescent lanthanide complexes, and molecular logic gates. Biocompatible, low-energy alternatives for computation and biosensing are provided by biological computing techniques such as strand-displacement architectures, enzyme-regulated classifiers, and DNA-based logic gates. At the same time, fault-tolerant quantum operations at room temperature are becoming possible thanks to developments in quantum physics, including topologically protected quantum units, ultracold dipolar molecule gates, and molecular spin qudits. These fields' convergence encourages the development of hybrid computing platforms that can interface with biology, process data in parallel, and make intelligent decisions. The review provides a thorough synthesis of the current state of the field and outlines strategic directions for future research in nanocomputing by highlighting significant experimental milestones, theoretical frameworks, and unresolved challenges.

KEYWORDS: Nanocomputing, molecular logic gates, DNA computing, quantum nanotechnology, synthetic chemistry, bio-quantum interfaces, molecular qubits, enzymatic logic circuits, hybrid computing systems, topological quantum computing..

I. INTRODUCTION

As scientists get closer to creating intelligent, self-governing systems at the molecular and atomic level, the paradigm of computation has changed significantly over the last 20 years. Synthetic chemistry, molecular biology, and quantum physics are all combined to create new computing architectures in nanocomputers, which are computational systems built from nanoscale components [1]–[3]. Nanocomputers, as opposed to traditional silicon-based computers, can process information in essentially different ways by taking advantage of the special behaviours of atoms, molecules, and biological systems.

The goal of creating nanocomputers stems from the understanding that complex issues in communication, materials science, medicine, and sensing require new types of computation in addition to the desire to reduce the size of existing devices. Heat dissipation, parallelism, and quantum inefficiencies at the nanoscale are challenges for conventional computers. On the other hand, chemical logic [4], [5], genetic circuits [6], [7], and quantum entanglement-based processing [8]–[10] can all be integrated into nanocomputing systems, allowing for previously unheard-of computational performance for particular task classes.

Molecular logic gates, rotaxanes, and supramolecular machines that serve as nanoscale processing units have been designed thanks to synthetic chemistry [1], [11], and [12]. These systems encode logical operations in chemical space by taking advantage of reversible covalent interactions, redox states, or conformational dynamics. The possibility of molecular-level programming with specially created molecules is further highlighted by recent advancements in systems chemistry and chemical artificial intelligence [4].



DOI:10.15680/IJMRSET.2025.0806201

ISSN: 2582-7219 | www.ijmrset.com | Impact Factor: 8.206| ESTD Year: 2018|



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

At the same time, biological computing has advanced rapidly, using proteins, DNA, RNA, and even entire cells as computational substrates [6, 13, 14]. Programmable, biocompatible nanocomputers that can make decisions in biological settings are made possible by DNA logic gates, which can be dynamically reconfigured and encoded in sequences [7], [15]. A few of these platforms have already shown promise in intracellular communication, metabolic regulation, and cancer diagnostics [6], [16].

Another frontier is quantum nanocomputing, which uses quantum mechanics to enable exponentially faster algorithms, especially in simulation, optimisation, and cryptography [8]–[10]. The creation of topologically protected logic gates, solid-state qubits, and molecular spin systems raises the possibility that computation can take place at scales and efficiencies that are not possible with classical physics [1], [17], and [18].

Crucially, the real innovation is found in the integration of disciplines rather than in each one alone. Bio-quantum interfaces, for instance, are currently being investigated in which biological environments house quantum sensors for neural mapping or medical imaging [9], [19]. Similar to this, new approaches to molecular quantum control are being explored through the development of chemical scaffolds for the stabilisation and manipulation of quantum states [1], [2], and [20].

With an emphasis on how synthetic chemistry, biology, and quantum physics each individually and in combination improve the architecture and functionality of nanocomputers, this review examines the state-of-the-art in nanocomputing technologies. We offer a thorough analysis of:

- fundamental ideas and computational structures in every field
- new platforms like quantum dots, molecular logic gates, and DNA nanostructures
- cross-disciplinary systems that combine chemical or quantum logic with biological control
- breakthroughs in applications, difficulties, and tactical chances for further advancement.

By doing this, we hope to shed light on the complex field of nanocomputing and pinpoint the areas where synergistic convergence holds the greatest promise for practical application.

II. FOUNDATIONS AND THEORETICAL FRAMEWORK

2.1 Synthetic Chemistry: Molecule Programming

2.1.1 Gates for Molecular Logic

Using their conformational or electronic changes, molecules can be chemically programmed to carry out logic operations such as AND, OR, and NOT. For example:

Rotaxanes are molecules that resemble rings and are attached to a linear "axle." The ring, which represents an ON/OFF logic switch, shifts to a different area of the axle in response to particular chemical stimuli (such as a proton or light) [1] Redox-based switches switch conductivity or fluorescence by altering their oxidation state in response to an applied voltage. These modifications function as output signals [5]. For instance, you create a molecule that only emits light when both protons (H⁺) and electrons are present. An AND logic gate is what that is.

This is the chemical counterpart of electronic logic, but instead of relying solely on electricity, it is based on molecular structure and interaction.

2.1.2 Lanthanide-Based Multi-State (Qudit) Systems

Lanthanide ions (rare earth metals) have multiple stable electron spin states, in contrast to binary systems that only have 0 or 1 states. Qudit logic, which represents more than two logical states per molecule, is made possible by this [3].

For instance, a 4-level logic state (0, 1, 2, 3) could be stored in a single lanthanide complex, increasing the system's computational capacity without growing its physical dimensions.

Higher-density computing is made possible by this, which is crucial in nanoscale environments with limited space.



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

2.1.3 Self-Regulating Chemical Systems and Molecular Machines

Thanks to recent developments in systems chemistry, molecules can now act like machines that react to various inputs and change their configuration accordingly.

• When exposed to chemical gradients or energy inputs (such as heat, light, etc.), molecular machines—like nanocars or synthetic motors—move directionally across a surface or alter their configuration. [6].

By associating motion with logical results, such as "move if input A AND input B are present," these are able to perform computation.

• Similar to early computers, chemical automata are molecules or reaction networks that use feedback loops and dissipative systems to sequentially carry out logic steps [4].

2.2 Biology: Using the Building Blocks of Life to Compute

2.2.1 Circuits for DNA Strand Displacement

DNA-based logic gates create input/output pathways using predictable base pairing.

The double-stranded portion of a normal DNA gate has an overhang. This overhang is bound by an incoming DNA strand, which then pushes out the output strand. It is possible to manipulate this sequence to mimic AND, OR, and NOT functions [10].

For instance, you can use cellular AND logic in diagnostics to program a DNA strand to emit a fluorescent signal only in the presence of two particular microRNA sequences.

2.2.2 Origami of DNA as Logical Structures

Folding DNA strands into exact nanostructures—such as boxes, hinges, or switches—is known as DNA origami.

In reaction to molecular inputs (proteins, enzymes, or ions), these structures can change their configuration, and the transformation itself turns into a logical process [11].

This technique is used by researchers to design "logic gates" that, in response to specific signals, physically open or close, regulate chemical reactions, or release therapeutic agents [12].

2.2.3 Cellular Logic Circuits and Proteins

Computational components include proteins (such as transcription factors and enzymes) and modified cell components: Synthetic gene circuits: These genes are designed to create an in vivo logic gate by expressing proteins only in response to specific molecular inputs, such as sugars or toxins [14].

CRISPR-based logic: Mechanisms that construct more intricate logical pathways inside cells by editing DNA only under particular molecular circumstances.

For living nanocomputers-cell-based devices that can sense, think, and act-these systems are particularly crucial.

2.2.4 Molecular Crystals as Platforms for Computing

Information can be processed by crystalline DNA or protein frameworks based on how their molecules come together: Self-putting together The logic rules governing how each component connects are encoded in DNA crystals. The computation is the assembly behaviour [15].

This is similar to molecular-scale cellular automata, in which complex global behaviour is produced by each building block adhering to local rules.

2.3 Quantum Physics: Quantum States in Computation

2.3.1 Qubits in Molecular Structure

Qubits, which are units of quantum information that exist in superpositions (both 0 and 1 at the same time), are used in quantum computers.



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

In the spin states of metal complexes such as organic radicals or lanthanides, molecular spin qubits encode quantum information [1].

Microwave pulses can be used to precisely alter the quantum state of these systems. Because molecular control allows for scalability and compactness, which are essential for integration with biology or chemistry, they hold promise.

2.3.2 Majorana Modes and Topological Qubits

Exotic particles known as Majorana zero modes can be found at the ends of particular nanowires or quantum materials. Since their data is nonlocally stored, they are resistant to noise and decoherence, which are significant issues in quantum computing [20].

Microsoft's "Majorana-1" processor is based on this methodology [20].

2.3.3 Quantum dots and NV centres

Quantum dots and NV centres (diamond vacancy centres) are nanoscale materials in which individual atoms or defects function as qubits:

- It is possible to optically read out NV centres (shine light and read the spin state).
- Information is encoded by quantum dots using charge/spin states that are confined in a nanostructure [17], [18].

Under ambient or nearly ambient conditions, they enable quantum sensing and computation.

2.3.4 Quantum Error Correction Based on Qudit

For quantum computing, error correction is essential. Qudits (d > 2 quantum states) are now used in some systems to encode more information per particle.

For example, qudits based on antimonide enable more complex information to be represented with greater stability using fewer particles [21].

This maintains coherence while scaling quantum systems to realistic sizes.

III. TECHNOLOGICAL PLATFORMS AND MATERIALS

Nanocomputing is based on both theoretical underpinnings and physical platforms that represent logic at the nanoscale. The combination of quantum physics, molecular biology, and synthetic chemistry has produced a range of architectures, each suited to different operational settings, input methods, and computational objectives

3.1 Nanostructures of DNA and RNA

DNA and RNA molecules are among the most adaptable materials in nanoscale computing. The technique of folding single-stranded DNA into predetermined 2D or 3D structures using short "staple" strands is known as DNA origami, and it has become a programmable logic scaffold. These nanostructures efficiently carry out logic operations by reconfiguring in response to particular inputs, such as complementary DNA strands, small molecules, or enzymes. In a biological context, for example, a DNA nanobox might only open when two specific microRNAs are present, carrying out an AND logic operation [11], [12].

Because RNA can both encode and catalyse, it provides an extra degree of computational flexibility. These naturally occurring RNA-guided DNA cleaving enzymes, known as CRISPR-Cas systems, are now used to create programmable logic inside living cells. For instance, Cas12a can be designed to cut only in the presence of particular activator and guide RNAs, creating a molecular AND gate [13], [14]. Especially in environments with limited resources, these systems have been used in biosensing, gene control, and molecular diagnostics.

3.2 Artificial Molecular Instruments

The foundation of chemically encoded computation is made up of supramolecular devices from the synthetic chemistry domain, including rotaxanes, catenanes, and photochromic molecules. When exposed to external stimuli such as light, pH, or redox changes, rotanes—which are made up of a ring molecule threaded onto an axle—can transition between



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

various states. These molecules act as molecular-scale logic gates when integrated into monolayers or self-assembled films, and this reversible switching can be mapped to binary logic [1], [6].

This logic architecture is further extended by assemblies of nanoparticles. Reconfigurable electrical networks can be created by functionalising semiconductor or gold nanoparticles with particular ligands. When other particles or chemical agents are present, their conductivity changes, allowing for a type of environmental logic computation. Mensing et al. modelled circuit-like behaviour at the molecular level by demonstrating such programmable behaviour in networks of gold nanoparticles [5].

Particularly promising are these molecular systems for the development of low-energy, self-governing, and adaptable devices that can function in intricate chemical or biological settings and provide computing power in scales and formats that silicon-based circuits cannot match.

3.3 Qubit Platforms and Quantum Materials

By utilising quantum phenomena like superposition and entanglement, quantum computing platforms push the limits of computational speed and complexity. Superconducting qubits, NV centres in diamond, and quantum dots are some of the most experimentally advanced platforms.

Discrete quantum energy states are produced by confining charge carriers in three dimensions using quantum dots, which are nanoscale semiconductor particles. These have been used in memory units, photon-based communication systems, and quantum logic gates. They are highly tunable for particular computational requirements due to their size-dependent optical and electronic characteristics [18].

Defect sites in diamond known as nitrogen-vacancy (NV) centres contain a single electron whose spin state can be initialised, controlled, and optically read out at room temperature. NV centres have been used in quantum sensing, such as intracellular thermometry and magnetic field mapping in neurones, due to their extended coherence times and biocompatibility [17].

Josephson junctions are used by superconducting qubits, like the 105-qubit Willow processor created by Google, to precisely control and measure quantum states. Currently leading the way in quantum supremacy demonstrations, these devices are scalable [19].

Topological qubits based on Majorana zero modes have demonstrated promise on the frontier of fault-tolerant quantum computing. Because their quantum information is stored nonlocally, these qubits are theoretically impervious to local decoherence; Microsoft's Majorana-1 project takes advantage of this feature [20].

3.4 Converging Modalities in Hybrid Platforms

The combination of quantum, chemical, and biological systems is creating hybrid platforms with previously unheard-of capabilities. One example is the nanometer-level organisation of quantum dots using DNA scaffolds, which enables controlled energy transfer and logic operations that combine quantum mechanics and biological programmability [11].

There is also the emergence of bio-quantum interfaces, in which quantum devices are housed within biological systems. For example, living cells internalise NV centres embedded in nanodiamonds, allowing for quantum-enhanced intracellular condition sensing [17]. Opportunities for quantum-controlled gene circuits or even real-time cellular diagnostics are presented by this integration.

By connecting reaction cascades to logical behaviour, enzyme-mediated logic gates serve as a link between chemistry and biology. Enzymes such as glucose oxidase or peroxidase, for instance, can be arranged so that their combined activity resembles a logic circuit. These have been used in environmental monitoring and point-of-care diagnostics, where the biochemical environment serves as the computational input [9].

These hybrid systems are prime examples of the fundamental idea behind nanocomputing: that completely new computational architectures—ones that are capable of thinking, sensing, and reacting at the nanoscale—can be created by combining the molecular accuracy of chemistry, the flexibility of biology, and the computational power of quantum physics.



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

IV. DISCIPLINE INTEGRATION: CROSSING BOUNDARIES

4.1 Chemical–Quantum Interfaces: Molecular-Level Coherent Control

Molecular quantum systems, in which individual molecules are designed to host and control qubits, are emerging as a result of the fusion of synthetic chemistry and quantum physics. These systems exploit the inherent quantum characteristics of lanthanide ions or transition metal complexes, whose orbital and spin states can act as stable quantum states at comparatively high temperatures [1].

For instance, a quantum simulator based on molecular spin qudits—multi-level quantum systems embedded in specially designed chemical scaffolds—was demonstrated by Carretta et al. [1]. In addition to being scalable through solution-phase synthesis, these molecular systems can be adjusted in terms of coherence times and interaction strength. Their usefulness in quantum networks can also be increased by altering their chemical environments to lessen decoherence or allow coupling with photons or phonons [2].

Moreover, molecular scaffolds offer a modular and chemically stable host for qubits, which may make roomtemperature quantum logic possible. This tackles the requirement for cryogenic infrastructure, one of the main obstacles in quantum computing.

4.2 Convergence of Biology and Chemistry: Biocomputing and Molecular Circuits

Biochemical logic circuits, which combine small-molecule sensors, nucleotide strands, or enzyme cascades into programmable logic networks, are the clearest example of the fusion of synthetic chemistry and biology. Molecular decision-making within living cells is made possible by these systems, which operate in physiological settings and in real time [6, 10].

To diagnose cancer, for example, DNA logic gates that react to microRNA inputs have been created. These gates use logical operations like AND, OR, and XOR to release signals or therapeutic agents only in response to the detection of particular intracellular biomarker combinations [9]. Chemically altered nucleotides or small-molecule inputs further improve these circuits, providing more intricate regulatory behaviour [10].

In contrast, catalytic activity serves as the logic function itself in enzyme-based logic. Platforms for pH-controlled enzymatic computing, for instance, have shown both digital and analogue outputs, allowing for more complex decision-making as opposed to binary outcomes [9]. Their translational potential is demonstrated by the growing integration of such systems into microfluidic diagnostic devices and wearable biosensors.

4.3 Interfaces between Biology and Quantum: Living Systems and Quantum Sensing

The relationship between biological environments and quantum systems is one of the most fascinating areas. It is now possible to measure intracellular magnetic fields, temperature, and even ion concentrations at nanoscale resolution thanks to the deployment of quantum sensors based on diamond's NV centres inside living cells [17].

Feedback-controlled bio-quantum systems can be created by functionally connecting these sensors with biological logic. As an illustration of a bio-quantum closed-loop controller, consider a system that uses a quantum magnetic sensor to identify mitochondrial dysfunction and a DNA logic circuit to initiate a gene-expression response.

Furthermore, the possibility of using proteins as quantum scaffolds is being investigated. Biologically informed quantum control is made possible by protein environments, which can stabilise particular spin states or allow for the targeted placement of metal-based qubits [2].

4.4 Three-Way Hybrid Systems: Moving Towards Integrated Nanocomputers

All three fields—chemistry, biology, and quantum physics—are now being integrated into integrated nanocomputing architectures by emerging platforms. With real-time feedback and low energy consumption, these interdisciplinary systems have the potential to carry out intricate computational tasks in biochemical environments.

The application of DNA nanostructures as organisational templates for quantum materials is a powerful illustration. Molecular qubits or quantum dots can be arranged spatially with nanometre accuracy using DNA origami scaffolds, allowing for coherent control and readout while preserving biocompatibility [11].



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

A related strategy involves integrating chemically stabilised NV centres into liposomes or synthetic vesicles, where they interact with cell signalling molecules. These nanodevices are potential candidates for next-generation nanomedical computing platforms because they can sense, process, and even interfere with biological processes [17]. Another new approach is the use of programmable artificial cells that integrate quantum sensors for communication, DNA for memory, and molecular machines for logic, thereby creating living nanocomputers that can function independently in a variety of settings.

4.5 Convergence's Implications

Where, how, and why we compute are all altered by this interdisciplinary convergence. The resulting nanocomputers can:

- function independently in biological settings, including cells;
- Real-time perception and reaction to molecular or quantum-level stimuli;
- Make decisions and use logic without the use of traditional electronics.

V. CURRENT BREAKTHROUGHS AND APPLICATIONS

5.1 Molecular-Level Intelligent Biosensing

Designing smart biosensors—systems that recognise particular biological signals and react with logic-driven outputs is one of the most direct and significant uses of nanocomputing. DNA-based logic gates have been incorporated into hydrogel matrices and nanoparticles to identify disease-specific biomarkers like metabolites, cytokines, or microRNAs. Only when certain logical conditions are satisfied do these gates generate a detectable signal, such as electrical output or fluorescence [6], [9].

The use of NV centres in diamond or quantum dots to detect molecular changes at high sensitivity is another emerging technique in quantum-enhanced biosensors. These allow for high-resolution, non-invasive diagnostics because they can function in biological fluids or even inside cells [17].

5.2 Architectures for Molecular Data Storage and Memory

Molecular-level data storage represents yet another important advance. Large volumes of digital data are increasingly being encoded in an ultra-dense, stable, and long-lasting format using DNA molecules. Scientists have used programmable enzymes or CRISPR-associated systems to read and rewrite synthetic DNA strands that contain text, video, and images [10].

Parallel to this, bistable systems like switchable lanthanide complexes or rotaxanes, as well as molecular logic gates, present the possibility of memory units that are both stable and sensitive to external stimuli [3], [6]. Smart storage media are made possible by this method, which enables storage devices to adjust or modify their behaviour in response to stimuli.

On the quantum side, long-term storage of quantum information is made possible by quantum memory systems built on molecular qubits or NV centres. Such systems are essential for future quantum internet nodes, quantum cloud systems, and quantum communication protocols, even though they are still primarily experimental [1], [19].

5.3 Therapeutic Logic Systems and Intracellular Computing

Logic-based therapeutic platforms have been made possible by the combination of synthetic biology and nanocomputing. These systems can detect intracellular conditions and start particular reactions, like stopping inflammatory pathways or causing cancer cells to undergo apoptosis.

Genetically encoded logic circuits that recognise combinations of biomarkers and subsequently activate or repress gene expression are a well-known example [13], [14]. These systems are programmable and adaptable to different disease models, such as neurodegenerative diseases and cancer.

Furthermore, it has been shown in vitro that DNA-based automata can move along a DNA "track" inside a cell and make decisions based on molecules they come across. These systems are the first steps towards programmable molecular robots that can perform subcellular targeted diagnosis and treatment.

© 2025 IJMRSET | Volume 8, Issue 6, June 2025|

ISSN: 2582-7219 | www.ijmrset.com | Impact Factor: 8.206| ESTD Year: 2018|



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

5.4 Interface and Communication Technologies

Additionally, new kinds of molecular-to-quantum communication interfaces are being made possible by nanocomputing. Information can be processed using quantum principles while being routed via biological pathways in hybrid systems that use DNA scaffolds to position quantum dots or NV centres [11], [17].

This kind of interface holds promise for the creation of:

- bio-quantum networks, in which data is exchanged between quantum sensors and living tissues;
- neuro-quantum interfaces, which might be able to read neuronal signals with quantum sensitivity;

• Intelligent particles dispersed throughout the body or surroundings can logically communicate with one another in molecular internet-of-things (IoT) systems.

Because each device can perform several functions at once, these technologies make it difficult to distinguish between sensing, computing, and communication.

5.5 Platforms for Environmental and Real-Time Sensing

Additionally, nanocomputing systems have been used for environmental monitoring, including the detection of pollutants, pathogens, and changes in the pH of water or air.

In autonomous cycles, chemically responsive logic systems that use pH-controlled DNA structures or enzyme-linked logic gates detect target compounds and initiate subsequent reactions such as colour change, catalysis, or data transmission [9].

Certain platforms are even made to function as disposable, single-use sensors for field diagnostics in disaster relief, healthcare, and agriculture. Rapid adaptation to new targets is made possible by their programmability, which makes them perfect for pandemic situations or changing environmental threats.

Future developments in bio-quantum-enhanced sensors may enable in situ real-time monitoring of chemical reactions, supporting planetary-scale sensing systems, industrial safety, or green chemistry.

5.6 In the direction of general-purpose nanocomputers

Advances are being made towards programmable, reconfigurable nanocomputers, although the majority of existing nanocomputing systems are application-specific. Similar to general-purpose microprocessors, these would function at the nanoscale and in the chemical, biological, and quantum domains.

Recent initiatives consist of:

- networks of molecular logic processors constructed from layered DNA circuits.
- hybrid quantum-classical logic gates that combine biochemical and photon-based control;

• computational modules in artificial cells that change their behaviour in response to chemical cues from the environment.

These advancements hint at a time when distributed nanocomputing networks—functioning inside organisms, environments, or even materials—will be able to sense, compute, remember, and act in real time. The following **Chart** 1 lists the main fields in which nanocomputing technologies are being used, along with illustrative platforms from quantum physics, synthetic chemistry, and biology.

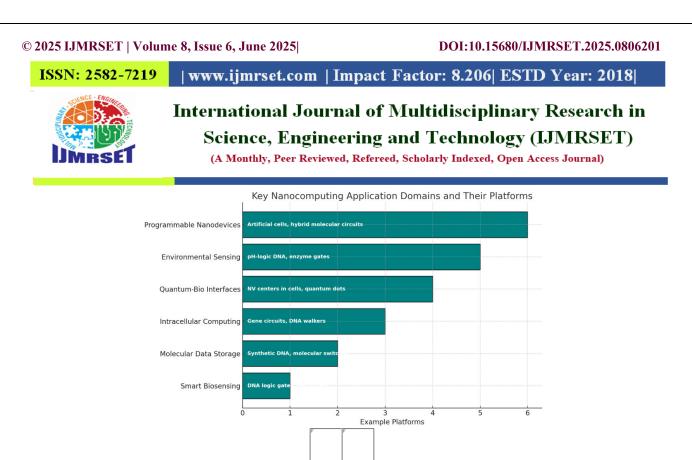


Chart 1 Application Domains of Nanocomputing and Representative Enabling Platforms This overview highlights the growing versatility and cross-disciplinary nature of nanocomputing, demonstrating how molecular, biological, and quantum systems are now coalescing into application-specific platforms [22].

VI. CHALLENGES AND LIMITATIONS

6.1 System Complexity and Scalability

The challenge of scaling from a few molecular gates or logic units to a complete, programmable system is one of the most urgent problems in nanocomputing. As more gates are added, molecular logic circuits in synthetic chemistry frequently experience environmental instability, cross-reactivity, and signal degradation [5, 6]. It gets exponentially more difficult to maintain clean ON/OFF states as circuit complexity increases.

Even though DNA and RNA provide elegant programmability, the sheer number of reactions and timing coordination required to operate large-scale molecular circuits in biological computing can result in inconsistent outputs [10], [13]. Diffusion kinetics and the possibility of off-target hybridisation frequently place restrictions on multi-gate biological systems.

However, qubit fidelity, gate error rates, and the exponential increase in decoherence risk with the number of entangled qubits limit quantum systems. Existing qubit architectures, like the Willow processor [19], still depend on sizable cryogenic infrastructures and have trouble providing fault-tolerant control for more than 100 qubits.

6.2 Production Accuracy at the Atomic Level

Accurate assembly of molecules, qubits, or biomolecules at the nanometre or even angstrom scale is necessary for nanocomputing platforms. The placement of external quantum elements (such as spin centres or quantum dots) with nanometre accuracy is still a significant challenge, even though DNA origami enables near-atomic patterning of logic structures [11].

Building multicomponent, spatially complex networks makes chemical synthesis less predictable, despite the fact that it is extremely controllable at the molecular level. Logic behaviour can be changed by even slight synthesis variations, producing non-deterministic results.

Defect-free nanostructures, like Majorana-supporting nanowires or NV centres, must be fabricated in quantum hardware using ultraprecise lithography and doping techniques, which are still expensive and low-yield [17], [20].

6.3 Error correction, noise, and decoherence

Decoherence, or the quick loss of quantum information as a result of environmental interactions, is a fundamental problem in quantum nanocomputing. Quantum signals are rapidly deteriorated by thermal noise, vibrational coupling,



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

and electromagnetic interference, despite the potential for coherence maintenance for microseconds to milliseconds demonstrated by molecular spin systems and NV centres [1], [18].

Error-correcting techniques are being developed to lessen this, particularly those that make use of topological encoding or qudits (higher-dimensional logic units). Nevertheless, these approaches frequently come with a high overhead—dozens of physical qubits for a single logical qubit [21]—which makes scalability challenging in the short term.

Even though they are not quantum, biological and chemical logic systems experience noise and signal loss, especially when they are subjected to the temperature, ionic strength, or pH variations found in biological fluids [9].

6.4 Cross-Modal Integration

Although distinct platforms, such as chemical, biological, or quantum, can function effectively when used separately, creating hybrid systems presents additional engineering challenges. For instance:

- The optimal function of both components may be limited when buffer and ionic compatibility are required when combining DNA logic with quantum dots;
- Bio-stability and targeting problems arise when NV centres are embedded in liposomes for intracellular sensing;
- It is still mostly experimental to chemically attach quantum spin centres to protein scaffolds without affecting function [2], [17].

Furthermore, nanocomputing lacks a common "operating system." It is still unclear how to design subsystem-tosubsystem shared communication protocols, timing systems, and energy delivery plans.

6.5 Biocompatibility and Energy Limitations

In contrast to conventional silicon-based systems, nanocomputers frequently require no external power to function, particularly in biological settings. Many depend on light, chemical energy from the environment, or catalytic reactions to operate. It is difficult to ensure consistent and dependable operation in such circumstances, particularly in harsh environments or inside living tissues [6], [9].

Moreover, there is no guarantee that chemical or quantum components will be biocompatible. For instance:

- Toxic metals, such as cadmium, can be found in quantum dots.
- In vivo, molecular machines could be immunogenic or unstable.
- Certain DNA devices might cause immunological reactions or degrade too quickly.

One of the main research goals is still to create inert, robust, and functional nanocomputers that can endure and function safely in real-world or in vivo settings.

6.6 Safety and Ethical Aspects

Ethical issues surface as nanocomputers become more autonomous and capable of making decisions, particularly within biological systems. These consist of:

- Unintentional actions or changes in artificial biological circuits,
- protection of molecular information contained in synthetic DNA,
- the possibility of technologies with two uses that could be repurposed for negative purposes.

There is an urgent need for transparent risk assessment frameworks, biological containment techniques, and regulatory guidelines for the deployment of nanocomputing, particularly as these systems transition from laboratory to field.

VII. FUTURE DIRECTIONS AND OPPORTUNITIES

7.1 Quantum Logic Meets Synthetic Biology

Integrating quantum sensors like diamond NV centers into artificial cells can enable highly sensitive, programmable biological responses to subtle physiological changes (e.g., pH, ROS, magnetic fields). Coupling these with CRISPR-based logic may allow real-time feedback loops for targeted therapy or neural repair.



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

7.2 Computational Intelligence for Artificial Life

Synthetic cells combining DNA/RNA logic, memory storage, and molecular decision-making could serve as programmable nanorobots for medicine, environmental sensing, or terraforming—blurring the line between computation and living systems.

7.3 Real-Time Nanomedical Computing

Future DNA-based nanoprocessors and quantum dot-linked nanosystems could detect mutations, monitor drug levels, and deliver therapies autonomously—pioneering smart, self-regulating nanotherapeutics.

7.4 Environmental and Planetary Sensing

Distributed nanosensors with quantum-enhanced sensitivity may enable long-term monitoring of pollutants, soil nutrients, or seismic activity. DNA-based, biodegradable devices could self-report via RF, light, or quantum signals.

7.5 Nano-AI and Molecular Learning

Machine learning is optimizing nanostructure design and chemical logic behavior. Emerging nano-AI hybrids—such as adaptive molecular systems or neuromorphic elements—can evolve behavior from experience, blending computation with cognition.

7.6 Smart, Computation-Embedded Materials

Next-gen materials may include nanocomputers that sense and respond autonomously—e.g., self-healing, shape-shifting, or stress-sensing surfaces—ideal for robotics, aerospace, and wearables.

7.7 Ethics and Governance

As nanocomputing scales up, ethical models must ensure transparency, data security, ecological safety, and responsible use in health, agriculture, and infrastructure.

Looking Ahead

Nanocomputers of the future may be molecular, adaptive, and invisible—integrated seamlessly into living systems and materials. Their development marks a shift from theoretical research to transformative, cross-disciplinary applications.

VIII. CONCLUSION

One of the most active and interdisciplinary areas of science and technology nowadays is nanocomputing. Researchers are creating platforms that surpass the capabilities of traditional silicon-based computing by utilising the molecular control of synthetic chemistry, the programmability of biological systems, and the unmatched computational power of quantum physics.

We have examined how these three fields support different but connected nanocomputing foundations throughout this review. Redox reactions, supramolecular machines, and dynamic molecular switches are examples of chemistry's use of logic. With living systems that can execute instructions, run logic gates, and even evolve, biology provides computing at the DNA and RNA level. At the same time, qubits, entanglement, and coherence are used in quantum physics to present radically new models of information processing.

Novel hybrid systems, such as chemically modulated spin systems, intracellular quantum sensors, and DNA-guided quantum dot arrays, are emerging as these fields increasingly overlap. These systems demonstrate the enormous potential of convergent frontiers. Applications in the real world are already beginning to take shape, ranging from nanomedical devices that compute directly inside cells to biosensors that can make molecular decisions. These advancements show that nanocomputers are evolving from conceptual to deployable systems.

Even with these developments, there are still a number of difficulties. Important topics for continued research include managing decoherence in quantum operations, ensuring biocompatibility, scaling systems while preserving stability and precision, and creating ethical governance frameworks. In addition to technological innovation, cooperation across conventionally divided fields will be necessary to address these issues.



International Journal of Multidisciplinary Research in Science, Engineering and Technology (IJMRSET)

(A Monthly, Peer Reviewed, Refereed, Scholarly Indexed, Open Access Journal)

Future technologies such as programmable matter, autonomous medical diagnostics, real-time planetary sensing, and even artificial lifeforms with the ability to learn and adapt are all expected to be built on nanocomputing. A future in which matter itself is intelligent—responding to stimuli, processing information, and changing with its surroundings— is suggested by the combination of machine learning, artificial cells, and quantum logic.

In conclusion, the convergence of quantum physics, synthetic chemistry, and biology is not merely an exercise in interdisciplinary research; rather, it is a prerequisite for the development of the next generation of computing. Nanocomputers have the potential to serve as the systems that connect theory and life, information and matter, energy and intelligence. Their ascent marks a significant change in the way we compute, and possibly in the definition of computation itself.

REFERENCES

[1] S. Carretta et al., "Proof-of-Concept Quantum Simulator Based on Molecular Spin Qudits," J. Am. Chem. Soc., vol. 146, no. 1, pp. 1053–1061, 2024.

[2] Wired Science, "Quantum Materials: Chiral Semiconductors and Metal Phthalocyanines as Room-Temperature Qubit Systems," Online Feature Article, 2023.

[3] Lanthanide-Based Logic: A Venture for Molecular Computing, Chem. Commun., 2023.

[4] P. L. Gentili, "Empowering Chemical AI Through Systems Chemistry," ChemSystemsChem, 2024.

[5] J. Mensing, W. G. van der Wiel, and A. Heuer, "Boolean Logic in Gold Nanoparticle Networks Using Kinetic Monte Carlo," arXiv preprint, 2023.

[6] K. Ariga et al., "Molecular Machines at Interfaces: Physics, Evolution, and Nanoarchitectonics," Phys. Chem. Chem. Phys., 2024.

[7] Enlightening Molecular Logic: Basics, Tools and Techniques, Mater. Horiz., 2025.

[8] M. Agiza et al., "pH-Controlled Enzymatic Computing for Digital and Analog Logic," Phys. Chem. Chem. Phys., 2024.

[9] S. Bi, R. Yang, H. Ju, and Y. Liu, "Dynamic Nanostructure-Based DNA Logic Gates for Cancer Diagnosis and Therapy," ChemBioChem, 2024.

[10] A. C. Bardales, V. Smirnov, K. Taylor, and D. M. Kolpashchikov, "DNA Logic Gates Integrated on DNA Substrates in Molecular Computing," ChemBioChem, vol. 25, no. 8, e202400080, 2024.

[11] W. Wang, "Dynamic Reconfigurable DNA Nanostructures, Networks and Materials," Angew. Chem. Int. Ed., 2023.

[12] Y. Zhang, "Implementing Logic Gates by DNA Crystal Engineering," Adv. Mater., 2023.

[13] C. Emanuelson, A. Bardhan, and A. Deiters, "DNA Logic Gates for Small Molecule Activation Circuits in Cells," ACS Synth. Biol., vol. 13, no. 2, pp. 538–545, 2024.

[14] M. Kieffer et al., "Molecular Computation for Molecular Classification Using DNA and Polymerase Logic," Adv. Biol., 2023.

[15] N. Liu et al., "Digital Computing by DNA Colloidal Crystal Engineering," J. Am. Chem. Soc., 2024.

[16] R. Li et al., "High-Fidelity CZ Gate Based on Double-Transmon Coupler," Phys. Rev. X, 2024.

[17] Google Quantum AI, "Willow Processor: A 105-Qubit Superconducting Chip," Nature, 2024.

[18] L. Picard et al., "iSWAP Gate in Individually Trapped NaCs Molecules," arXiv preprint, 2024.

[19] Y. Zhang et al., "Fault-Tolerant Quantum Algorithms for Quantum Molecular Systems: A Survey," arXiv preprint, 2025.

[20] Microsoft Research, "Majorana 1: Topological Quantum Processing Unit," Microsoft Research Release, 2025.

[21] UNSW Sydney et al., "Antimonide-Based Qudit Error Correction for Scalable QEC Systems," Institutional Research Report / Preprint, 2024.

[22] S. Carretta, A. Chiesa, F. Luis et al., "Blueprint of a Molecular Spin Quantum Processor," Preprint, 2023.





INTERNATIONAL JOURNAL OF MULTIDISCIPLINARY RESEARCH IN SCIENCE, ENGINEERING AND TECHNOLOGY

| Mobile No: +91-6381907438 | Whatsapp: +91-6381907438 | ijmrset@gmail.com |

www.ijmrset.com